

*Basic statistical tools for analytical laboratories*

# **Chapter 5**

## **Determination of outliers**

# Determination of Outliers

- Odd or extreme data in a given set of measurement results must be rejected with statistical justification
- **PaHTa's Rule,**
- **Chauvenet  $\omega$  Test**
- **Dixon's Q Test**
- **Thompson's *tau*  $\tau$  Test**
- Other outlier tests include: Grubb's, Cochran's, Bartlett's, Hartley's, Levene's and Brown-Forsythe's.

# Determination of Outliers

- **PaHTa's Rule**

- For a series of test values,  $x_1, x_2, \dots, x_n$
- If  $v_i = x_i - \bar{x}$ , with standard deviation  $s$ , and,
- if  $v_i > 3*s$ , then,
- $x_i$  is a significant outlier.

# Determination of Outliers

- **Chauvenet Test**

- For a series of test values,  $x_1, x_2, \dots, x_n$
- If  $v_i = x_i - \bar{x}$ , with standard deviation  $s$ , and
- when  $|v_i| > \omega_i * s$ , where  $\omega_i$  is referred to the Chauvenet's table, based on the number of data,  $n$ , then the extreme value  $x_i$  is an outlier.

**Table 2: Chauvenet's  $\omega_i$  values against number of data,  $n$**

$n$	$\omega$	$n$	$\omega$	$n$	$\omega$
<b>3</b>	1.38	<b>13</b>	2.07	<b>23</b>	2.3
<b>4</b>	1.53	<b>14</b>	2.10	<b>24</b>	2.3
<b>5</b>	1.65	<b>15</b>	2.13	<b>25</b>	2.3
<b>6</b>	1.73	<b>16</b>	2.15	<b>30</b>	2.4
<b>7</b>	1.80	<b>17</b>	2.17	<b>40</b>	2.5
<b>8</b>	1.86	<b>18</b>	2.20	<b>50</b>	2.6
<b>9</b>	1.92	<b>19</b>	2.22	<b>75</b>	2.7
<b>10</b>	1.96	<b>20</b>	2.24	<b>100</b>	2.8
<b>11</b>	2.00	<b>21</b>	2.26	<b>200</b>	3.0
<b>12</b>	2.03	<b>22</b>	2.28	<b>500</b>	3.2

# Determination of Outliers

- **Dixon's  $Q$  Test**

- $Q = | \text{suspected value} - \text{nearest value} | / (\text{largest value} - \text{smallest value})$

- For values  $X_1, X_2, \dots, X_{n-1}, X_n$  where  $X_n$  is suspected to be extremely high:

- For sets of 3 through 7 values:

- $Q = (X_n - X_{n-1}) / (X_n - X_1)$

- For sets of 8 through 12 values:

- $Q = (X_n - X_{n-1}) / (X_n - X_2)$

- For sets of 13 through 40 values:

- $Q = (X_n - X_{n-2}) / (X_n - X_3)$

# Determination of outliers

- For values  $X_1, X_2, \dots, X_{n-1}, X_n$  where  $X_1$  is suspected to be extremely low:
  - For sets of 3 through 7 values:
    - $Q = (X_2 - X_1) / (X_n - X_1)$
  - For sets of 8 through 12 values:
    - $Q = (X_2 - X_1) / (X_{n-1} - X_1)$
  - For sets of 13 through 40 values:
    - $Q = (X_3 - X_1) / (X_{n-2} - X_1)$

***Compare the estimated  $Q$  against the critical values at  $n$  sets of tests in the Dixon's Table (Table 3 next page).***

***If  $Q >$  Dixon's critical value, the result is an outlier with 95% confidence.***

**Table 3 : Critical Values for the Dixon Test**

Test Criteria	N	95%	99%
	3	0.970	0.994
$D(3...7) = [x(2) - x(1)] / [x(n) - x(1)]$	4	0.829	0.926
Or	5	0.710	0.821
$D(3...7) = [x(n) - x(n-1)] / [x(n) - x(1)]$	6	0.628	0.740
(Whichever is the greater)	7	0.569	0.680
	8	0.608	0.717
$D(8...12) = [x(2) - x(1)] / [x(n-1) - x(1)]$	9	0.564	0.672
Or	10	0.530	0.635
$D(8...12) = [x(n) - x(n-1)] / [x(n) - x(2)]$	11	0.502	0.605
(Whichever is the greater)	12	0.479	0.579



## Critical Values for Dixon's Test

	13	0.611	0.697
	14	0.586	0.670
	15	0.565	0.647
	16	0.546	0.633
	17	0.529	0.610
	18	0.514	0.594
	19	0.501	0.580
	20	0.489	0.567
	21	0.478	0.555
	22	0.468	0.544
	23	0.459	0.535
$D(13...40) = [x(3) - x(1)] / [x(n-2) - x(1)]$	24	0.451	0.526
Or	25	0.443	0.517
$D(13...40) = [x(n) - x(n-2)] / [x(n) - x(3)]$	26	0.436	0.510
(Whichever is the greater)	27	0.429	0.502
	28	0.423	0.495
	29	0.417	0.489
	30	0.412	0.483
	31	0.407	0.477
	32	0.402	0.472
	33	0.397	0.467
	34	0.393	0.462
	35	0.388	0.458
	36	0.384	0.454
	37	0.381	0.450
	38	0.377	0.446
	39	0.374	0.442
	40	0.371	0.438

# Example of Dixon's test

## Repeated drug assay values

Original		Sorted	
Trial #	Value, %	Trial #	Value, %
1	98.0	6	96.8
2	98.5	1	98.0
3	99.0	2	98.5
4	98.6	4	98.6
5	99.3	7	98.8
6	96.8	3	99.0
7	98.8	5	99.3
8	99.4	8	99.4

- Dixon's  $Q$  value =  $(98.0 - 96.8) / (99.3 - 96.8) = 1.20 / 2.50 = 0.48$
- Dixon's critical value for  $n = 8$  is 0.608 (95% confidence)
- Conclusion: Value 96.8% is not an outlier.

# Determination of outliers

- **Thompson's tau ( $\tau$ ) Test**

145	155	153	154	158	161	148	155
147	146	156	155	159	160	<b>172</b>	160
157	153	147	154	157	158	149	152

- $\bar{x} = 154.6$  and  $s = 6.00$
- Note the suspected outlier : 172
- Calculate the **absolute** delta value  $\delta =$  suspected value  $-$  mean  $x$
- Here,  $\delta = 172 - 154.6 = 17.4$
- Use Thompson's critical value table (95% confidence)

## Table of Critical Values for Thompson's $\tau$ at 95% Confidence Level

Sample size	$\tau$	Sample size	$\tau$
3	1.150	21	1.889
4	1.393	22	1.893
5	1.572	23	1.896
6	1.656	24	1.899
7	1.711	25	1.902
8	1.749	26	1.904
9	1.777	27	1.906
10	1.798	28	1.908
11	1.815	29	1.910
12	1.829	30	1.911
13	1.840	31	1.913
14	1.849	32	1.914
15	1.858	33	1.916
16	1.865	34	1.917
17	1.871	35	1.919
18	1.876	36	1.920
19	1.881	37	1.921
20	1.885	38	1.922

# Determination of outliers

- From the table,  $\tau = 1.899$
- Calculate the product of  $\tau$  and  $s$  :
- Here,  $\tau s = 1.899 \times 6.00 = 11.4$
- Compare  $\delta$  and the product  $\tau s$
- If  $\delta > \tau s$ , then the suspected value is an outlier or else, the suspected value is not an outlier.
- In this case, as  $17.4 > 11.4$ , the data 172 is indeed an outlier.