Statistical treatment of data
CHEM 212

Learning Objectives:

- Articulate the use and importance of statistics.
- Be able to calculate the area under the curve of a Gaussian distribution.
- Be able to apply the appropriate statistical tests (Student's T test, F-test, Grubbs test) to critically evaluate dataset(s).

Why do we need statistics?

What is the most common population distribution? Draw an example.

Do problem 4-2 parts a-c.

4-2. Use Table 4-1 to state what fraction of a Gaussian population lies within the following intervals:

(a) $\mu \pm \sigma$ (c) μ to $+\sigma$ (e) $-\sigma$ to -0.5σ

What is the purpose of a T-test? How do you know if data is statistically different?

Equations

T-test case	Criteria for statistical comparison
T-test case 1	
T-test case 2, similar St Dev	
T-test case 2, different St Dev	
T-test case 3	

Example Case 1
Determine if the three sets of replicate analyses shown in the table are statistically different from the a certified reference material (48 ppb) at the 50% and 95% CI.

Table 2. Fire assay results from two Fire Assay-AA runs of the CANMET UMT-1 versus fNAA gold values. Example of improper fluxing not in homogeneity of sample.

First Run Fire Assay-AA 30 g Aliquot		Second Run Fire Assay-AA 30 g Aliquot		INAA 30 g Aliquot	
14	9	38	40	49	
11	13	26	39	49	
4	10	37	42	48	
10	11	39	34	51	
16	6	40	42	49	
21	11	45	40	47	
13	25	30	41	55	
11	19	23	43	53	
12	21	35	36	53	
8	22	41	37	54	
12	15		43	48	
16	25				53
12	18				61
11	14				57
15	12				48
14	24				53
Average = 14 +/– 5		Average = 38 +/– 6		Average = 52 +/–4	

Average fire assay 14 ppb (32 aliquots) range: 4 to 25
Average fire assay 38 ppb (21 aliquots) range: 26 to 45
Average INAA 52 ppb (16 aliquots) range: 48 to 61

Example Case 2
Determine if the two FIRE ASSAY sets of analysis are statistically different at the 50 and 95% CI.

Example Case 3

I recently had some samples analyzed by one method, but there was incomplete dissolution of some samples. I had the samples reanalyzed, but didn't get data for an important analyte. I need to determine if the methods produce data that are significantly different at a 90%, 95%, and 99% confidence interval.

	Method 1	Method 2	di	di- d	$(di-d)^2$
C-366895	6.9	6.15	0.75	-0.668	0.446224
C-366899	1.2	1.57	0.37	-1.048	1.098304
C-366900	6.1	5.64	0.46	-0.958	0.917764
C-366901	0.4	0.69	0.29	-1.128	1.272384
C-366906	1.3	1.72	0.42	-0.998	0.996004
C-366907	47.1	54.56	7.46	6.042	36.505764
C-366908	5.3	6.51	1.21	-0.208	0.043264
C-366909	3.8	4.69	0.89	-0.528	0.278784
C-366910	3.8	4.71	0.91	-0.508	0.258064
n=9			d= 1.418	**Σ**$(di-d)^2$=41.82	

What is Tcalc?

Is there a statistical difference at the 90% CI?

Is there a statistical difference at the 95% CI?

Is there a statistical difference at the 99% CI?

When do you need an F-test? What does the F-test compare?

F-test

What is a Grubbs test and how do you know when to use it?

Grubbs test

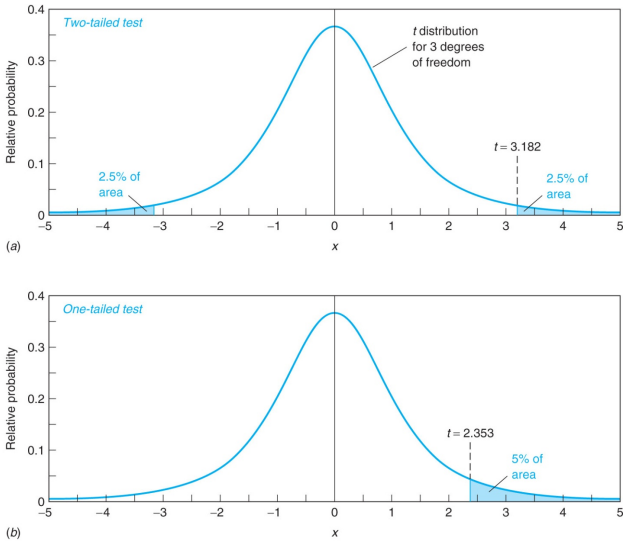
4-21. A Standard Reference Material is certified to contain 94.6 ppm of an organic contaminant in soil. Your analysis gives values of 98.6, 98.4, 97.2, 94.6, and 96.2 ppm. Do your results differ from the expected result at the 95% confidence level? If you made one more measurement and found 94.5, would your conclusion change?

4-23. Should the value 216 be rejected from the set of results 192, 216, 202, 195, and 204?

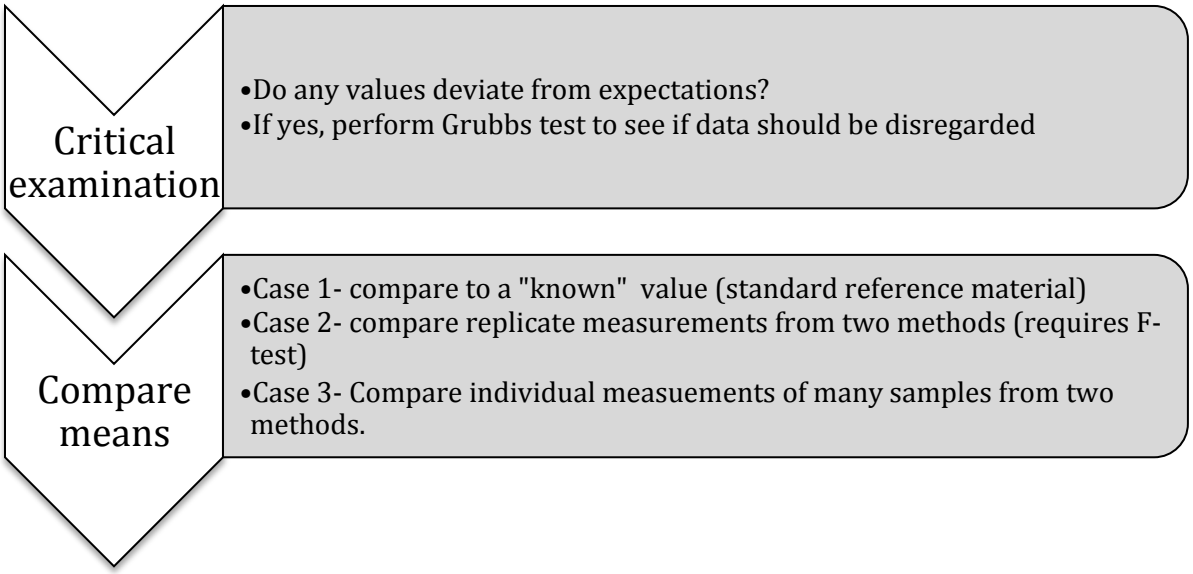
One or two tailed test?

The T-test relies on having methods that have the same probability of being different in the positive or negative direction. Thus the 95% confidence interval has 2.5% of the probability on the high and low sides of the Gaussian curve (check out the figure). This is the standard 2-tailed test.

If, however, you know that your method is likely to only be high or low, then using the same 95% confidence interval will have the entire 5% of the area on the high or low side of the curve. Conversely, in order to have compareable data with the two tailed test, you would need to use a 97.5% confidence interval



Below is a very general idea of how I approach a new data set.



Draw a more detailed diagram of your own demonstrating how you might approach a dataset.