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The Use of Hodges-Lehmann Estimator in Multiple Response Optimization with Replication

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Abstract

透過反應曲面法(RSM)，發展一近似的模型，在探討多反應值最佳化中，常以樣本平均數做爲探討的基準，然而樣本平均數裡通常包括了許多outliers的影響，故在此篇文章中，引用**Hodges-Lehmann** 較爲健全性的估計值。

keywords

- Response surface methodology
- Hodges-Lehmann estimator
- Optimization
- Generalized reduced gradient

Introduction

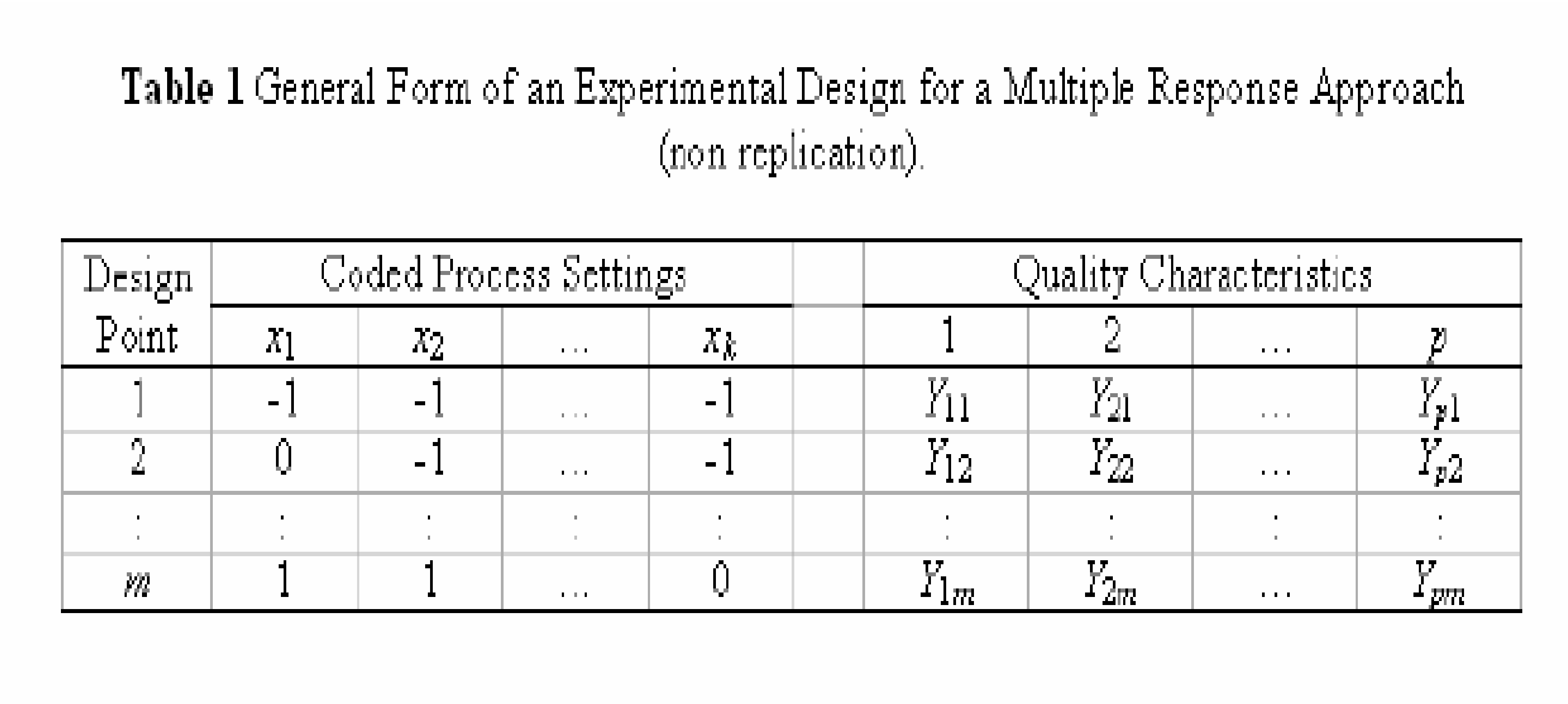


Table 1 General Form of an Experimental Design for a Multiple Response Approach (non replication).

Design Point	Coded Process Settings					Quality Characteristics			
	x_1	x_2	…	x_k		1	2	…	p
1	-1	-1	…	-1		Y_{11}	Y_{21}	…	Y_{p1}
2	0	-1	…	-1		Y_{12}	Y_{22}	…	Y_{p2}
:	:	:	:	:		:	:	:	:
m	1	1	…	0		Y_{1m}	Y_{2m}	…	Y_{pm}

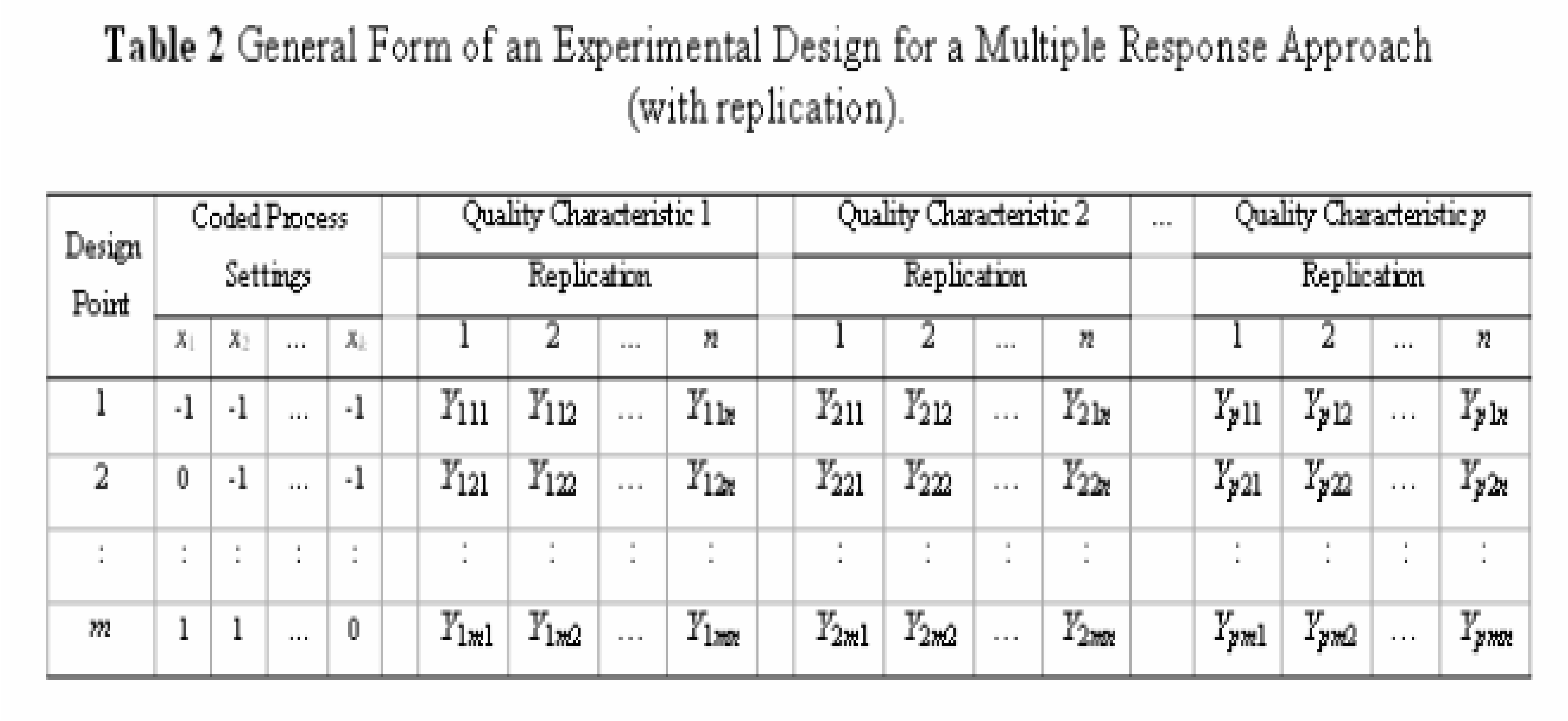


Table 2 General Form of an Experimental Design for a Multiple Response Approach (with replication).

Design Point	Coded Process Settings					Quality Characteristic 1					Quality Characteristic 2				…	Quality Characteristic p			
						Replication					Replication					Replication			
	x_1	x_2	…	x_k		1	2	…	n		1	2	…	n		1	2	…	n
1	-1	-1	…	-1		Y_{111}	Y_{112}	…	Y_{11n}		Y_{211}	Y_{212}	…	Y_{21n}		Y_{p11}	Y_{p12}	…	Y_{p1n}
2	0	-1	…	-1		Y_{121}	Y_{122}	…	Y_{12n}		Y_{221}	Y_{222}	…	Y_{22n}		Y_{p21}	Y_{p22}	…	Y_{p2n}
⋮	⋮	⋮	⋮	⋮		⋮	⋮	⋮	⋮		⋮	⋮	⋮	⋮		⋮	⋮	⋮	⋮
m	1	1	…	0		Y_{1m1}	Y_{1m2}	…	Y_{1mn}		Y_{2m1}	Y_{2m2}	…	Y_{2mn}		Y_{pm1}	Y_{pm2}	…	Y_{pmn}

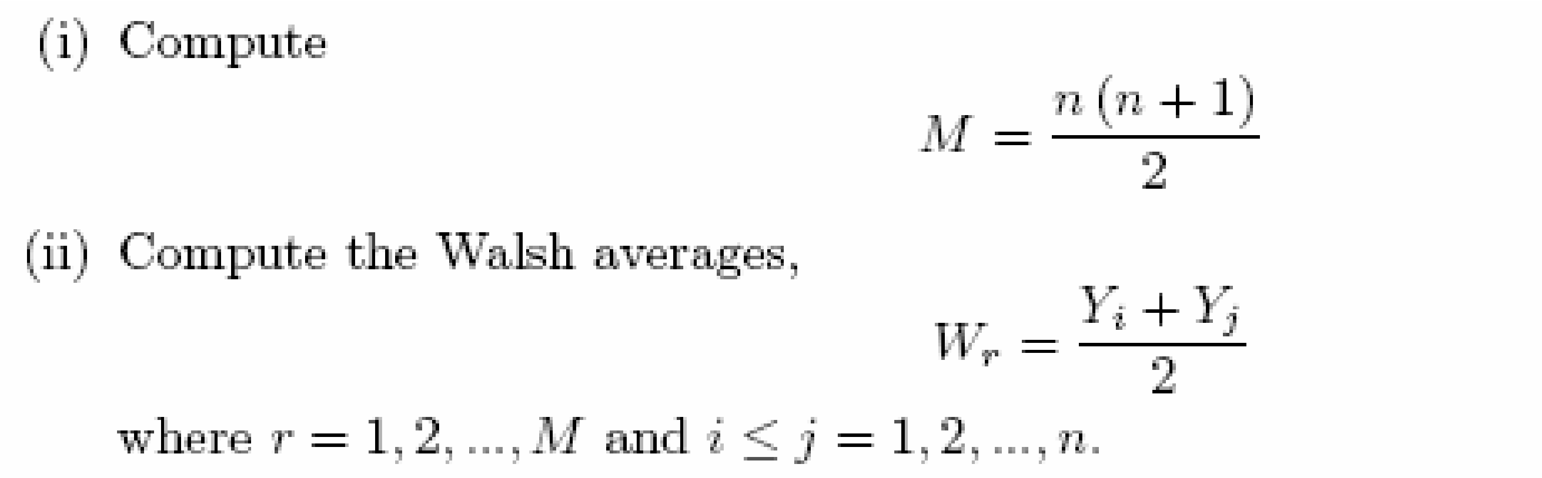
The Hodges-Lehmann estimator

- 假設：

  估計值對稱於 θ 且爲一連續型的對稱分配

The computations of the HL.E follow four steps

- Let Y1,Y2….Yn be a random sample obtained form some distribution , which is continuous and symmetrical about θ ,then,



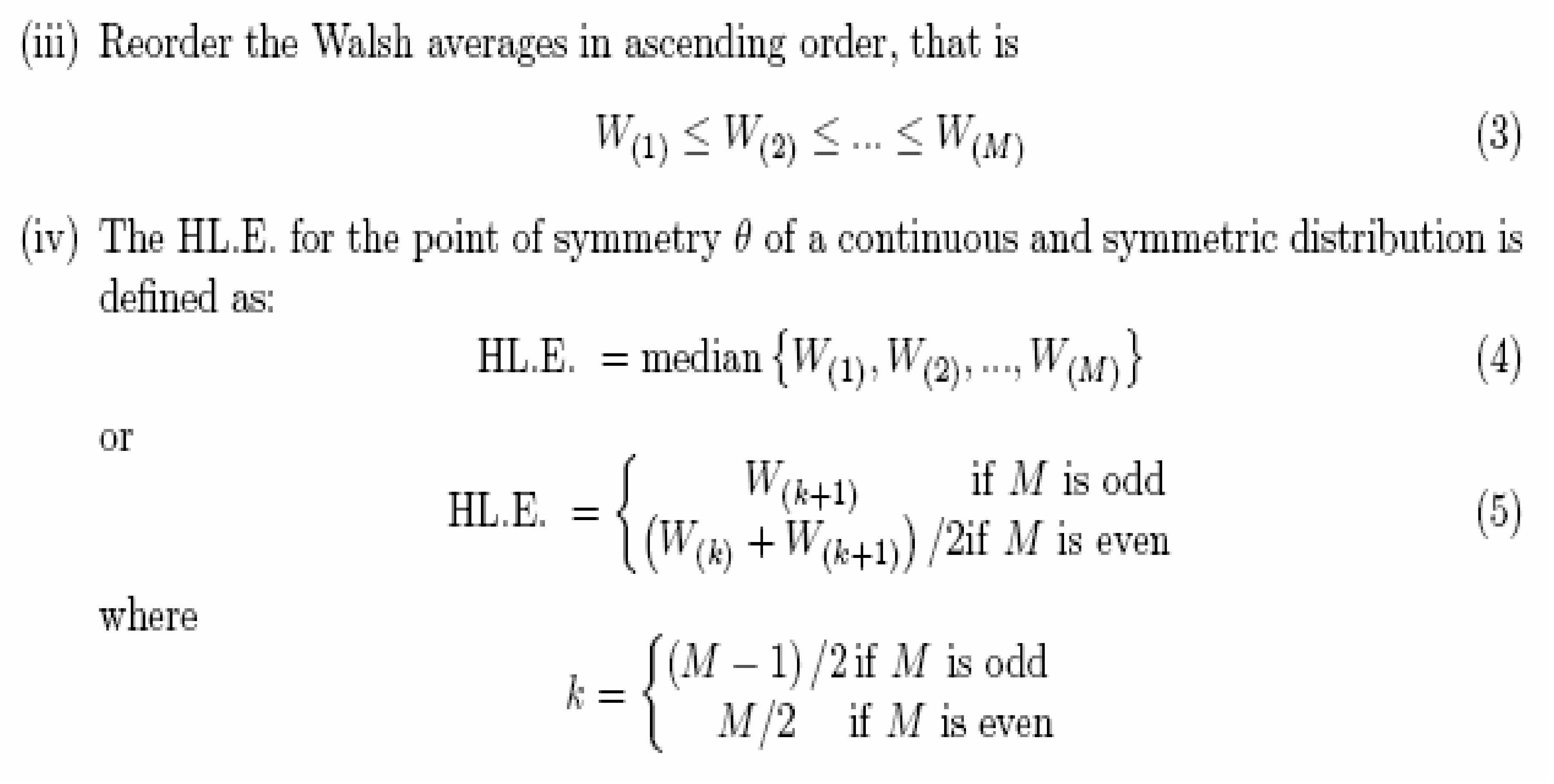
(i) Compute

$$M = \frac{n(n+1)}{2}$$

(ii) Compute the Walsh averages,

$$W_r = \frac{Y_i + Y_j}{2}$$

where $r = 1, 2, ..., M$ and $i \leq j = 1, 2, ..., n$.



(iii) Reorder the Walsh averages in ascending order, that is

$$W_{(1)} \leq W_{(2)} \leq \ldots \leq W_{(M)} \tag{3}$$

(iv) The HL.E. for the point of symmetry θ of a continuous and symmetric distribution is defined as:

$$\text{HL.E.} = \text{median}\left\{W_{(1)}, W_{(2)}, \ldots, W_{(M)}\right\} \tag{4}$$

or

$$\text{HL.E.} = \begin{cases} W_{(k+1)} & \text{if } M \text{ is odd} \\ \left(W_{(k)} + W_{(k+1)}\right)/2 & \text{if } M \text{ is even} \end{cases} \tag{5}$$

where

$$k = \begin{cases} (M-1)/2 & \text{if } M \text{ is odd} \\ M/2 & \text{if } M \text{ is even} \end{cases}$$

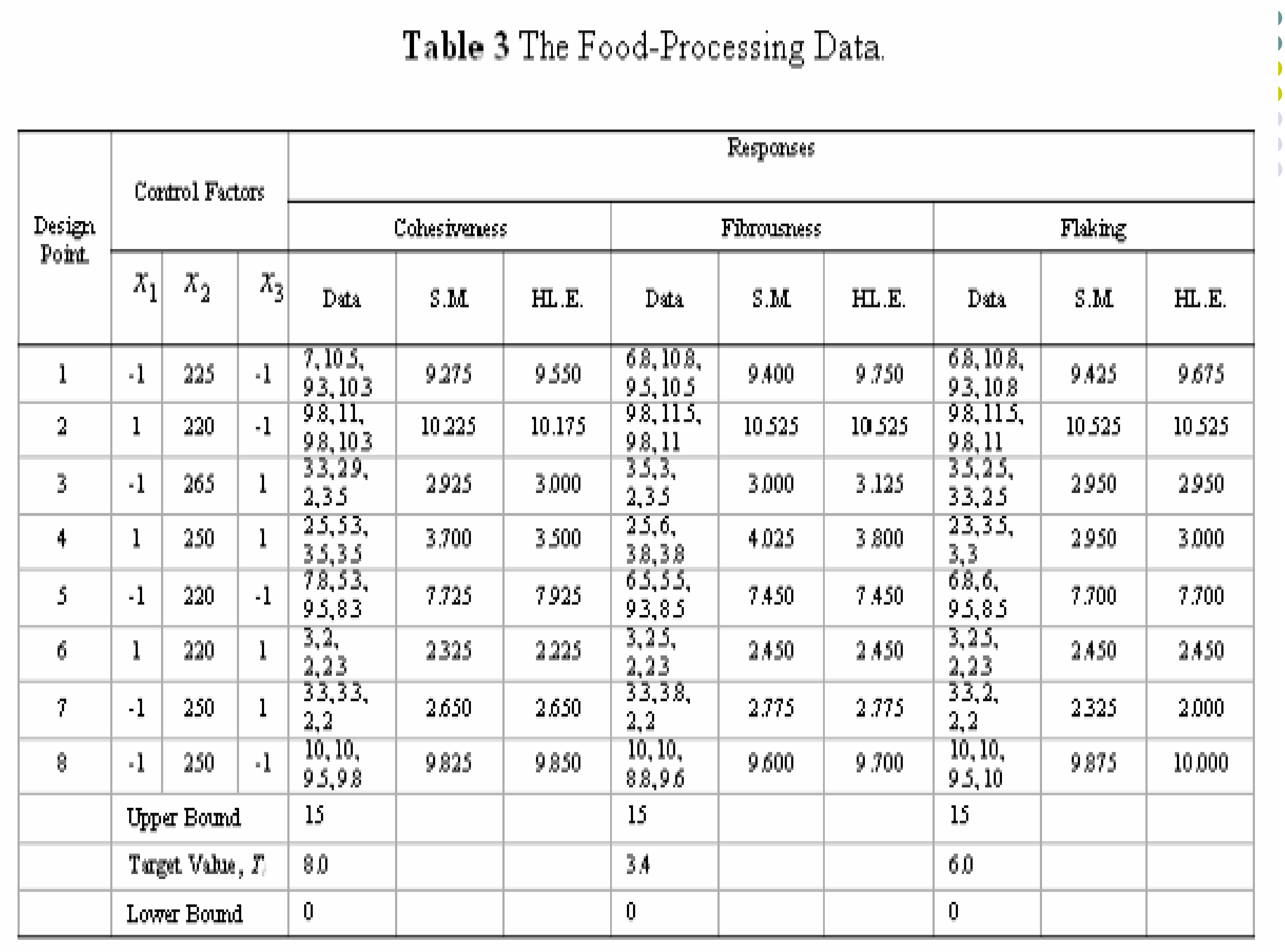


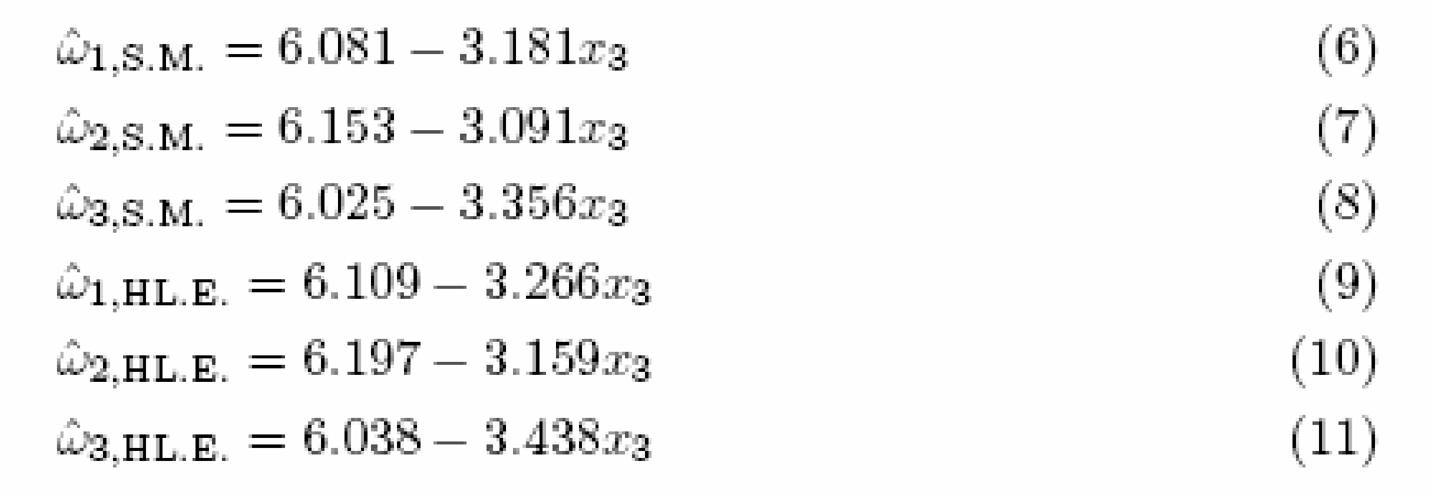
Table 3 The Food-Processing Data.

Design Point	Control Factors			Responses								
				Cohesiveness			Fibrousness			Flaking		
	x_1	x_2	x_3	Data	S.M	HL.E.	Data	S.M	HL.E.	Data	S.M	HL.E.
1	-1	225	-1	7, 10.5, 9.3, 10.3	9.275	9.550	6.8, 10.8, 9.5, 10.5	9.400	9.750	6.8, 10.8, 9.3, 10.8	9.425	9.675
2	1	220	-1	9.8, 11, 9.8, 10.3	10.225	10.175	9.8, 11.5, 9.8, 11	10.525	10.525	9.8, 11.5, 9.8, 11	10.525	10.525
3	-1	265	1	3.3, 2.9, 2, 3.5	2.925	3.000	3.5, 3, 2, 3.5	3.000	3.125	3.5, 2.5, 3.3, 2.5	2.950	2.950
4	1	250	1	2.5, 5.3, 3.5, 3.5	3.700	3.500	2.5, 6, 3.8, 3.8	4.025	3.800	2.3, 3.5, 3, 3	2.950	3.000
5	-1	220	-1	7.8, 5.3, 9.5, 8.3	7.725	7.925	6.5, 5.5, 9.3, 8.5	7.450	7.450	6.8, 6, 9.5, 8.5	7.700	7.700
6	1	220	1	3, 2, 2, 2.3	2.325	2.225	3, 2.5, 2, 2.3	2.450	2.450	3, 2.5, 2, 2.3	2.450	2.450
7	-1	250	1	3.3, 3.3, 2, 2	2.650	2.650	3.3, 3.8, 2, 2	2.775	2.775	3.3, 2, 2, 2	2.325	2.000
8	-1	250	-1	10, 10, 9.5, 9.8	9.825	9.850	10, 10, 8.8, 9.6	9.600	9.700	10, 10, 9.5, 10	9.875	10.000
	Upper Bound			15			15			15		
	Target Value, T_i			8.0			3.4			6.0		
	Lower Bound			0			0			0		

分析的方法

- 將上述資料中的三個變數所計算出之樣本平均數及HL.E.，分別建立迴歸模型，並透過spss採Stepwise ,Backward and Forward三種方式分析之
- 計算出adjusted R squared，值越大表較爲適合的模型。

Model Selection Procedure：Stepwise



$$\hat{\omega}_{1,\text{S.M.}} = 6.081 - 3.181x_3 \quad (6)$$

$$\hat{\omega}_{2,\text{S.M.}} = 6.153 - 3.091x_3 \quad (7)$$

$$\hat{\omega}_{3,\text{S.M.}} = 6.025 - 3.356x_3 \quad (8)$$

$$\hat{\omega}_{1,\text{HL.E.}} = 6.109 - 3.266x_3 \quad (9)$$

$$\hat{\omega}_{2,\text{HL.E.}} = 6.197 - 3.159x_3 \quad (10)$$

$$\hat{\omega}_{3,\text{HL.E.}} = 6.038 - 3.438x_3 \quad (11)$$

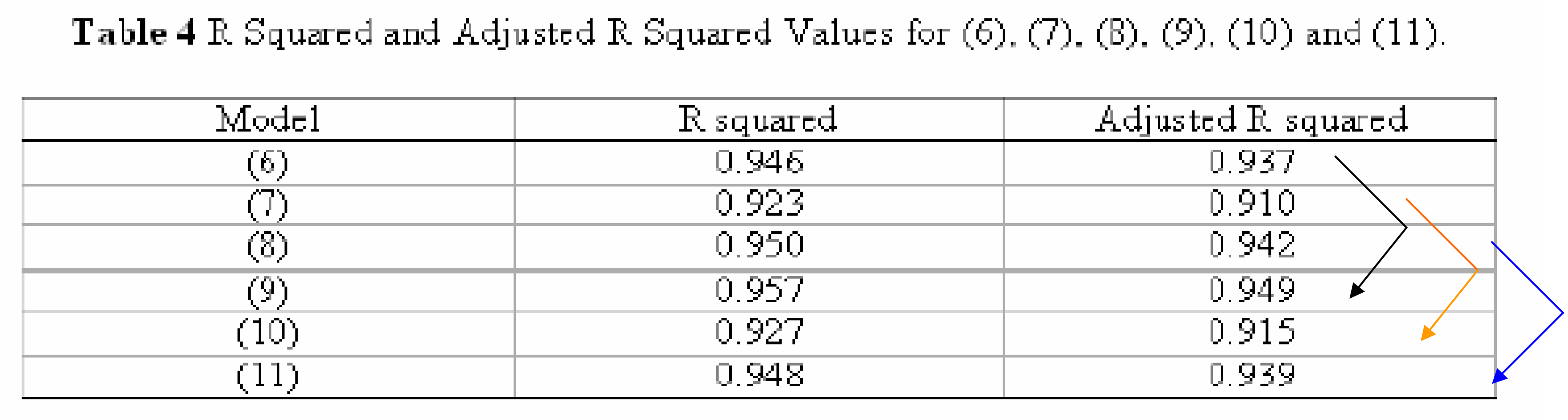


Table 4 R Squared and Adjusted R Squared Values for (6), (7), (8), (9), (10) and (11).

Model	R squared	Adjusted R squared
(6)	0.946	0.937
(7)	0.923	0.910
(8)	0.950	0.942
(9)	0.957	0.949
(10)	0.927	0.915
(11)	0.948	0.939

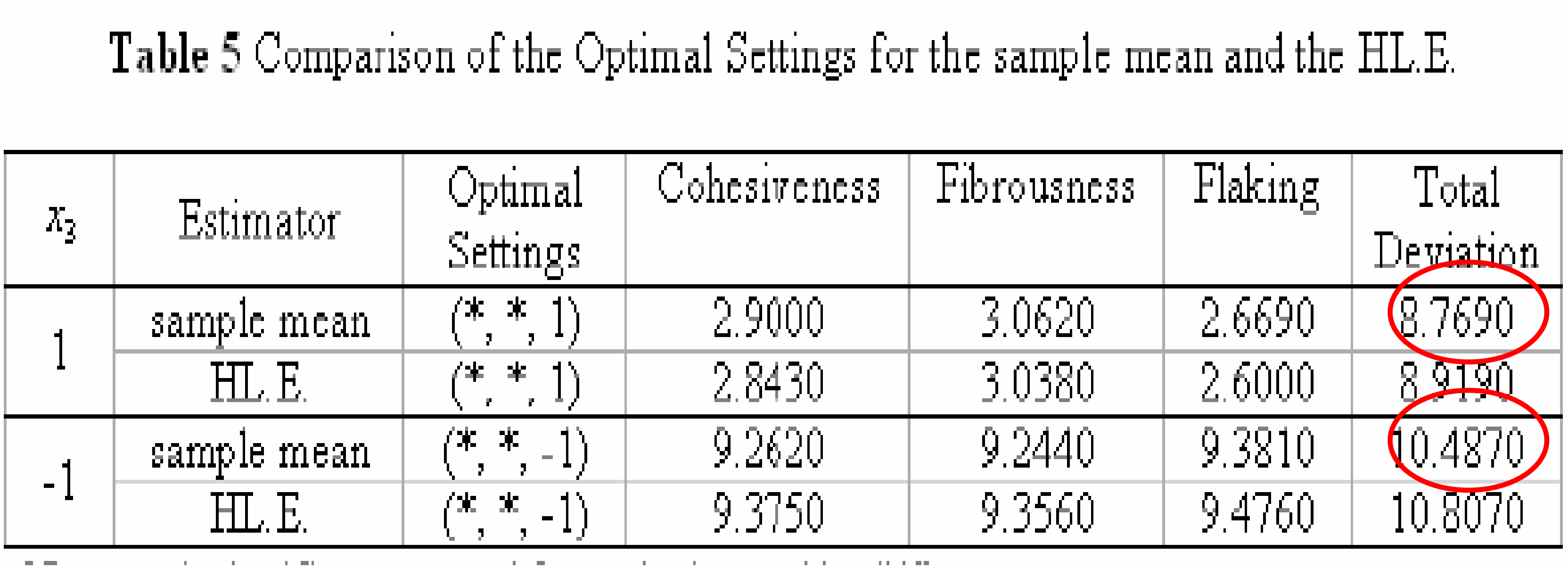


Table 5 Comparison of the Optimal Settings for the sample mean and the HL.E.

x_3	Estimator	Optimal Settings	Cohesiveness	Fibrousness	Flaking	Total Deviation
1	sample mean	(*, *, 1)	2.9000	3.0620	2.6690	8.7690
	HL.E.	(*, *, 1)	2.8430	3.0380	2.6000	8.9190
-1	sample mean	(*, *, -1)	9.2620	9.2440	9.3810	10.4870
	HL.E.	(*, *, -1)	9.3750	9.3560	9.4760	10.8070

Model Selection Procedure：Backward

$$\hat{\omega}_{1,\mathrm{S.M.}} = -5.450 + 0.780x_1 + 0.04938x_2 - 3.808x_3 \quad (13)$$

$$\hat{\omega}_{2,\mathrm{S.M.}} = -5.819 + 0.925x_1 + 0.05138x_2 - 3.771x_3 \quad (14)$$

$$\hat{\omega}_{3,\mathrm{S.M.}} = -3.752 + 0.719x_1 + 0.04192x_2 - 3.903x_3 \quad (15)$$

$$\hat{\omega}_{1,\mathrm{HL.E.}} = -4.451 + 0.642x_1 + 0.04514x_2 - 3.821x_3 \quad (16)$$

$$\hat{\omega}_{2,\mathrm{HL.E.}} = -5.208 + 0.820x_1 + 0.04889x_2 - 3.792x_3 \quad (17)$$

$$\hat{\omega}_{3,\mathrm{HL.E.}} = -4.225 + 0.764x_1 + 0.04402x_2 - 4.014x_3 \quad (18)$$

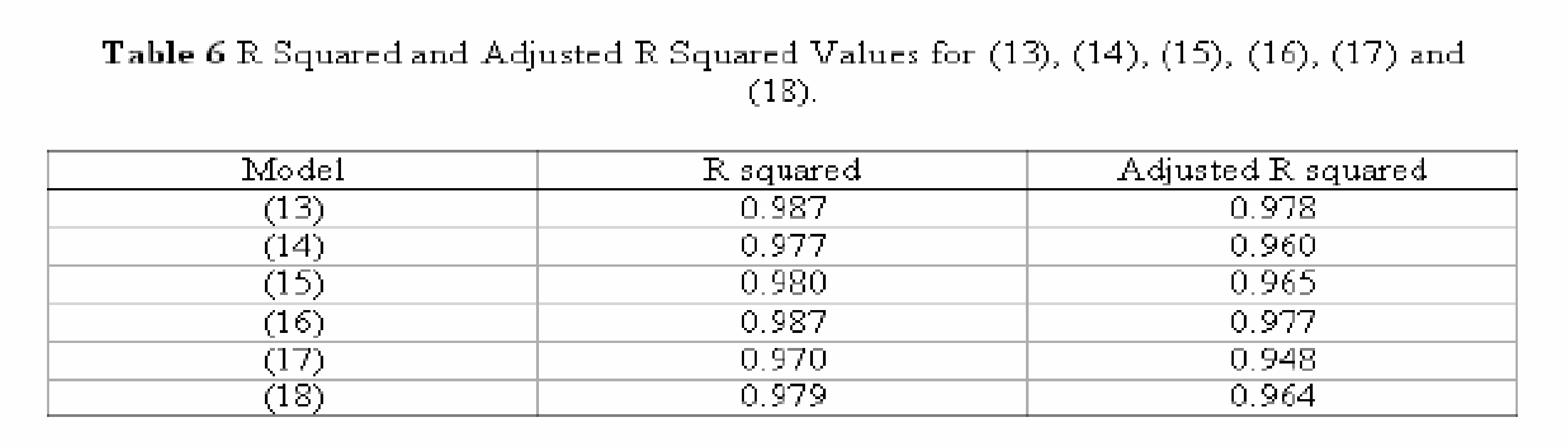


Table 6 R Squared and Adjusted R Squared Values for (13), (14), (15), (16), (17) and (18).

Model	R squared	Adjusted R squared
(13)	0.987	0.978
(14)	0.977	0.960
(15)	0.980	0.965
(16)	0.987	0.977
(17)	0.970	0.948
(18)	0.979	0.964

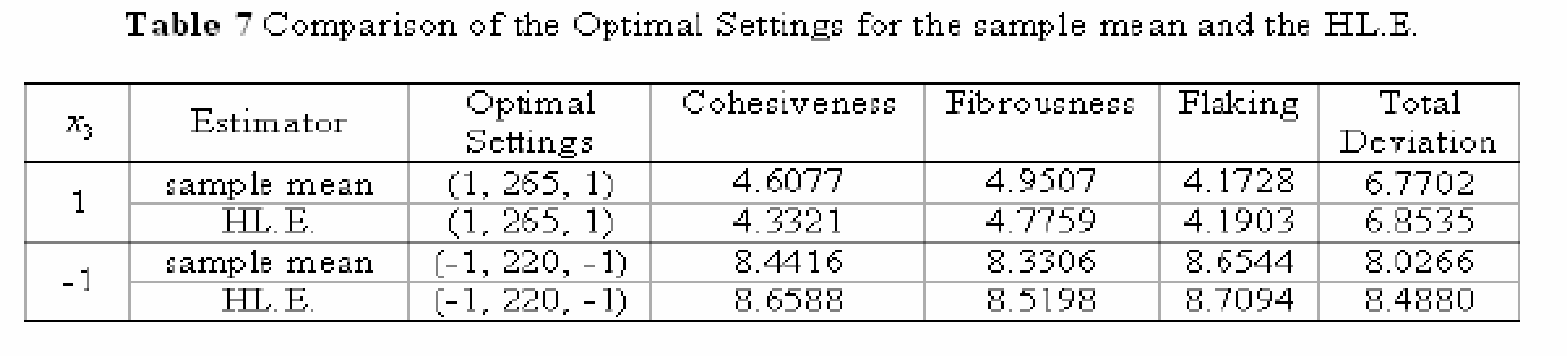


Table 7 Comparison of the Optimal Settings for the sample mean and the HL.E.

x_3	Estimator	Optimal Settings	Cohesiveness	Fibrousness	Flaking	Total Deviation
1	sample mean	(1, 265, 1)	4.6077	4.9507	4.1728	6.7702
	HL.E.	(1, 265, 1)	4.3321	4.7759	4.1903	6.8535
-1	sample mean	(-1, 220, -1)	8.4416	8.3306	8.6544	8.0266
	HL.E.	(-1, 220, -1)	8.6588	8.5198	8.7094	8.4880

Model Selection Procedure：forward

在本paper中的例子，以forward的方式所計算出之R squared and adjusted R squared如同Stepwise一樣，所呈現的結果也相同

Conclusion

- 當沒有Outliers存在時，使用**Hodges-Lehmann estimator**會比使用樣本平均數還來得好。
- **Hodges-Lehmann estimator**有助於經驗不足的人，更容易查出Outliers。