Reporting Data, Units, Propagation of Error, and Error Analysis Analytical Cume
12/06/2018

DON'T PANIC

1. Here is a sentence from a manuscript; there are 9 errors. Find as many as you can. Hint- there are grammatical, mathematical, and scientific mistakes. **(10 pts)**

"The result of the experiments demonstrate that the sum of mass and length: 5.1(±1.5) kg + 6.0(±2) m, are 11.1 ± 2.35 kg·m, which is in contrast to those repored by Zoe Gato et. al."

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2. a. What are the proper S. I. units of the following? For derivative units, please also give the underlying pure units. For example, force is in Newtons, which are kg·m/s^2.

Pure units-	Mass:	Length:	Time:	Charge:
Derivative units-	Volume:	Energy:	Pressure:	

b. Is molarity a standard S.I. unit? Why or why not? **(10 pts)**

The formula for propagation of error of a function f(x,y) is:

$$\sigma_f = \sqrt{\left(\frac{\partial f(x,y)}{\partial x}\right)^2 \sigma_x^2 + \left(\frac{\partial f(x,y)}{\partial y}\right)^2 \sigma_y^2}$$

This assumes that the measured distributions of x and y are "normal" (i.e. bell-shaped Gaussian) and that the measurements of x and y are uncorrelated. Use this formula to answer questions 3-6, which are derivations of error formulas.

3. You have a function f(x) that describes the result of an experiment. The measurements in the lab yield $x \pm \sigma_x$. You need to report: $f(x) \pm \sigma_f$ for your paper, with $f(x) = \frac{x}{c}$ where c is a constant that has no associated error. Can you show that $\sigma_f = \frac{|\sigma_x|}{|c|}$? **(5 pts)**

4. You have a function f(x,y) that describes the result of an experiment. The measurements in the lab yield $x \pm \sigma_x$ and $y \pm \sigma_y$. You need to report $f(x,y) \pm \sigma_f$ for your paper, with $f(x,y) = x + y$. Can you show that $\sigma_f = \sqrt{\sigma_x^2 + \sigma_y^2}$? **(5 pts)**

5. You have a function f(x,y) that describes the result of an experiment. The measurements in the lab yield $x \pm \sigma_x$ and $y \pm \sigma_y$. You need to report: $f(x,y) \pm \sigma_f$ for your paper, with $f(x,y) = x \cdot y$. Can you show that $\sigma_f = (x \cdot y)\sqrt{\frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2}}$? **(7 pts)**

6. You have a function f(x) that describes the result of an experiment. The measurements in the lab yield $x \pm \sigma_x$. You need to report: $f(x) \pm \sigma_f$ for your paper, with $f(x) = \ln(x)$. Can you show that $\sigma_f = \frac{|\sigma_x|}{|x|}$? **(7 pts)**

7. You have a function f(x,y) that describes the result of an experiment. The measurements in the lab yield $x \pm \sigma_x$ and $y \pm \sigma_y$. You need to report $f(x,y) \pm \sigma_f$ for your paper with: $f(x, y) = x \cdot \ln(y)$. Can you derive the formula for the error of f(x,y)? Hint: you should be able to answer this question using the results from #5 and #6, you simply have to get the order of operations correct.

(10 pts)

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8. The following measurements were made: Mass of sample A: 1.50 ± 0.15 kg with a molar mass of 150.0 g/mol. The volume of flask is 1000.0 mL ± 1.0 mL. Find the molar concentration and report the error as well. Hint: this is an order of operations question, and the relevant equations are provided above, and in the case of $f(x, y) = {}^{x}/_{y}$ the error is $\sigma_f = \frac{|x|}{|y|}\sqrt{\frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2}}$. You can assume that the molar mass is a constant with no associated error. **(10 pts)**

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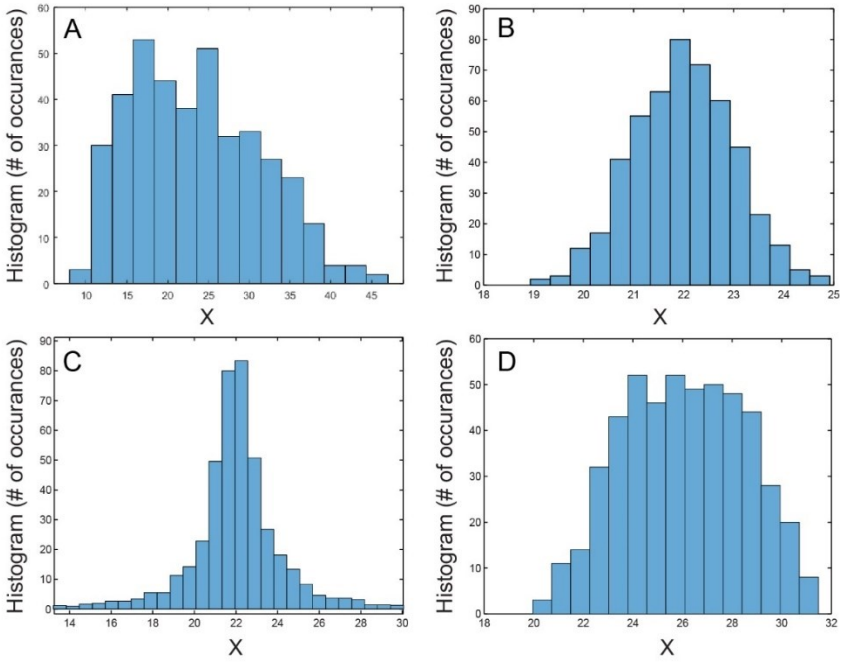
9. If you make a measurement 100×, you can determine the signal to noise (**S**/**N**) ratio. Let's say you need to make more measurements for your paper and you wish to double your **S**/**N** ratio- how many measurements do you need to make in total? (For clarity, if you state 200×, this means you need to make 100 additional measurements to the 100 you already have).
Hint: If you double the number of measurements then the signal and variance doubles, but the **S**/**N** ratio is the magnitude of the signal over the standard deviation, i.e. ${}^{S}/_{\sigma}$. **(7 pts)**

10. You make a measurement 100× and calculate the standard deviation, which is σ. Do you expect to get a significantly different standard deviation if you make 100,000× measurements? In other words, will you get a much greater σ, smaller σ, or about the same? **(5 pts)**

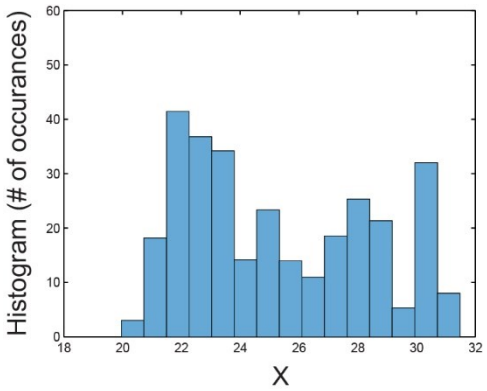
11. Shown here are 4 histograms of datasets (A→D). The histograms are relatively "normal", i.e. Gaussian-like, although three of them seem a bit off. In fact, they have skew or kurtosis. Please label which ones display either skew or kurtosis or are normal.

(4 pts)



12. The formula for standard deviation: $\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2}$ is based on the idea that lab measurements of "x" have "normal" or bell-shaped Gaussian distributions. What if that is not the case (for example, the dataset here)? If you have a non-normal distribution, the use of the standard deviation formula may not deliver a proper representation of the error. How would you approach reporting the error in this situation? Note that there are well-established methods for such situations, you either know one of them or not.

(5 pts)



Ethics (5 pts)

13. The subject of your PhD thesis will be published in a paper, where you set out to prove that A = B. You have measured $A \pm \sigma_A$ and $B \pm \sigma_B$, and it turns out that: $A + \sigma_A = B - \sigma_B$. Thus, your hypothesis is true due to the overlap of values within the error, but just barely.

However, you suspect that the data distribution is not Gaussian-type, which means that the standard deviation may not represent the error accurately. You're not totally sure though, and unfortunately you have run out of sample and can't make any more measurements.

How do you approach this issue in terms of your paper, which is central to your PhD thesis? For example, you could simply not publish it; if so, defend your decision. Or maybe you publish it without discussion of this potential problem? If so, defend your decision. Or propose another solution and defend your decision.

Safety (10 pts)

14. Can you pour methanol down the sink (at least some)?

15. Which is more dangerous: 12 M HCl or 1M HF acid?

16. Certain chemicals should be handled differently than others. For example, let's say that your lab receives diethyl zinc, trimethyl aluminum, trimethyl phosphine, and/or butyl lithium. What precautions should be taken with these chemicals? Hint: all these chemicals have the same special handling condition.

17. What kind of gloves can be worn without needing to replace them if contacted with chemicals?

18. What is an SOP?

EQUATIONS

$$\frac{\partial x}{\partial x} = 1 \qquad \frac{\partial ln(x)}{\partial x} = \frac{1}{x} \qquad \frac{\partial 1/x}{\partial x} = \frac{-1}{x^2} \qquad \frac{\partial x}{\partial x} = 1 \qquad |x| = \sqrt{x^2}$$

$$\sqrt{\frac{a}{b}} = \frac{\sqrt{a}}{\sqrt{b}} \qquad \text{Var} = \frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{x_i} - \bar{\mathrm{x}})^2 \qquad \sigma = \sqrt{\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{x_i} - \bar{\mathrm{x}})^2} = \sqrt{Var}$$

$$\text{Skew} = \frac{\sqrt{\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{x_i}-\bar{\mathrm{x}})^3}}{\sigma^3} \qquad \text{Kurtosis} = \frac{\sqrt{\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{x_i}-\bar{\mathrm{x}})^4}}{\sigma^4}$$

$$\text{Gaussian f(x)} = \sqrt{\frac{1}{2\pi\sigma^2}}\, e^{-(x-\bar{x})^2/2\sigma^2} \qquad \text{Liter} = \mathrm{dm}^3$$