ANALYTICAL CHEMISTRY

Tutorial 1: Statistical Treatment of Data

Question 1

The Ti content (mass %) of two different ore samples was measured several times by the same method. Are the mean values significantly different at the 95% confidence level?

Sample 1: 0.0134; 0.0138; 0.0128; 0.0133; 0.0137
Sample 2: 0.0135; 0.0142; 0.0137; 0.0141; 0.0143

Question 2

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 results at the 95 % confidence level?

Question 3

The following data were obtained for the titration of 10 mL of 0.250 M HCl with 0.126 M NaOH:

20.14 20.09 20.10 20.17 19.78

a) Should any of the values be rejected at the 90% confidence interval?
b) Taking into account any outliers, calculate the mean and the standard deviation of the volumes obtained.
c) The theoretical volume calculated for this titration was 20.16 mL. Are the experimental results significantly different at the 90% confidence level?

Question 4

A certified reference material is known to contain 21.37% arsenic. A student from the 2nd year class analysed a sample of the material and obtained the results below.

Determination	% Arsenic
1	21.40
2	21.35
3	21.32
4	21.39
5	21.30

a) Calculate
- The mean of the data set
- The relative standard deviation of the data set
- The absolute average error of the data set

b) Calculate the 90% confidence interval for the data set and explain what this represents.

c) Determine if there is a significant difference between the experimental and true values at the 90% confidence level.

Question 5

The presence of iron (II) in beer is thought to adversely affect its taste. Samples of beer were analyzed for iron (II) using an atomic absorption method and a titration method. The results obtained are given below in mg kg^{-1}.

Sample	$[Fe^{2+}]$ atomic absorption	$[Fe^{2+}]$ titration
1	7.3	8.0
2	8.4	7.5
3	8.3	8.3
4	7.8	7.7
5	8.9	8.1

a) Determine if the two methods are significantly different from each other at the 90% confidence interval.

b) Using the 95% confidence interval, determine if there is a significant difference in the precision obtained by the two different techniques?

Question 6

A trainee in a medical lab will be released to work on her own when her results agree with those of an experienced worker at the 95 % confidence level. Results for a blood urea nitrogen analysis are shown below:

Trainee:

$\bar{x}$ = 14.57 mg/dL s = 0.53 mg/dL n = 6

Experienced worker:

$\bar{x}$ = 13.95 mg/dL s = 0.42 mg/dL n = 5

Should the trainee be allowed to work alone? Show your reasoning.

Data Sheet

$$t_{calculated} = \frac{|\bar{x} - \mu|}{s}\sqrt{N} \qquad t_{calculated} = \frac{\bar{d}}{s_d}\sqrt{n} \qquad t_{calculated} = \frac{|\bar{x}_a - \bar{x}_b|}{s_{pooled}} \times \sqrt{\frac{n_a \times n_b}{n_a + n_b}}$$

Confidence

degrees Freedom	50%	90%	95%	99%
1	1.000	6.314	12.706	63.656
2	0.816	2.920	4.303	9.925
3	0.765	2.353	3.182	5.841
4	0.741	2.132	2.776	4.604
5	0.727	2.015	2.571	4.032
6	0.718	1.943	2.447	3.707
7	0.711	1.895	2.365	3.499
8	0.706	1.860	2.306	3.355
9	0.703	1.833	2.262	3.250
10	0.700	1.812	2.228	3.169
11	0.697	1.796	2.201	3.106
12	0.695	1.782	2.179	3.055
13	0.694	1.771	2.160	3.012
14	0.692	1.761	2.145	2.977
15	0.691	1.753	2.131	2.947
16	0.690	1.746	2.120	2.921
17	0.689	1.740	2.110	2.898
18	0.688	1.734	2.101	2.878
19	0.688	1.729	2.093	2.861
20	0.687	1.725	2.086	2.845
21	0.686	1.721	2.080	2.831
22	0.686	1.717	2.074	2.819
23	0.685	1.714	2.069	2.807
24	0.685	1.711	2.064	2.797
25	0.684	1.708	2.060	2.787
26	0.684	1.706	2.056	2.779
27	0.684	1.703	2.052	2.771
28	0.683	1.701	2.048	2.763
29	0.683	1.699	2.045	2.756
30	0.683	1.697	2.042	2.750
31	0.682	1.696	2.040	2.744
32	0.682	1.694	2.037	2.738
33	0.682	1.692	2.035	2.733
34	0.682	1.691	2.032	2.728
35	0.682	1.690	2.030	2.724

Critical Values for the Rejection Quotient

	Q_{crit} (Reject if $Q_{exp} > Q_{crit}$)		
N	**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

***N* = number of observations**

Critcal values of F at the 5% Probability Level (95% confidence)

Degrees of Freedom (Denominator)	Degrees of Freedom (Numerator)								
	2	3	4	5	6	7	8	9	10
2	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40
3	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79
4	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96
5	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74
6	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06
7	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64
8	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35
9	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14
10	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98
15	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54
20	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35
25	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24
26	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22
27	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20
28	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19
29	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18
30	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16