

行政院國家科學委員會補助專題研究計畫成果報告

半折疊與雙半折疊解析度為 IV 之二水準部份因子設計

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摘要

在二水準部份因子設計的領域中，「半折疊設計」(semifolding design)的觀念和技巧在解析度 III 和 IV 的設計中已有詳盡的探討，如 Mee and Peralta (2000)和 Ting and Hsu (2002)，本研究報告主要是針對 16-run, 32-run 及 64-run 解析度 IV 的設計，利用 Ting and Hsu (2002)所提之概念與方法，進行半折疊與雙半折疊(double semifolding)。本研究報告所建議之雙半折疊過程為先將原始設計分成四個部份，然後在對其中一部份進行折疊。本研究報告之表列最佳子集選取的因子組合，礙於篇幅，無法提供，請參閱葉紫君(2002)，報告最後將應用實例來對雙半折疊設計、半折疊設計與全折疊設計做一比較與建議。

關鍵詞：折疊設計，全折疊設計，半折疊設計，雙半折疊設計。

Abstract

In the area of two-level fractional factorial design, the concept and techniques of semifolding have been developed for resolution III and IV designs, e.x., Mee and Peralta (2000) and Ting and Hsu (2002). This research report, however, focuses on 16-run, 32-run, and 64-run resolution IV designs. We apply the semifolding procedure proposed by Ting and Hsu (2002) and extend it to double-semifolding. The procedure we suggest in doing double-semifolding is to block the original design into four sections, and then to fold over on one section only. The “optimal” blocking factors are listed in tables, which can be found in 葉紫君(2002), and the performance of double-semifolding designs in comparisons with that of full foldover designs and semifolding designs are shown by means of examples.

Keywords and phrases: Foldover designs, full foldover designs, semifolding designs, double-semifolding designs.

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性或許沒有全折疊設計高，但若從可估計效果的總個數方面來看，在許多情況下，半折疊設計的表現和全折疊設計是不分上下，其相關做法及結果在 Mee and Peralta (2000)與 Ting and Hsu (2002)的文章中均有詳細的說明。

Mee and Peralta (2000)提到半折疊設計的做法，在解析度 IV 的設計下，將某一主效應，假設將因子 A 當作是固定的折疊因子，讓整個設計對因子 A 進行全折疊，然後在折疊後設計中，選取一半的試驗組合進行實驗。文中作者考慮若干不同的選取試驗組合的方法，並將所有不同的選取法歸成五大類，且分別比較這五種類型選取法的優缺點。再者作者亦證明，若實驗者有興趣的因子是因子 A，將因子 A 當成是折疊因子，如此便可打斷所有與 A 有關的主效應與二因子交互作用中的別名結構，亦即可估計出因子 A 的主效應及所有與 A 有關的二因子交互作用。

Ting and Hsu (2002)亦提及半折疊設計的做法，該論文主要建構在解析度 III 的設計下，作者認為進行半折疊的過程中，應分為兩個步驟，先將原始設計的試驗組合分成兩個部分(section)，且盡可能的讓這兩個部分設計的解析度均維持在 III，或是接近 III，然後再對任一部分進行折疊，而在折疊過程方面，則是將 Li and Mee (2000)的觀念延伸到半折疊設計中，而使用的技巧就是將最短的字的符號變號做折疊，以達到增加解析度，便能夠估計出更多的主效應及二因子交互作用。Ting and Hsu (2002)所提之方法相較於 Mee and Peralta (2000)更為簡易且有效率，文中並指出在許多參數之組合下半折疊設計所估計出之主效應與二因子交互作用害和全折疊一致。

二、研究動機與方向

如前所述，Mee and Peralta (2000)的文章中，作者所討論的半折疊設計主要是建構在解析度 IV 的設計情況下，由作者所舉的例子中，可發現其進行半折疊的方式非常複雜，且在選取一半的試驗組合上花費太多的時間，尤其當因子太多、設計太大時，確實會有實行上的困難，而且該文僅針對 2_{IV}^{6-2} , 2_{IV}^{7-3} , 2_{IV}^{8-4} 做特別探討，而未歸納出一個具體的結論。Ting and Hsu (2002)將半折疊設計之可能結果做一個有系統的整理，作者將半折疊設計的過程分成兩個部分，分別為選取子集方面與折疊過程方面，文中採用的實例皆示取自於 Chen, Sun and Wu (1993)，並將其所選取子集的做法，和 Mee and Peralta (2000)之選取一半試驗組合的做法，兩者互相比較，前者的做法更直覺且容易，然而該論文主要是建構在解析度 III 的設計情況下，所以引起我們繼續探討將 Ting and Hsu (2002)之半折疊做法運用到解析度 IV 的設計，並與 Mee and Peralta (2000)所展現的例子作比較。

再者我們亦想將 Ting and Hsu (2002)在解析度 III 的設計情況下，所使用的選取子集觀念，就是該如何有效的將原設計分成兩個解析度均為 III 或接近 III 之部份設計概念，推廣到解析度 IV 的設計，使用雙半折疊(double semifolding)，亦即將原設計的試驗組合分成四個部分，且盡可能的讓這四個部分設計的解析度均維持在 IV，或是達到最大，然後再對任一部分進行折疊，看是否在解析度 IV 的設計下，雙半折疊設計所得到的結果和半折疊或甚至全折疊之結果一樣。

一般在折疊解析度 IV 的設計下，如前所述，研究者都是考慮全因子折疊來

增加設計之解析度，以估計出更多的主效應及二因子交互作用，但是 Li and Mee (2000)認為在某些情況下，只需考慮將所有長度為三的字變號作折疊，即可達到和全因子折疊一樣的效果，或甚更好。在 Ting and Hsu (2002)的文章中，作者考慮不同選取折疊因子的方式，其中有採用 Li and Mee (2000)所提之方法，亦即盡量讓定義關係中長度短的字變號，或者進行全因子折疊，或者選擇重要因子當折疊因子，並且從中比較半折疊設計與全折疊設計的效果。而在本研究中，我們並不考慮全因子折疊，其主要原因，如前所述，在解析度 III 的設計中，只要透過全因子折疊，所有主效應及部分二因子交互作用便皆可估計，但在解析度 IV 的設計中，其定義關係裡長度為四的字太多，就算將全部因子之水準均反折，亦無法有效的估計出所有的二因子交互作用，所以從效率性來考量，單因子折疊似較為符合我們的需求。

研究基礎：

在解析度 IV 的設計情況下，分成 16-run, 32-run 和 64-run 三部分，施行全折疊、半折疊、雙半折疊並一起做探討，所採用的實例皆取自於 Chen, Sun and Wu (1993)。

研究方向：

1. 比較全折疊、半折疊和雙半折疊所估計出之結果，探討半折疊後，其估計的結果是否大致上和全折疊相同，或雙半折疊後，其估計的結果是否大致上和半折疊以及全折疊相同。
2. 針對 16-run, 32-run 和 64-run 之設計，由折疊後的結果來判斷何時該採用全折疊，何時該採用半折疊以及何時該採用雙半折疊。

三、半折疊設計與雙半折疊設計

Ting and Hsu (2002)建議進行半折疊設計的過程應分為兩步驟，其先後順序分別為：(一) 將原設計之試驗組合分成兩個部分，此步驟稱為選取子集 (blocking)；(二) 然後再對任一部分進行折疊。例如，文章中所提到的 2_{III}^{5-1} 設計，其定義關係為 $I=ABC$ ，作者先用 ACD 將原設計分為二部分，此二部分設計之定義關係分別為 $I=ABE=ACE=BCDE$, $I=ABE=-ACD=-BCDE$ ，然後選擇定義關係為 $I=ABE=ACE=BCDE$ 之部分設計做折疊，接著選擇因子 A 當成是折疊因子，將該部分設計中所有有關 A 之高低水準進行反折。文中作者僅針對解析度 III 的設計做探討，在選取子集方面，盡可能的讓這兩個部分的解析度均維持在 III 或接近 III；在折疊過程方面，則是採用 Li and Mee (2000)所提之方法，亦即盡量讓定義關係長度短的字變號，其目的是希望在進行完整個半折疊過程的步驟後，能估計出最多的主效應與二因子交互作用。從上述的過程中，我們發現若採用 Ting and Hsu (2002)所提的方法來進行半折疊，在選取試驗組合上所花費的時間較 Mee and Peralta (2000)的做法來得少，且半折疊設計的表現和全折疊設計非常接近或一致。

在本研究報告中，當我們針對解析度 IV 的設計進行半折疊時，亦同樣採用 Ting and Hsu (2002)所提出的兩個步驟，在選取子集方面，我們盡可能的讓這兩

個部分的解析度均維持在 IV，或是接近 IV；在折疊過程方面，亦是採用 Li and Mee (2000)所提之方法，盡量讓定義關係中長度短的字變號，希望在進行完整個半折疊過程的步驟後，能估計出最多的二因子交互作用。

另外，當我們進行雙半折疊的過程時，同樣分成兩個步驟，依先後順序分別為：(一) 將原設計之試驗組合分成四個部分，我們亦稱此步驟稱為選取子集，並盡可能的讓這兩個部分的解析度均維持在 IV，或是接近 IV；(二) 然後再對任一部分進行折疊，在折疊過程方面則是採用單因子折疊或 Li and Mee (2000)的方法，希望在進行完整個雙半折疊過程的步驟後，能估計出最多的二因子交互作用。

至於在做半折疊時如何有效地將原設計分成兩個解析度均為 IV 或是接近 IV 之部分，我們使用的技巧是利用部份因子設計的正負表(table of plus and minus)來判斷。假設 X 是一個元素均為 ± 1 之 $n \times k$ 的矩陣，其中 n 為原設計之試驗單位， k 為因子個數， X 中之正負號與正負表中主效應之正負號相同， X 又稱之為設計矩陣(design matrix)；若根據不同的因子或因子組合來分兩個部分，則 X 可分成上下二個各為 $(n/2) \times k$ 之矩陣 X_1, X_2 ，亦即 $X = [X_1', X_2']'$ ，其中 X_1 和 X_2 的正負號分別與此二部分所對應之主效應的正負表。由於正規(regular)之解析度 III 或 III 以上的設計，其 $X'X = nI_k$ ，又因為 $X'X = X_1'X_1 + X_2'X_2$ ，所以當 $X_1'X_1 = (n/2)I_k$ 時，則 $X_2'X_2 = (n/2)I_k$ ，且 X_1, X_2 二集區皆為解析度 III，但若當 $X_1'X_1 = (n/2)I_k$ 無法達到時，我們則會考慮選擇讓 $X_1'X_1$ (或 $X_2'X_2$) 最接近 $(n/2)I_k$ 之選取子集法，亦即非 0 之元素之個數為最小的視為最佳之選取方法。因此，對解析度 IV 的設計而言，此種選取子集方法可以使這二部分之解析度為 I 或至少為 III，而若想更進一步找出是否有解析度為 IV 的兩部分，可藉由其定義關係中得知。

例一、Chen et al. (1993)中的設計 6-2.1，此為 2_{IV}^{6-2} 設計，其衍生器為 $E=ABC, F=ABD$ ，且定義關係為 $I=ABCE=ABDF=CDEF$ ，則 X 如下所示。首先我們考慮半折疊設計，若根據 ACD 來分兩部分，則 X_1, X_2 亦如下所示，經由簡單的計算可得 $X'X = 16I_6$ ， $X_1'X_1 = 8I_6$ ， $X_2'X_2 = 8I_6$ 亦即此二部分設計所對應之解析度為 I 或至少為 III，又此二部分設計之定義關係分別如後：

- (1) $I=ABCE=ABEF=CDEF=ACD=BDE=BCF=AEF$,
- (2) $I=ABCE=ABDF=CDEF=-ACD=-BDE=-BCF=-AEF$,

故兩個部分的解析度均為 III。

$$X' = \begin{bmatrix} -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \end{bmatrix},$$

$$X_1 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \quad X_2 = \begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix},$$

X 我們根據來分兩部分，則如下所示，且此二部分的定義關係分別為，

$$I=ABCE=ABDF=CDEF=AC=BE=BCDE=ADEF,$$

$$I=ABCE=ABDF=CDEF=-AC=-BE=-BCDE=-ADEF,$$

故兩個部分的解析度均為 II。

$$X_1 = \begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix},$$

$$X_1'X_1 = \begin{bmatrix} 8 & 0 & 8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 8 & 0 \\ 8 & 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 8 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix}, \quad X_2'X_2 = \begin{bmatrix} 8 & 0 & -8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & -8 & 0 \\ -8 & 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & -8 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix}$$

所以由上述的結果可以看出 ACD 是較佳之子集選取。

而在做雙半折疊時如何有效地將原設計分成四個解析度均為 IV 或是接近 IV 之部分，所使用的技巧也是利用部份因子設計的正負表來判斷。我們先採取上述選取子集的方法，根據不同的因子或是因子組合來分四個部分，則 X 將可劃分成四個各為 $(n/4) \times k$ 之矩陣 X_1, X_2, X_3, X_4 ，亦即 $X = [X_1', X_2', X_3', X_4']'$ ，其中 X_1, X_2, X_3, X_4 的正負號分別為此四部份所對應之主效應之正負表。由於 $X'X = X_1'X_1 + X_2'X_2 + X_3'X_3 + X_4'X_4$ ，故當 $X_1'X_1 = (n/4)I_k$ ， $X_2'X_2 = (n/4)I_k$ ， $X_3'X_3 = (n/4)I_k$ ， $X_4'X_4 = (n/4)I_k$ 時，則 X_1, X_2, X_3, X_4 四個部分皆是解析度為 I 或至少為 III，但若當 $X_1'X_1 = (n/4)I_k$ 無法達到時，則我們會考慮選擇讓 $X_1'X_1$ （或 $X_2'X_2$ 或 $X_3'X_3$ 或 $X_4'X_4$ ）最接近 $(n/4)I_k$ 之選取子集法，亦即非 0 之元素之個數

為最小的視為可能之最佳選取方法，此為選取子集的第一步驟。

接著進行第二步驟選取，假設 $m = k + C_2^k$ ，令 $W = (X_1^*, Z)$ 是一個元素均為 ± 1 之 $n \times m$ 的矩陣，其中 X_1^* 為第一步驟中所篩選出之可能最佳子集選取所對應之設計矩陣， Z 為其所對應之二因子交互作用之矩陣。計算 $W'W$ ，並將非 0 之元素之個數最小的視為最佳子集之選取，本研究報告所有子集的選取皆以上述的情況考慮，以下舉例說明之。

例二、沿用上例 2_{IV}^{6-2} ，當我們進行第一步驟選取子集，以 A 與 C 來分四部份，和以 A 與 CD 來分四部份，均可讓 $X_1'X_1$ 中非 0 之元素之個數最小，亦即十個，詳述如後：

以 A 與 C 來分四部份，則 X_1, X_2, X_3, X_4 如下所示，而其定義關係分別如下：

$$X_1 = \begin{bmatrix} 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix},$$

$$X_3 = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix}, \quad X_4 = \begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix},$$

- (1) $I=ABCE=ABDF=CDEF=A=BCE=BDF=C=ABE=DEF=AC=BE=BCDE=ADEF,$
- (2) $I=ABCE=ABDF=CDEF=A=BCE=BDF=-C=-ABE=-DEF=-AC=-BE=-BCDE$
 $=-ADEF,$
- (3) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=C=ABE=DEF=-AC=-BE=-BCDE$
 $=-ADEF,$
- (4) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=-C=-ABE=DEF=AC=BE=BCDE$
 $=ADEF,$

故四個部分的解析度均為 I。經簡單的計算可得 $X_1'X_1$ (或 $X_2'X_2$ 或 $X_3'X_3$ 或 $X_4'X_4$) 中不為 0 之元素之個數為十個。若以 A 與 CD 來分四部份，則 X_1, X_2, X_3, X_4 如下所示，而其定義關係分別如下：

$$X_1 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix},$$

$$X_3 = \begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix}, \quad X_4 = \begin{bmatrix} -1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix},$$

- (1) $I=ABCE=ABDF=CDEF=A=BCE=BDF=CD=ABDE=ABCF=EF=ACD=BDE=BCF=AEF,$
- (2) $I=ABCE=ABDF=CDEF=A=BCE=BDF=-CD=-ABDE=-ABCF=-EF=-ACD=-BDE=-BCF=-AEF,$
- (3) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=CD=ABDE=ABCF=EF=-ACD=-BDE=-BCF=-AEF,$
- (4) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=-CD=-ABDE=-ABCF=-EF=ACD=BDE=BCF=AEF,$

故四個部分的解析度均為 I。接著進行第二步驟子集的選取，以 A 與 C 來分四部份之 W 矩陣為：

$$W = \begin{bmatrix} 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 \end{bmatrix},$$

$W'W$ 中不為 0 之元素之個數為 115 個，而以 A 與 CD 來分四部份之 W 矩陣為：

$$W = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 \end{bmatrix},$$

$W'W$ 中不為 0 之元素之個數為 117 個。

續沿用上例 2_{IV}^{6-2} ，若以 A 與 C 將原設計分成四部份，並將其定義關係分別列在下面之(1), (2), (3)和(4)，並將因子 A 當其折疊因子，而將折疊過後之定義關係列在(5)，亦即 $\mathbf{block}=[A,C]$ ， $\mathbf{fold}=A$ ，故整個雙半折疊設計的定義關係如下：

- (1) $I=ABCE=ABDF=CDEF=A=BCE=BDF=C=ABE=DEF=AC=BE=BCDE=ADEF,$
- (2) $I=ABCE=ABDF=CDEF=A=BCE=BDF=-C=-ABE=-DEF=-AC=-BE=-BCDE=-ADEF,$
- (3) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=C=ABE=DEF=-AC=-BE=-BCDE=-ADEF,$
- (4) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=-C=-ABE=DEF=AC=BE=BCDE=ADEF,$
- (5) $I=-ABCE=-ABDF=CDEF=-A=BCE=BDF=C=-ABE=DEF=-AC=BE=BCDE=-ADEF,$

原設計之定義關係為 $I=ABCE=ABDF=CDEF$ ，

- (1) + (5) 之定義關係為 $I=CDEF=BCE=BDF=-ABE=-AC=-ADEF$ ，
- (3) + (5) 之定義關係為 $I=CDEF=-A=C=DEF=-AC=-AEDF$ ，
- (4) + (5) 之定義關係為 $I=CDEF=-A=DEF=BE=BCDF$ ，

利用上面組合出的之義關係，可估計之效果如下：

- (1) + (5): AD, AF.
- (2) + (5): None.
- (3) + (5): BD, BE, BF.
- (4) + (5): None.

- (3) + (5): BD, BE, BF.
 (4) + (5): None.

所以在此雙半折疊之 20-run 設計中，可估計之總效果為 A, B, C, D, E, F, AD, AF, BD, BE, BF，亦即六個主效應與五個二因子交互作用。

若以 A 與 CD 將原設計分成四部份，並將因子 A 與因子 C 當其折疊因子，亦即 **block**=[A, CD], **fold**=A, C，故整個雙半折疊設計的定義關係如下：

- (1) $I=ABCE=ABDF=CDEF=A=BCE=BDF=CD=ABDE=ABCF=EF=ACD=BDE=BCF=AEF$,
 (2) $I=ABCE=ABDF=CDEF=A=BCE=BDF=-CD=-ABDE=-ABCF=-EF=-ACD=-BDE=-BCF=-AEF$,
 (3) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=CD=ABDE=ABCF=EF=-ACD=-BDE=-BCF=-AEF$,
 (4) $I=ABCE=ABDF=CDEF=-A=-BCE=-BDF=-CD=-ABDE=-ABCF=-EF=ACD=BDE=BCF=AEF$,
 (5) $I=ABCE=-ABDF=-CDEF=-A=-BCE=BDF=-CD=-ABDE=ABCF=EF=ACD=BDE=-BCF=-AEF$,

原設計之定義關係為 $I=ABCE=ABDF=CDEF$ ，

- (1) + (5) 之定義關係為 $I=ABCE=BDF=ABCF=EF=ACD=BDE$ ，
 (2) + (5) 之定義關係為 $I=ABCE=BDF=-CD=-ABDE=-BCF=-AEF$ ，
 (3) + (5) 之定義關係為 $I=ABCE=-A=-BCE=ABCF=EF=-BCF=-AEF$ ，
 (4) + (5) 之定義關係為 $I=ABCE=-A=-BCE=-CD=-ABDE=ACD=BDE$ ，

利用上面組合出的之義關係，可估計之效果如下：

原設計：A, B, C, D, E, F.

- (1) + (5): None.
 (2) + (5): None.
 (3) + (5): BD, CD.
 (4) + (5): BF, EF.

所以在此雙半折疊之 20-run 設計中，可估計之總效果為 A, B, C, D, E, F, BD, BF, CD, EF，亦即六個主效應與四個二因子交互作用。

不論是全折疊設計、半折疊設計或者雙半折疊設計，在進行折疊過程方面，我們由可估計效果個數的觀點來看，希望能估計出最多的二因子交互作用，並將這三種設計做比較，看是否半折疊設計所估出來的效果和全折疊相同，是否雙半折疊設計所估出來的效果和半折疊或全折疊也相同，是列舉一例說明。

例三、我們採用 Chen et al (1993) 中 5-1.2 設計，在進行全折疊設計時，對定義關係 $I=ABCE$ 做折疊，並利用 Li and Lin (2002) 的方法，亦即將因子 E 當其折疊因子，將設計中所有有關 E 的部分進行折疊，所以此設計之總試驗組合的個數為 32 runs。

「全折疊設計」：**fold**=E 則原設計(1)和折疊後之設計(2)的定義關係如下。

- (1) $I=ABCE$, (2) $I=-ABCE$,
 由於此(1)+(2)之全折疊的 32-run 設計為一 2^5 之因子設計，所以所有效果均可估計。

分為兩個部分，並將其定義關係分別列在下面之(1)和(2)，並選擇定義關係 $I=ABCE=ABD=CDE$ 之部分做折疊，並將因子 A 當其折疊因子，而將折疊後之定義關係列在(3)，所以此設計之總試驗組合個數為 24 runs。

「半折疊設計」： $\text{block}=ABD$ ； $\text{fold}=A$ ，則此三部分之定義關係如下。

(1) $I=ABCE=-ABD=-CDE$, (2) $I=ABCE=ABD=CDE$, (3) $I=-ABCE=-ABD=CDE$,

則 (1)+(2)的定義關係為 $I=ABCE$ (原設計)，

(2)+(3)的定義關係為 $I=CDE$ ，

(1)+(3)的定義關係為 $I=-ABD$ ，

利用上面組合出的定義關係，可分別求得下列可估計效果：

(1)+(2)：A,B,C,D,E,AD,BD,CD,DE,

(2)+(3)：A,B,AB,AC,AD,AE,BC,BD,BE,

(1)+(3)：C,E,AC,AE,BC,BE,CD,CE,DE.

所以在此半折疊之 24-run 設計中，可估計之效果為 A,B,C,E,D,AB,AC,AD,AE,BC, BD,BE,CD,CE,DE，亦即所有的主效應與二因子交互作用。

「雙半折疊」：在進行雙半折疊時，最佳之子集選取之一為[A,D]，我們用 A 和 D 將原設計分成四個部份，並將其定義關係分別列在下面之(1), (2), (3)和(4)，並將因子 A 當其折疊因子，而將折疊後之定義關係列在(5)，亦即 $\text{block}=A,D$ ； $\text{fold}=A$ ，故整個雙半折疊設計之定義關係如下。

(1) $I=ABCE=A=BCE=D=ABCDE=AD=BCDE$ ，

(2) $I=ABCE=A=BCE=-D=-ABCDE=-AD=-BCDE$ ，

(3) $I=ABCE=-A=-BCE=D=ABCDE=-AD=-BCDE$ ，

(4) $I=ABCE=-A=-BCE=-D=-ABCDE=AD=BCDE$ ，

(5) $I=-ABCE=-A=BCE=D=-ABCDE=-AD=BCDE$ ，

則原設計之定義關係為 $I=ABCE$ ，

(1)+(5)的定義關係為 $I=BCE=D=BCDE$ ，

(2)+(5)的定義關係為 $I=BCE=-ABCDE=-AD$ ，

(3)+(5)的定義關係為 $I=-A=D=-AD$ ，

(4)+(5)的定義關係為 $I=-A=-ABCDE=BCDE$ ，

利用上面組合出的定義關係，可分別求得下列可估計效果：

原設計：A,B,C,E,D,AD,BD,CD,DE.

(1)+(5)：AB,AC,AE,

(2)+(5)：None,

(3)+(5)：BE,BE,CE,

(3)+(5)：None.

所以在此雙半折疊之 20-run 設計中，可估計之效果為 A,B,C,E,D,AB,AC,AD,AE, BC,BD,BE,CD,CE,DE，亦即所有的主效應與二因子交互作用。

由上述的過程中可看出，雖然半折疊設計所估計出之效果的精確度不如全折疊設計高，但因所增加的試驗組合只有全折疊設計的一半，所以從可估計效果和其個數的觀點來看，半折疊設計的表現和全折疊設計不分上下；而雙半折疊設計所估計出之效果的精確度不如全折疊設計或半折疊設計高，因所增加的試驗組合只有半折疊設計的一半（全折疊設計的四分之一），然而其所估計的效果和全折疊設計亦一致，所以若實驗對估計之精確度無疑問時，我們建議使用雙半折疊設計。

計，因為只需增加四分之一個試驗組合便可估計出所有的主效應與二因子交互作用。在本研究報告中我們將給出在 2_{IV}^{k-p} 設計中，當 k, p 值為何時，我們建議使用雙半折疊設計，以及當 k, p 值為何時，雙半折疊設計表現不佳，而應採用半折疊設計，以及何時應採用全折疊設計。

Mee and Peralta (2000)的文章中針對解析度為 IV 的設計之半折疊做法提出，若實驗者有興趣的因子是因子 Q，就選擇將因子 Q 當成是折疊因子，亦即將設計中所有有關 Q 的部份進行折疊，如此便可打斷所有與 Q 有關的二因子交互作用中的別名結構，所以可以估計出因子 Q 的主效應以及所有與 Q 有關的二因子交互作用。我們亦可對雙半折疊設計證出類似的定理。

定理一、對於解析度為 IV 之部分因子設計，在進行雙半折疊設計時，用因子 A 與因子 B 將原始設計分成四個部份，並選擇將因子 A (B)當成是折疊因子，如此便可打斷部份與因子 A (B)有關的二因子交互作用中的別名結構，可以估計出部份與 A (B)有關的二因子交互作用。

證明：詳見葉紫君(2002)。

3.1 16-Run 之半折疊與雙半折疊設計

對於 16-Run 之半折疊與雙半折疊設計，我們將最佳之子集選取列成二表，限於篇幅，請參閱葉紫君(2002)。總結與建議如後：

1. 當因子個數小於 9 時，半折疊設計的表現和全折疊設計一致，基於經濟與效率的考量，我們建議採用半折疊之 24-run 設計。
2. 當因子個數小於 6 時，雙半折疊設計的表現和半折疊設計非常接近，基於經濟與效率的考量，我們建議採用雙半折疊之 20-run 設計。

3.2 32-Run 之半折疊與雙半折疊設計

對於 32-Run 之半折疊與雙半折疊設計，我們將最佳之子集選取列成二表，限於篇幅，請參閱葉紫君(2002)。總結與建議如後：

1. 當因子個數小於等於 16 時，半折疊設計的表現和全折疊設計一致，基於經濟與效率的考量，我們建議採用半折疊之 48-run 設計；而因子個數小於 9 時，我們建議採用雙半折疊之 40-run 設計。
2. 當因子個數大於 6 時，無論雙半折疊設計或半折疊設計，我們只進行單因子折疊，因為在解析度為 IV 之設計中，其目的是估計出較多的二因子交互作用，基於經濟與效率的考量，單因子折疊較符合研究者的需求。

3.3 64-Run 之半折疊與雙半折疊設計

對於 64-Run 之半折疊與雙半折疊設計，我們將最佳之子集選取列成二表，限於篇幅，請參閱葉紫君(2002)。總結與建議如後：

1. 半折疊設計在因子個數等於 9 或 10 時，其表現均和全折疊設計一致或接近，

僅在少數情形下無法達到和全折疊設計一樣。

2. 雙半折疊設計在因子個數等於 9 或 10 的例子中，其表現若非和半折疊設計一致，亦是很接近，僅在少數情形下無法達到和半折疊設計一樣。
3. 當因子個數等於 9 或 10 時，雙半折疊設計、半折疊設計之表現和全折疊設計一致或非常接近，基於經濟與效率的考量，我們建議採用雙半折疊之 80-run 設計。

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四、研究成果評估

研究內容與原計畫一致，研究成果亦達到預期效果，目前本研究之結果已寫成論文並送審中。

出席國際會議心得報告

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協辦單位：中國現場統計學會，均勻設計學會，南開大學，中國統計學會

發表論文：Families of A-optimal Diallel Crosses for Test Line Versus Control Comparisons

心得報告：

本研討會共計二日，發表篇數二十一篇，參與人數將近百人，其中包括 K. T. Fang, D. J. K. Lin, Geoff Vining, Scott Kowalski, Shu Yamada, Mong-Na Lo, Shao-Wei Cheng, Jianfang Zhang, Liangping Hu, Jian Zhang, Rongxian Yue, Mingqian Liu, and Xiru Chen 等，會議報告安排方式共分五組，第一組、國際組，第二組、實驗設計研究在台灣組，第三組、應用組，第四組、均勻設計組，第五組、正交設計組。

此研討會最特殊的地方在於打破以往認為中國大陸統計學者的專精在數理方面，會議中之應用組，讓我們看到統計學在中國大陸主要應用範圍，雖仍是以生物統計為主，但發表文章內容之精采，發表者口才之好，足以令我們大開眼界。我所發表之文章雖非屬於均勻設計亦或是正交設計之範疇，但亦得到許多參與者之寶貴建議，以及日後可能發展之方向，可謂收穫豐盛。發表之文章如附件，近日分別獲得 *Statistics and Probability Letters* 和中國統計學報接受刊登。

A-Optimal and Efficient Diallel Cross Experiments for Comparing
Test Treatments with a Control

By

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Abstract

A-optimality of diallel cross experiments for comparing two or three test lines with a control line under the model for block designs is studied. Families of A-optimal and efficient Type S_0 block designs are derived. The construction methods of these designs are given.

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1. Introduction

The problem of simultaneously comparing p test treatments with a control in the set up of block design in diallel cross experiment is considered. Design of experiments for diallel crosses are used in plant and animal breeding experiment to study the genetic properties of inbred lines. Suppose there are $p + 1$ inbred lines, and are denoted as $0, 1, \dots, p$, with 0 denotes the control line, and $1, \dots, p$ denote the p test lines, respectively. For $i < j = 0, 1, \dots, p$, let a cross between lines i and j be denoted as (i,j) , and the lines are to be compared with respect to their general combining abilities. The study of optimal designs for all pairwise comparisons between lines has been receiving considerable attention recently, see e.g. Gupta and Kageyama (1994), Gupta, Das, and Kageyama (1995), Dey and Midha (1996), Mukerjee (1997), Das, Dey, and Dean (1998), Das, Dean, and Gupta (1998). Not until Choi, Gupta, and Kageyama (2002), the problem of test line versus control comparisons is under investigation. Choi, Gupta, and Kageyama (2002) define type S block design, and tabulate its efficiency, which is computed by comparing to the best unblocked type S design, for up to 24 test lines. The “best” design in their paper means the design that estimates the test line versus control comparisons with the minimum constant variance. Das, Gupta, and Kageyama (2002) derive a sufficient condition for designs to be A-optimal, and define type S_0 block designs, a special group of type S block designs for which all p test lines occur almost the same number of times within each block and in every block, and the control line occurs almost the same number of times in every block. The optimality and efficiency of type S_0 block design are also shown.

The objective of the present communication, however, is to find families of optimal

and efficient type S_0 block designs and to develop a construction method for small p , that is, when the number of test lines is two and three. The paper is organized as follows. Section 2 contains preliminaries, definitions, and some needed theorems. Families of A-optimal and efficient type S_0 block designs when the number of test lines is three are given in section 3. A construction method is also provided. Section 4 is devoted to the calculation of the efficiencies and the construction of efficient type S_0 block designs when the number of test lines is two. Some examples are also presented.

2. Preliminaries

The diallel crosses involving $p(p+1)/2$ distinct crosses are considered in here. Let d be a block design for a diallel cross experiment with p test lines, one control line, and b blocks of size k each, and let $n = bk$ denote the total number of crosses in d . The model for a block design for diallel crosses is assumed to be

$$\bar{Y}_d = \mu \bar{1}_n + \Delta_{1d} \bar{\tau} + \Delta_{2d} \bar{\beta} + \bar{\varepsilon},$$

where \bar{Y}_d is the $n \times 1$ vector of observed responses, μ is the overall mean, $\bar{1}_n$ denotes the $n \times 1$ vector of 1's, $\bar{\tau} = (\tau_0, \tau_1, \dots, \tau_p)'$ is the vector of $p+1$ general combining ability effects, $\bar{\beta} = (\beta_1, \dots, \beta_b)'$ is the vector of b block effects, Δ_{1d}, Δ_{2d} are the corresponding design matrices, that is, the (s, h) th element of Δ_{1d} is 1 if the s th observation pertains to line h , and is zero, otherwise; and the (s, l) th element of Δ_{2d} is 1 if the s th observation pertains to block l , and is zero, otherwise; $\bar{\varepsilon}$ is the $n \times 1$ vector of independent random errors with mean zero and constant variance σ^2 . The coefficient matrix of the reduced normal equations for estimating $\bar{\tau}$ is given by

$$C_d = G_d - (1/k)N_d N_d',$$

where $G_d = (g_{dii'}) = \Delta'_{1d} \Delta_{1d}$, $N_d = (n_{dij}) = \Delta'_{1d} \Delta_{2d}$, $g_{dii'}$ is the number of times cross (i, i') appears in d , $g_{dii} = s_{di}$ is the number of times line i occurs in crosses in d , and n_{dij} is the number of times line i occurs in block j in d . In this paper, however, our focus is on the estimation of the test line versus control contrasts $(\tau_1 - \tau_0, \dots, \tau_p - \tau_0)'$, and by Bechhofer and Tamhane (1981), and Das, Gupta, and Kageyama (2002) the information matrix, $M_d = (m_{dii'})$, for the estimation of $(\tau_1 - \tau_0, \dots, \tau_p - \tau_0)'$ is obtained by deleting the first row and first column of C_d , where $m_{dii} = s_{di} - (1/k) \sum_{j=1}^b n_{dij}^2$, $i = 1, \dots, p$, and $m_{dii'} = g_{dii'} - (1/k) \sum_{j=1}^b n_{dij} n_{di'j}$, $i \neq i'$, $i, i' = 1, \dots, p$.

Let $D(p+1, b, k)$ be a collection of all connected designs with p test lines, one control line, b blocks of size k . A design $d^* \in D(p+1, b, k)$ is said to be A-optimal if it minimizes $\sum_{i=1}^p \text{Var}(\hat{\tau}_i - \hat{\tau}_0)$, where $\hat{\tau}_i - \hat{\tau}_0$ is the best linear unbiased estimator (BLUE) of $\tau_i - \tau_0$, $i = 1, \dots, p$, over all designs in $D(p+1, b, k)$, that is, d^* satisfies

$$\sum_{i=1}^p \text{Var}(\hat{\tau}_{d^*i} - \hat{\tau}_{d^*0}) = \min_{d \in D(p+1, b, k)} \sum_{i=1}^p \text{Var}(\hat{\tau}_{di} - \hat{\tau}_{d0}), \text{ or}$$

$$\text{tr} M_{d^*}^{-1} = \min_{d \in D(p+1, b, k)} \text{tr} M_d^{-1}.$$

For all designs $d \in D(p+1, b, k)$, applying the averaging technique in Kiefer (1975), Majumdar and Notz (1983), and Jacroux and Majumdar (1989), one has

$$\begin{aligned} \text{tr} M_d^{-1} &\geq \text{tr} \bar{M}_d^{-1} \\ &= \frac{p}{s_{d0} - k^{-1} \sum_{j=1}^b n_{d0j}^2} + \frac{(p-1)^2}{2bk - s_{d0} - k^{-1} \sum_{i=1}^p \sum_{j=1}^b n_{dij}^2 - p^{-1} (s_{d0} - k^{-1} \sum_{j=1}^b n_{d0j}^2)}, \end{aligned}$$

where $\bar{M}_d = (1/p!) \sum_{\pi} \pi M_d \pi'$, is the average of all possible permutations of the p test lines on M_d , and π is the corresponding $p \times p$ permutation matrix. We should note that \bar{M}_d is completely symmetric, i.e., $\bar{M}_d = aI_p + bJ_{p,p}$, where I_p is the $p \times p$ identity matrix, and $J_{p,p}$ is a $p \times p$ matrix of 1's, and the eigenvalues of \bar{M}_d are $p^{-1}(s_{d0} - k^{-1} \sum_{j=1}^b n_{d0j}^2)$ with multiplicity 1, and $(p-1)^{-1}(2bk - s_{d0} - k^{-1} \sum_{i=1}^p \sum_{j=1}^b n_{dij}^2 - p^{-1}(s_{d0} - k^{-1} \sum_{j=1}^b n_{d0j}^2))$ with multiplicity $p-1$. The designs having completely symmetric information matrices are called type S block designs by Choi, Gupta, and Kageyama (2002).

Definition 2.1. (Choi, Gupta, and Kageyama (2002)) A design $d \in D(p+1, b, k)$ is a type S block design if it satisfies $g_{d0i} = g_0$, $g_{dii'} = g_1$, $\sum_{j=1}^b n_{d0j} n_{dij} = \lambda_0$, and $\sum_{j=1}^b n_{dij} n_{di'j} = \lambda_1$, for $i \neq i'$, $i, i' = 1, \dots, p$, and $g_0, g_1, \lambda_0, \lambda_1$ are integers.

A type S block design d has the following properties.

- (i) $s_{d0} = pg_0$,
- (ii) $s_{d1} = \dots = s_{dp} = (2bk - s_{d0})/p = g_0 + (p-1)g_1 = s_1$, say,
- (iii) $pg_0 + (p(p-1)/2)g_1 = bk$,
- (iv) $\sum_{j=1}^b n_{d0j}^2 = p(2kg_0 - \lambda_0)$,
- (v) $\sum_{j=1}^b n_{dij}^2 = 2k(g_0 + (p-1)g_1) - (p-1)\lambda_1 - \lambda_0$, $i = 1, \dots, p$, and
- (vi) $M_d = ((p\lambda_1 + \lambda_0)/k - g_0 - pg_1)I_p + (g_1 - \lambda_1/k)J_p$.

Among all type S block designs, there is a special group of designs called type S_0 block designs by Das, Gupta, and Kageyama (2002), and their A-optimality property has been shown.

Definition 2.2. (Das, Gupta, and Kageyama (2002)) A type S block design d is said to be

a type S_0 block design, denoted as $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$, if it satisfies $|n_{d_{0j}} - n_{d_{0j'}}| \leq 1$, and $|n_{d_{ij}} - n_{d_{i'j'}}| \leq 1$, for $i, i' = 1, \dots, p; j, j' = 1, \dots, b$.

Let $g(s; p, b, k) = \frac{p}{s - k^{-1}h(s)} + \frac{(p-1)^2}{2bk - s - k^{-1}a(s) - p^{-1}(s - k^{-1}h(s))}$, where

$$h(s) = s(2y+1) - by(y+1), \quad a(s) = (2bk - s)(2x+1) - pbx(x+1), \quad x = [(2bk - s)/pb],$$

$y = [s/b]$, and $[\cdot]$ is the greatest integer function. For an $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$ design d

it can be shown that $n_{d_{0j}} = [s_{d_0}/b]$ or $[s_{d_0}/b] + 1$, $\sum_{j=1}^b n_{0j}^2 = h(s_{d_0}) = 2ks_{d_0} - p\lambda_0$,

$n_{d_{ij}} = [(2bk - s_{d_0})/pb]$ or $[(2bk - s_{d_0})/pb] + 1$, and $\sum_{j=1}^b n_{ij}^2 = h(s_1) = 2ks_1 - (p-1)\lambda_1 - \lambda_0$,

for $i = 1, \dots, p, j = 1, \dots, b$. Das, Gupta, and Kageyama (2002) show that for given values

of p, b , and k , design $d \in D(p+1, b, k)$ satisfies $trM_d^{-1} \geq tr\bar{M}_d^{-1} \geq g(s_{d_0}; p, b, k)$, and

the equalities hold when M_d is completely symmetric. By minimizing $g(s; p, b, k)$ over s

and using the fact that the information matrix of a type S_0 block design is completely

symmetric, a type S_0 block design having the value of s_{d_0} which minimizes $g(s; p, b, k)$, if

exists, is A-optimal.

Theorem 2.1. (Das, Gupta, and Kageyama (2002)) For given values of p, b , and k ,

an $S_0(p, b, k, g_0, g_1, \lambda_0, \lambda_1)$ design d^* is A-optimal if it satisfies

(i) $s_{d^*0} = s_0$, and s_0 is a positive integer such that $g(s_0; p, b, k) = \min_{1 \leq s \leq c} g(s; p, b, k)$,

where $c = bk$ if (1) $p = 5, k = 3$, or (2) $p = 4, k$ is odd, or (3) $p = 3$; else $c = b[k/2]$,

(ii) $s_1 = (2bk - s_0)/p$,

(iii) $g_0 = s_0/p, g_1 = (s_1 - g_0)/(p-1)$,

(iv) $\lambda_0 = (2ks_0 - h(s_0))/p, \lambda_1 = (2ks_1 - h(s_1) - \lambda_0)/(p-1)$.

3. Optimal and Efficient Designs for $p = 3$

To find families of A-optimal designs and efficient designs, we derive the following inequality by substituting x with $(2bk - s)/pb$, and y with s/b in $g(s; p, b, k)$,

$$\begin{aligned} g(s; p, b, k) &\geq pbk \left(\frac{1}{bks - s^2} + \frac{(p-1)^2}{bk(2bk(p-2) - (p-3)s)} \right) \\ &= pbk(g^*(s; p, b, k)), \text{ say,} \end{aligned} \quad (1)$$

and the equality holds when $(2bk - s)/pb$ and s/b are integers.

For $p = 3$, $g^*(s; 3, b, k) = (bks - s^2)^{-1} + 2(bk)^{-2}$, and by taking the derivative of $g^*(s; 3, b, k)$ with respect to s , the minimum value of $g^*(s; 3, b, k)$ is achieved at $s = s_0 = bk/2$, and $g^*(bk/2; 3, b, k) = 6/(bk)^2$. In the following, the problems of finding and constructing families of A-optimal type S_0 block designs having $s_0 = bk/2$ are investigated.

A type S_0 block design $S_0(3, b, k, g_0, g_1, \lambda_0, \lambda_1)$ with $s_0 = bk/2$ has the following values for $s_1, g_0, g_1, \lambda_0, \lambda_1$, and

$$\begin{aligned} s_1 &= bk/2, \quad g_0 = g_1 = bk/6, \text{ and} \\ \lambda_0 = \lambda_1 &= \begin{cases} bk^2/4, & \text{if } k \text{ is even,} \\ bk^2/4 - b/12, & \text{if } k \text{ is odd.} \end{cases} \end{aligned}$$

For these designs to exist, $s_0, s_1, g_0, g_1, \lambda_0, \lambda_1$ must all be integers, and the possible combinations of the values of such b and k are as follows.

- (I) $b \equiv 0 \pmod{3}$, $k \equiv 0 \pmod{2}$, (II) $k \equiv 0 \pmod{6}$,
 (III) $b \equiv 0 \pmod{6}$, $k \equiv 1 \pmod{2}$.

In cases (I) and (II), k is an even number, and both $(2bk - s_0)/3b = k/2$ and

$s_0 / b = k / 2$ are integers, hence, the minimum values of $g^*(s;3,b,k)$ or $g(s;3,b,k)$ can be achieved by the corresponding type S_0 block designs. Then by Theorem 2.1, these designs are A-optimal in their respective classes.

Lemma 3.1. For $b = 0 \pmod{3}$, $k = 0 \pmod{2}$, that is, $b = 3t$, $k = 2q$, where $t, q \geq 1$ are integers, a type S_0 block design $S_0(3,3t,2q,tq,tq,3tq^2,3tq^2)$ if exists, is A-optimal in $D(3+1,3t,2q)$.

Lemma 3.2. For $k = 0 \pmod{6}$, that is, $b = t$, $k = 6q$, where $t, q \geq 1$ is an integer, a type S_0 block design $S_0(3,t,6q,tq,tq,9tq^2,9tq^2)$ if exists, is A-optimal in $D(3+1,t,6q)$.

The optimal designs in Lemmas 3.1 and 3.2 can always be constructed by using the following two initiate designs d_A and d_B in Examples 3.1 and 3.2, respectively. These two designs are A-optimal by the above two lemmas.

Example 3.1. For $b = 3$, $k = 2$, that is, $t = q = 1$, the following design d_A with columns as blocks is a $S_0(3,3,2,1,1,3,3)$, and is A-optimal in $D(3+1,3,2)$.

$$d_A : \begin{array}{ccc} (0,1) & (0,2) & (0,3) \\ (2,3) & (1,3) & (1,2) \end{array}$$

Example 3.2. For $b = 1$, $k = 6$, that is, $t = q = 1$, the following design d_B with column as block is a $S_0(3,1,6,1,1,9,9)$, and is A-optimal in $D(3+1,1,6)$.

$$d_B : \begin{array}{c} (0,1) \\ (0,2) \\ (0,3) \\ (1,2) \\ (1,3) \\ (2,3) \end{array}$$

Case (I): For $b = 0 \pmod{3}$, $k = 0 \pmod{2}$, that is, $b = 3t$, $k = 2q$, where $t, q \geq 1$ are integers, an A-optimal $S_0(3, 3t, 2q, tq, tq, 3tq^2, 3tq^2)$ design d_I with columns as blocks can be constructed by repeating d_A t times in the column direction and q times in the row direction, and is illustrated in the following.

$$d_I : \left. \begin{array}{cccc} & \overbrace{\hspace{10em}}^t & & \\ & d_A & d_A & \cdots & d_A \\ & d_A & d_A & \cdots & d_A \\ & \vdots & \vdots & \ddots & \vdots \\ & d_A & d_A & \cdots & d_A \end{array} \right\} q \quad (2)$$

Case (II): For $k = 0 \pmod{6}$, that is, $b = t$, $k = 6q$, where $t, q \geq 1$ is an integer, an A-optimal $S_0(3, t, 6q, tq, tq, 9tq^2, 9tq^2)$ design d_{II} can be constructed as (2) by replacing d_A with d_B .

Remark: For $b = 3t$, $k = 6q$, no matter how differently the optimal designs, constructed by using the above two methods, might appear, they all are type S_0 block designs, and hence they all are A-optimal designs. For example, for $b = 3$, $k = 6$, by Lemmas 3.1 and 3.2, the following two designs d and d' both are A-optimal type S_0 block designs in $D(3+1, 3, 6)$.

$$d : \begin{array}{ccc} (0,1) & (0,2) & (0,3) \\ (0,1) & (0,2) & (0,3) \\ (0,1) & (0,2) & (0,3) \\ (2,3) & (1,3) & (1,2) \\ (2,3) & (1,3) & (1,2) \\ (2,3) & (1,3) & (1,2) \end{array}, \quad d' : \begin{array}{ccc} (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) \\ (0,3) & (0,3) & (0,3) \\ (1,2) & (1,2) & (1,2) \\ (1,3) & (1,3) & (1,3) \\ (2,3) & (2,3) & (2,3) \end{array}$$

For values of b and k in case (III), type S_0 block designs, though exist, can not be

proved to be A-optimal by existing methods. Their efficiencies are thus investigated.

Case (III): For $b = 0 \pmod{6}$, $k = 1 \pmod{2}$, that is, $b = 6t$, $k = 2q + 1$, where $t, q \geq 1$ are integers, a type S_0 block design d_{III} with $s_0 = s_1 = 3t(2q + 1)$, $g_0 = g_1 = t(2q + 1)$, and $\lambda_0 = \lambda_1 = t(6q^2 + 6q + 1)$, can be constructed by using the following two initiate designs d_1 for $b = 6, k = 3$, and d_2 for $b = 6, k = 2$, respectively, where

$$d_1 : \begin{pmatrix} (0,1) & (0,2) & (0,1) & (0,1) & (0,2) & (0,3) \\ (0,2) & (0,3) & (0,3) & (1,2) & (1,3) & (1,2) \\ (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (2,3) \end{pmatrix},$$

$$d_2 : \begin{pmatrix} (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) \\ (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) \end{pmatrix},$$

and

$$d_{III} : \left. \begin{array}{cccc} & \overbrace{\hspace{2cm}}^t & & \\ & d_1 & d_1 & \cdots & d_1 \\ & d_2 & d_2 & \cdots & d_2 \\ d_{III} : & d_2 & d_2 & \cdots & d_2 \\ & \vdots & \vdots & \ddots & \vdots \\ & d_2 & d_2 & \cdots & d_2 \end{array} \right\} q-1. \quad (3)$$

Example 3.3. For $b = 12, k = 7$, that is, $t = 2, q = 3$, the following design is a $S_0(3,12,7, 14,14,146,146)$.

$$\begin{pmatrix} (0,1) & (0,2) & (0,1) & (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,1) & (0,1) & (0,2) & (0,3) \\ (0,2) & (0,3) & (0,3) & (1,2) & (1,3) & (1,2) & (0,2) & (0,3) & (0,3) & (1,2) & (1,3) & (1,2) \\ (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (2,3) & (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (2,3) \\ (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) \\ (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) \\ (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) & (0,1) & (0,2) & (0,3) \\ (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) & (2,3) & (1,3) & (1,2) \end{pmatrix}$$

As for the efficiency of design $d \in D(p+1, b, k)$, the same definition is used as in Das, Gupta, and Kageyama (2002), that is,

$$E(d) = \sum_{i=1}^p \text{Var}(\hat{\tau}_{d_{opt}i} - \hat{\tau}_{d_{opt}0}) / \sum_{i=1}^p \text{Var}(\hat{\tau}_{di} - \hat{\tau}_{d0}), \quad (4)$$

where d_{opt} is an A-optimal design in $D(p+1, b, k)$. Now for $p = 3$, and by applying inequality (1),

$$\sum_{i=1}^p \text{Var}(\hat{\tau}_{d_{opt}i} - \hat{\tau}_{d_{opt}0}) \geq (3bk)g^*(bk/2, 3, b, k)\sigma^2 = (18/bk)\sigma^2,$$

hence, $E(d) \geq (18/bk)\sigma^2 / \sum_{i=1}^p \text{Var}(\hat{\tau}_{di} - \hat{\tau}_{d0}) = e(d)$, say.

For design d_{III} in case (III), through some straightforward calculation one can see that $\sigma^{-2} \sum_{i=1}^p \text{Var}(\hat{\tau}_{d_{III}i} - \hat{\tau}_{d_{III}0}) = 3(2q+1)/4tq(q+1)$, and $e(d_{III}) = 1 - 1/(2q+1)^2$. For $q = 1$, that is, $b = 6t, k = 3, E(d_{III}) \geq 0.89$; for $q \geq 2$, that is, $b = 6t, k \geq 5$ is an odd number, $E(d_{III}) \geq 0.96$. One can thus conclude that the type S_0 block designs in case (III) are highly efficient designs in $D(3+1, 6t, 2q+1)$.

4. Efficient Designs for $p = 2$

For $p = 2$, then $g^*(s; 2, b, k) = 1/(bks - s^2) + 1/bks$, by taking the derivative of $g^*(s; 2, b, k)$ with respect to s , the minimum value of $g^*(s; 2, b, k)$ is achieved at $s = s_0 = bk(2 - \sqrt{2})$, and $g^*(bk(2 - \sqrt{2}); 2, b, k) = (3 + 2\sqrt{2})/(bk)^2$. Now $bk(2 - \sqrt{2})$ is not an integer, the method we use in section 3 to find families of A-optimal designs for $p = 3$ can not be applied here. Though $bk(2 - \sqrt{2})$ is not an integer, it is close to $bk/2$, hence, in the following, the efficiencies of type S_0 block designs having $s_0 = bk/2$ are investigated.

A type S_0 block design $S_0(2, b, k, g_0, g_1, \lambda_0, \lambda_1)$ with $s_0 = bk/2$, has the following

values for $s_1, g_0, g_1, \lambda_0, \lambda_1$, and

$$s_1 = 3bk/4, \quad g_0 = bk/4, \quad g_1 = bk/2,$$

$$\lambda_0 = \begin{cases} 3bk^2/8, & \text{if } k \text{ is even,} \\ b(3k^2 - 1)/8, & \text{if } k \text{ is odd,} \end{cases}$$

$$\lambda_1 = \begin{cases} 9bk^2/16, & \text{if } k \equiv 0 \pmod{4}, \\ 9bk^2/8 - h(s_1), & \text{if } k \text{ is even, and } k \not\equiv 0 \pmod{4}, \\ b(9k^2 + 1)/8 - h(s_1), & \text{otherwise,} \end{cases}$$

where $h(\cdot)$ is as in section 2. For these designs to exist, $s_0, s_1, g_0, g_1, \lambda_0, \lambda_1$ must all be integers, and the possible combinations of the values of such b and k are as follows.

- (I) $k \equiv 0 \pmod{4}$, (II) $b \equiv 0 \pmod{4}, k \equiv 1 \pmod{4}$,
 (III) $b \equiv 0 \pmod{2}, k \equiv 2 \pmod{4}$, (IV) $b \equiv 0 \pmod{4}, k \equiv 3 \pmod{4}$.

Using the same efficiency definition in (4), for $p = 2$, $d \in D(2+1, b, k)$, the lower bound to the efficiency is obtained as follows.

$$e(d) = \frac{2(3+2\sqrt{2})\sigma^2/bk}{\sum_{i=1}^p \text{Var}(\hat{\tau}_{d_i} - \hat{\tau}_{d_0})}.$$

For designs $\tilde{d}_I, \tilde{d}_{II}, \tilde{d}_{III}$, and \tilde{d}_{IV} in cases (I), (II), (III), and (IV), respectively, through some straightforward calculation, one has

$$(I) \quad \sigma^{-2} \sum_{i=1}^p \text{Var}(\hat{\tau}_{\tilde{d}_{Ii}} - \hat{\tau}_{\tilde{d}_{I0}}) = 12/bk, \text{ and } E(\tilde{d}_I) \geq e(\tilde{d}_I) = (3+2\sqrt{2})/6 = 0.9714,$$

$$(II) \quad \sigma^{-2} \sum_{i=1}^p \text{Var}(\hat{\tau}_{\tilde{d}_{IIi}} - \hat{\tau}_{\tilde{d}_{II0}}) = 12/(bk - b/k), \text{ and}$$

$$E(\tilde{d}_{II}) \geq e(\tilde{d}_{II}) = (3+2\sqrt{2})(1-1/k^2)/6,$$

$$(III) \quad \sigma^{-2} \sum_{i=1}^p \text{Var}(\hat{\tau}_{\tilde{d}_{IIIi}} - \hat{\tau}_{\tilde{d}_{III0}}) = 8/bk + 4/(bk - 2b/k), \text{ and}$$

$$E(\tilde{d}_{III}) \geq e(\tilde{d}_{III}) = (3+2\sqrt{2})/(4+2/(1-2/k^2)),$$

(IV) $\sigma^{-2} \sum_{i=1}^p \text{Var}(\hat{\tau}_{\tilde{d}_{IVi}} - \hat{\tau}_{\tilde{d}_{IV0}}) = 12/(bk - b/k)$, and

$$E(\tilde{d}_{IV}) \geq e(\tilde{d}_{IV}) = (3 + 2\sqrt{2})(1 - 1/k^2)/6.$$

Almost all of the above lower bounds to the efficiencies are greater than or equal to 0.9325, the only two exceptions are in Case (III), when $k = 2$, and $E(\tilde{d}_{III}) \geq 0.7286$, and in Case (IV), when $k = 3$, and $E(\tilde{d}_{IV}) \geq 0.8635$. One can therefore conclude that the type S_0 block designs in the above four cases are highly efficient designs in $D(2+1, b, k)$ for $k \geq 3$.

The efficient type S_0 block designs can be constructed by using the same techniques as in section 3.

Case (I): For $k \equiv 0 \pmod{4}$, that is, $b = t$, $k = 4q$, where $t, q \geq 1$ is an integer. By replacing d_A with \tilde{d}_1 in (2), an efficient $S_0(2, t, 4q, tq, 2tq, 6tq^2, 9tq^2)$ design \tilde{d}_1 can thus be constructed, and

$$\tilde{d}_1 : \begin{matrix} (0,1) \\ (0,2) \\ (1,2) \\ (1,2) \end{matrix}.$$

Example 4.1. For $b = 2$, $k = 4$, that is, $t = 2$, $q = 1$, the following design is a $S_0(2,2,4,2,4,12,18)$, and $e(d) = 0.9714$.

$$\begin{matrix} (0,1) & (0,1) \\ (0,2) & (0,2) \\ (1,2) & (1,2) \\ (1,2) & (1,2) \end{matrix}$$

Case (II): For $b = 0 \pmod{4}$, $k = 1 \pmod{4}$, that is, $b = 4t$, $k = 4q + 1$, where $t, q \geq 1$ are integers. By replacing d_1 with \tilde{d}_{21} , and d_2 with \tilde{d}_{22} in (3), an efficient $S_0(2, 4t, 4q + 1, t(4q + 1), 2t(4q + 1), t(24q^2 + 12q + 1), 2t(18q^2 + 9q + 1))$ design \tilde{d}_{II} can thus be constructed, and

$$\tilde{d}_{21} : \begin{matrix} (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) \\ (0,2) & (0,1) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \end{matrix}, \quad \tilde{d}_{22} : \begin{matrix} (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \end{matrix}.$$

Example 4.2. For $b = 8$, $k = 13$, that is, $t = 2$, $q = 3$, the following design is a $S_0(2, 8, 13, 26, 52, 506, 760)$, and $e(d) = 0.9657$.

$$\begin{matrix} (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) \\ (0,2) & (0,1) & (1,2) & (1,2) & (0,2) & (0,1) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) \\ (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) \\ (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) \\ (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) \\ (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) & (0,2) \\ (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) & (1,2) \end{matrix}$$

Case (III): For $b = 0 \pmod{2}$, $k = 2 \pmod{4}$, that is, $b = 2t$, $k = 4q - 2$, where $t \geq 1$, $q \geq 1$ are integers. By replacing d_1 with \tilde{d}_{31} , and d_2 with \tilde{d}_{32} in (3), an efficient $S_0(2, 2t, 4q - 2, t(2q - 1), 2t(2q - 1), 3t(2q - 1)^2, 2t(9q^2 - 9q + 2))$ design \tilde{d}_{III} can thus be constructed, and

$$\tilde{d}_{31} : \begin{matrix} (0,1) & (0,2) \\ (1,2) & (1,2) \end{matrix}, \quad \tilde{d}_{32} : \begin{matrix} (0,1) & (0,1) \\ (0,2) & (0,2) \\ (1,2) & (1,2) \\ (1,2) & (1,2) \end{matrix}.$$

Example 4.3. For $b = 4$, $k = 6$, that is, $t = 2$, $q = 2$, the following design is a $S_0(2,4,6,6,12, 54,80)$, and $e(d) = 0.9527$.

$$\begin{matrix} (0,1) & (0,2) & (0,1) & (0,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \\ (0,1) & (0,1) & (0,1) & (0,1) \\ (0,2) & (0,2) & (0,2) & (0,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \end{matrix}$$

Case (VI): For $b = 0 \pmod{4}$, $k = 3 \pmod{4}$, that is, $b = 4t$, $k = 4q - 1$, where $t \geq 1$, $q \geq 1$ are integers. By replacing d_1 with \tilde{d}_{41} , and d_2 with \tilde{d}_{22} (as in Case (II)) in (3), an efficient $S_0(2,4t,4q-1,t(4q-1),2t(4q-1),t(24q^2-12q+1), 2t(18q^2-9q+1))$ design \tilde{d}_{IV} can thus be constructed, and

$$\tilde{d}_{41} : \begin{matrix} (0,1) & (0,1) & (0,1) & (0,2) \\ (0,2) & (0,2) & (1,2) & (1,2) \\ (1,2) & (1,2) & (1,2) & (1,2) \end{matrix}.$$

Example 4.4. For $b = 8$, $k = 7$, that is, $t = 2$, $q = 2$, the following design is a $S_0(2,8,7,14, 28,146,220)$, and $e(d) = 0.9516$.

(0,1)	(0,1)	(0,1)	(0,2)	(0,1)	(0,1)	(0,1)	(0,2)
(0,2)	(0,2)	(1,2)	(1,2)	(0,2)	(0,2)	(1,2)	(1,2)
(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)
(0,1)	(0,1)	(0,1)	(0,1)	(0,1)	(0,1)	(0,1)	(0,1)
(0,2)	(0,2)	(0,2)	(0,2)	(0,2)	(0,2)	(0,2)	(0,2)
(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)
(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)	(1,2)

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