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On generalizing the foldover technique to 3^{f-s} regular fractional factorial designs

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Abstract

The foldover technique allows for an expansion of a fractional factorial experiment with two level factors to achieve a resolution IV design from a resolution III design. Resolution IV designs allow for unbiased estimation of main effects if third order interactions and higher are 0. This paper lays out a scheme that generalizes the foldover technique to regular fractional factorial experiments with three level factors by augmenting the design matrix by a rotation vector. The criterion for choosing an optimal rotation vector is discussed in detail. It is shown that no perfect analog exists to always achieving resolution IV designs for regular fractional factorial experiments with three level factors although minimum aberration can be gained in all situations where resolution IV designs are not available.

1 Purpose

Many factorial experiments do not involve all treatments for a host of reasons (time, money, logistics, etc...). For example a complete experiment with six factors all with three levels will need 729 runs to support estimation of all factorial effects. To find standard errors or preform inference will require even more runs without making more assumptions. So it is common that only a fraction of the complete factorial experiment is preformed to reduce run size cost. Continuing the example if we include only the treatments for which any two factorial effects are held constant through the whole experiment we will reduce run costs to a more manageable 81. Such a design is referred to as regular fractional factorial design.

In a complete factorial experiment when all factors have three levels any one effect would have a specific level for 1/3 of the treatments in the experiment. To reduce costs, a regular fractional factorial experiment will include only those runs for which a specific effect occurs at one level, reducing the experiment size to a third of the original size (or a ninth if two effects are held constant through the whole experiment, et cetera). It is often seen as conceptually equivalent to blocking on an effect(s) and then preforming the experiment using only one of the blocks.

The reduction in run size comes with a penalty of confounding effects. Any given effect of interest, will, necessarily, be confounded with a string of effects which are impossible to isolate from one another without more runs. And more so, there will be some number of effects which are held constant through the whole experiment, confounding them with the intercept of the model.

The set of effects that are held constant through the whole experiment are referred to as the generating relation and are individually referred to as generators. The generating relation dictates how all factorial effects are confounded (aliased) with each other. Any given effect that is held constant will be referred to as a generator and it's coded vector of length f will be denoted **g**, a row vector. For example ABC^2 in a regular fractional factorial experiment with f = 5 factors is coded as **g** = (1, 1, 2, 0, 0).

We will rely on two important concepts when comparing candidate fractional factorial experimental designs to find which is best. The first is resolution, introduced by Box and Hunter (1961), which is defined as the number of the factors in the "shortest" effect in the generating relation. The higher the resolution the better. The second concept is aberration, introduced by Fries and Hunter (1980), which is the count of the "shortest" words in the generating relation. This number should be as low as possible and is considered the secondary crition for comparing designs.

Suppose a resolution III design for three two-level factors has $I = ABC$ as it's generating relation. This then implies that the main effect of factor A is completely confounded with the interaction of factors B and C. The point estimate of A then is also the point estimate of BC and their relative effects on the model cannot be isolated. What often occurs with a situation like this is that a *strong* assumption is made that the effect of $BC = 0$. A more realistic but less definitive assumption is that, *ceteris paribus*, effects of relatively higher order are relatively more likely (*a priori*) to be zero. Large resolution is desirable in order to relax this assumption to only high order generalized interactions.

The foldover technique, introduced by Box and Wilson (1951) and discussed in section 2, is commonly used in experimental design for expanding designs with 2 level factors from resolution III to resolution IV. The natural question is "Is there an analogous technique for foldover when the number of levels is not 2?". Margolin (1969) stated that attempts to extend the foldover to higher levels had not yet been developed although he made no attempt to solve the problem that we can tell. Margolin did find that the minimal run size for a three level factor design to be resolution IV is bounded below by 6*f - 3 with f being the number of factors. This paper attempts to generalize the foldover to experiments that have 3 levels for all factors, referring to it as the triple foldover. It will be shown that while it is not guaranteed that tripling the size of the experiment will produce a resolution IV design, in the case where is is not possible there is an optimum that produces a minimum aberration design of resolution III.

We will restrict ourselves to looking at only regular fractional factorial designs with f factors, f $\in$ N. All factors will have 3 levels denoted {0, 1, 2}. The initial designs will be regular fractions defined by s generators, i.e. 3^{-s} fractions containing 3^{f-s} unique treatments, where s $\in$ {1, 2, ..., f-1}. A rotation vector, denoted as **x**, will be used to define how each row of the original design matrix is rotated to create the augmented triple foldover design matrix. This operation will result in an augmented experimental design in $3^{f - s + 1}$ unique treatments , i.e. 3 times the size of the initial design. Finding the optimal rotation vector **x** is the main goal of this paper.

2 Foldover for 2 Level Factors

The original foldover method as described in Box and Wilson (1951) can be applied to a design of resolution III inlcuding factors of only two levels The foldover is the augmentation of the original design matrix by changing all signs to their opposites if one is using the +/- system. In 0/1 notation all 0's become 1's and all 1's become 0's. The advantage of this system is that all generators of odd length in the generating relation, most importantly generators of length three, will drop out. So if the original design was resolution III then the augmented design is of resolution IV. A very small example follows.

Suppose we have a regular fractional factorial design with 5 factors each at 2 levels, with the following design matrix

A	B	C	D	E
0	0	0	1	1
1	1	0	1	1
1	1	0	0	0
1	0	1	1	0
0	1	1	1	0
1	0	1	0	1
0	1	1	0	1
0	0	0	0	0

The generating relation is

$$\begin{aligned} I &= -ABC \\ &= -CDE = -ABDE \end{aligned}$$

since all of those effects are held as constants in the design. This is a resolution III design with aberration II because the shortest words in the generating relation are of length 3 and there are 2 of them. The prefix "-" and "+" are used to indicate the level at which the effects are being held (level 0 for "- "). The original foldover technique then will do a reversal of these 0's and 1's to create a second matrix to supplement the above design matrix. The new half of the augmented matrix will be

A	B	C	D	E
1	1	1	0	0
0	0	1	0	0
0	0	1	1	1
0	1	0	0	1
1	0	0	0	1
0	1	0	1	0
1	0	0	1	0
1	1	1	1	1

and the complete augmented design in 16 treatments has generating relation

$$I = -ABDE$$

since all odd length generators (specifically ABC and CDE) are now orthogonal to the intercept. For example, in any given row of the first matrix, the effect of ABC is a constant 0 but in this second matrix the effect of ABC is a constant 1 for any row. A pattern occurs for the CDE effect. But the $ABDE$ effect remains confounded with the intercept since in both generating relations the effect remains constant at level 0.

In the notation introduced in section 3 of this paper, the rotation vector, which is a row vector, for the two level foldover would be $\mathbf{x} = \{1, 1, ..., 1\}$. This rotation vector will be added to all row vectors $\mathbf{d}$, the rows of the original design matrix $\mathbf{D}$. The new rows in the augmented design matrix, $\mathbf{d} + \mathbf{x}$, will have the modulo 2 function applied element-wise. The result is such that $\mathbf{d}$ is reflected through the midpoint of the design region to determine the location of the point to be added. More generally we say that $\mathbf{d}$ will "rotate" to the new corresponding levels. This is the design augmentation that we seek to generalize by finding the optimal rotation vector for a design with 3 levels.

There is also a second type of 2 level foldover design. The second type is appropriate when the data collected in the original experiment indicates that one factor is acting "interestingly". In this case, the sign of only that factor will be changed in the second half of the design while all other factors remain at their original levels. Alternatively the rotation vector will be $\mathbf{x} = \{0, 0, ..., 0, 1, 0,..., 0\}$ with the single 1 being the corresponding location of the factor of interest. The overall design's resolution may not change but for the factor of interest it will have the behavior of a resolution V design. That is, for that factor the main effect is unconfounded by two- and three-factor interactions and the factor's second order interactions will be unconfounded by other two factor interactions. This has a direct analogy in experiments with 3 levels and will be shown later. Our approach to transforming the design matrix using rotation vectors does not treat these as two different techniques but the same technique with different goals driving which rotation vector is chosen (increased resolution/minimized aberration vs. higher resolution for a given factor).

Taking the example from above, allow the original design matrix to remain the same and allow for a rotation for factor A, arbitrally assuming that is the factor that is acting interestingly. The new rows in the augmented matrix will be

A	B	C	D	E
1	0	0	1	1
0	1	0	1	1
0	1	0	0	0
0	0	1	1	0
1	1	1	1	0
0	0	1	0	1
1	1	1	0	1
1	0	0	0	0

and the augmented design in 16 treatments has generating relation

$$I = -CDE$$

since both the effect of ABC and $ABDE$ will drop out. In the augmented new rows the levels of these effects are both 1 as compared to 0 in the original design matrix. Note that the main effect of A is unbiased by two level interactions and three level interactions. Indeed the only alias that the main effect of A has is $ACDE$, a fourth order interaction. Also worth noting is that the second order interactions involving A are biased by third order interactions ($AC = ADE$ for example) such that with respect to factor A, the augmented design has characteristics of a resolution V design.

3 Foldover for 3 level Factors Setup

For the triple foldover an explanation of notation is needed first. From there we will introduce the concept of rotationally tolerant and intolerant generators.

For coding an effect that has factors of three levels, the levels will be represented as 0, 1, and 2. A factor will be denoted with a capital letter. A string of capital letters will also be used to denote a factorial effect; if more than one capital letter is listed, the effect is an interaction. A squared capital letter in an effect string will represent the effect of the second generalized interaction of that factor (with the square) and the other terms in the effect string.

A simple example for a regular fractional factorial design matrix with three level factors is

A	B	C	D	E
0	0	0	0	0
0	0	1	1	2
0	0	2	2	1
0	1	0	2	0
0	1	1	0	2
0	1	2	1	1
0	2	0	1	0
0	2	1	2	2
0	2	2	0	1
1	0	0	1	1
1	0	1	2	0
1	0	2	0	2
1	1	0	0	1
1	1	1	1	0
1	1	2	2	2
1	2	0	2	1
1	2	1	0	0
1	2	2	1	2
2	0	0	2	2
2	0	1	0	1
2	0	2	1	0
2	1	0	1	2
2	1	1	2	1
2	1	2	0	0
2	2	0	0	2
2	2	1	1	1
2	2	2	2	0

for which we will denote a generating relation as

$$\begin{aligned} I &\propto AC^2E^2 \\ &\propto ABDE \propto AB^2CD^2 \propto BCDE^2 \end{aligned}$$

This notation is non-standard and some explanation is required. Let $\mathbf{d}$ be any of the 5-element rows form the design matrix. The presence of AC^2E^2 in the generating relation means that for $\mathbf{g}$ = (1, 0, 2, 0, 2), $\mathbf{gd}$' mod 3 takes the same value for all treatments. This is also true for $\mathbf{g}$ = (1, 1, 0, 1, 1) because $ABDE$ is a generator. Our notation does not specify the particular constant value taken for each of these terms, but this is not especially important for our purposes.

Note please that we are including only 27 runs out of a possible 243. This small fraction of the complete collection of treatments comes with the consequence of having no information on the above effects in the generating relation and having certain effects completely aliased with others. For example, the main effect of A is aliased with the interactions CE, $AB^2D^2E^2$, BDE, ABC^2D, BC^2D, $ABCDE^2$, and $AB^2C^2D^2E$.

4 Foldover for 3 level Factors

Our proposal on extending the foldover technique is to find some rotation vector $\mathbf{x}$ that can maximize the the resolution and minimize the aberration of an augmented design that triples the size of the originial experiment. The vector to be chosen has a particular relationship to the generators of the fraction such that the rotation introduces new levels to the generators of length three. For simplicity, please assume that any equation in the proceeding paper has the modulo 3 function applied, and where necessary, element-wise. Unbeknownst to us when this paper was originally written, similar work has been done by Ai et al (2008) but who lack the flexibility to define non-standard goals for expanding the experiment and fail to show certain relationships between generators and the choice of rotation vectors.

For every treatment (i.e. row) $\mathbf{d}$ in the initial design, $\mathbf{d} + \mathbf{x}$ is the corresponding first rotation of the augmented design matrix and $\mathbf{d} + 2\mathbf{x}$ is the corresponding second rotation. For example, using $\mathbf{x} = (1, 1, 2, 2, 0)$ to augment the example design, the augmented runs corresponding to the second row $\mathbf{d} = (0, 0, 1, 1, 2)$ will produce $\mathbf{d} + \mathbf{x} = (1, 1, 0, 0, 2)$ for the first rotation and $\mathbf{d} + 2\mathbf{x} = (2, 2, 2, 2, 2)$ for the second rotation. We refer to this as the *rotation vector method* for constructing the triple foldover.

Augmenting the original design matrix with new treatments in this way for all $\mathbf{d}$ in $\mathbf{D}$ will produce a new regular fractional factorial design with a generating relation

$$I \propto AB^2CD^2.$$

A generator (an element of the generating relation) is defined as *rotationally intolerant* (RI) with respect to a rotation vector $\mathbf{x}$ if $\mathbf{gx}' \neq 0$. If $\mathbf{gx}' = 0$, $\mathbf{g}$ is *rotationally tolerant* (RT). The rational for the naming scheme is that when the original design matrix is "rotated" by $\mathbf{x}$ the level of a rotationally tolerant generator does not change. As a result, the level of the generator remains constant for all runs in the augmented design. The following proof gives justification for this statement with an example to follow using the above design.

CLAIM 1: An effect $\mathbf{g}$ aliased with the intercept in the original design will continue to be aliased with the intercept in a triple foldover design if $\mathbf{gx}' = 0$ (i.e. is rotationally tolerant). Alternatively if $\mathbf{gx}' \neq 0$ (i.e. is rotationally intolerant) then the effect will be orthogonal to the intercept in the triple foldover design.

PROOF: Define $J_1 = \mathbf{gx}' = \text{k}$ as the first rotation of the design along the $\mathbf{x}$ rotational path. Define $J_2 = \mathbf{g}2\mathbf{x}' = 2\mathbf{gx}' = 2\text{k}$ as the second rotation of the design along the $\mathbf{x}$ rotational path.

Allow $\mathbf{x}$ to be some rotational vector that will be applied with $x_i \in \{0, 1, 2\}$ and i $\in \{1, 2, ..., \text{f}\}$ such that $\mathbf{gx}' = 0$.

Note please that if $J_1 = 0$ then immediately we know $J_2 = 0$.

Let **d** be any row vector from the original design matrix **D** such that **gd**' = L, for some L $\in$ {0, 1, 2}. This will be true for all **d** in **D** because **D** is a regular fraction and g is an element of it's defining relation.

The application of the first rotation along the **x** pathway will result in **g**(**d** + **x**)' = **gd**' + **gx**' = **gd**' = L

Similarly, the second rotation along the **x** pathway will be **g**(**d** + **2x**)' = **gd**' + **g**2**x**' = **gd**' = L.

Then neither the first nor the second rotation changes the level of the effect **g**, implying that the effect is still aliased with the intercept in the triple foldover design.

Alternatively if **gx**' $\neq$ 0, then **gd**' + **gx**' = L + **gx**'. And **gd**' + **g2x**' = L + 2**gx**'. If we allow **gx**' = 1, then the first rotation will change the level of the treatments to L + 1. Similarly the second rotation will then produce L + 1(2) = L + 2. Similarly if **gx**' = 2, then the first rotation will produce L + 2 and the second rotation will produce L + 4 = L + 1. Then all levels of the previously aliased effect will be present in the augmented experiment, each for the same number of experimental runs, implying orthogonality with the intercept.

$\square$

Remark: A byproduct of Claim 1 is that even applying the triple foldover to a fractional factorial design with a rotation vector chosen as a generator in the original factorial fraction will not necessarily make that generator orthogonal to the intercept in the augmented design. For example, if a generator in the original design is ABC (or **g'** = (1,1,1,0,0,....)) and this is also chosen as the rotation vector **x**' = (1,1,1,0,0,.....), the level of ABC will remain unchanged in the triple foldover design as per Claim 1 because **g**(**d** + **x**)' = **g**(**d** + 2**x**)' = **gd**' = L, an unchanged level.

The original design matrix had a generating relation

$$
\begin{aligned}
I &\propto AC^2E^2 \\
&\propto ABDE \propto AB^2CD^2 \propto BCDE^2
\end{aligned}
$$

with a proposed rotation vector **x** = (1, 1, 2, 2, 0). To find which generators are rotationally tolerant one must find the values of **gx**' which are

Generator	Coded Values	**gx**'	Rotation Status
AC^2E^2	[1 0 2 0 2]	1	RI
$ABDE$	[1 1 0 1 1]	1	RI
AB^2CD^2	[1 2 1 2 0]	0	RT
$BCDE^2$	[0 1 1 1 2]	2	RI

and as was noted earlier the new generating relation for the augmented design is

$$I \propto AB^2CD^2.$$

Appendix B gives some interesting results on the rotationally tolerant/intolerant status of generalized interactions for any two generators. The most noteworthy being that any two rotationally intolerant generators will have one generalized interaction that is rotationally tolerant and one that is rotationally intolerant.

The following shows that if the original design is a regular fractional factorial, the new augmented triple foldover will also be a regular fractional factorial. This is in direct parallel to the two level foldover where the designs continued to be regular fractions as well. There exist some benefits to using regular fractions as compared to irregular designs.

CLAIM 2: For any regular fractional factorial design with s generators, $3^{\text{f - s}}$, applying a triple foldover will produce a regular fractional factorial design with s - 1 defining generators, $3^{\text{f - s + 1}}$, for any rotation vector **x** such that at least for one generator **g**, $\mathbf{g}'\mathbf{x} \neq 0$.

PROOF: In the initial fraction, for every factorial effect **c**, either **cd**' = L for all $\mathbf{d} \in \mathbf{D}$ or **cd**' = 0, 1, or 2 each for 1/3 of the rows $\mathbf{d} \in \mathbf{D}$.

Let the triple foldover design be generated by **d** + **x** and **d** + 2**x**. Then for any **c** there are four possible cases.

Case 1: Suppose **cd**' = L for all $\mathbf{d} \in \mathbf{D}$ and **cx**' = 0. Then in the augmented design

$$\begin{aligned} \mathbf{cd}' &= \text{L in the initial fraction} \\ \mathbf{c}(\mathbf{d}+\mathbf{x})' = \mathbf{cd}' &= \text{L in the first rotation} \\ \mathbf{c}(\mathbf{d}+2\mathbf{x})' = \mathbf{cd}' &= \text{L in the second rotation} \end{aligned}$$

Then despite the augmentation the original design the effect **c** still only takes on one level in the design. As such, it is still fully aliased with the intercept.

Case 2: Suppose **cd**' = 0, 1, or 2 for 1/3 of the rows $\mathbf{d} \in \mathbf{D}$ and **cx**' = 0. Then in the augmented design

$$\begin{array}{rrrl} \mathbf{cd}' = 0 & \mathbf{cd}' = 1 & \mathbf{cd}' = 2 & \text{in the initial fraction} \\ \mathbf{c}(\mathbf{d}+\mathbf{x})' = \mathbf{cd}' = 0 & \mathbf{c}(\mathbf{d}+\mathbf{x})' = \mathbf{cd}' = 1 & \mathbf{c}(\mathbf{d}+\mathbf{x})' = \mathbf{cd}' = 2 & \text{in the first rotation} \\ \mathbf{c}(\mathbf{d}+2\mathbf{x})' = \mathbf{cd}' = 0 & \mathbf{c}(\mathbf{d}+2\mathbf{x})' = \mathbf{cd}' = 1 & \mathbf{c}(\mathbf{d}+2\mathbf{x})' = \mathbf{cd}' = 2 & \text{in the second rotation} \end{array}$$

In the augmented design the corresponding new rows will still take all three levels an equal number of the time. The effect **c** will be orthogonal to the intercept.

Case 3: Suppose **cd**' = L for all $\mathbf{d} \in \mathbf{D}$ and **cx**' = 1 or 2. Then in the augmented design

$$\begin{aligned} \mathbf{cd}' &= \text{L in the initial fraction} \\ \mathbf{c}(\mathbf{d}+\mathbf{x})' &= \text{L} + (1,2) \ \text{ in the first rotation} \\ \mathbf{c}(\mathbf{d}+2\mathbf{x})' &= \text{L} + (2,4) \ \text{ in the second rotation} \end{aligned}$$

For either **cx**' = 1 or **cx**' = 2 the overall result is the same. The effect **c** has taken on the two levels not present in the initial design in the two rotations and all three levels are represented an equal number of times in the initial design indicating that the effect **c** is now orthogonal to the intercept.

Case 4: Suppose **cd**' = 0, 1, or 2 for 1/3 of the rows $\mathbf{d} \in \mathbf{D}$ and **cx**' = 1 or 2. Then in the augmented design

$$\begin{array}{rrrl} \mathbf{cd}' = 0 & \mathbf{cd}' = 1 & \mathbf{cd}' = 2 & \text{in the initial fraction} \\ \mathbf{c}(\mathbf{d}+\mathbf{x})' = (1,2) & \mathbf{c}(\mathbf{d}+\mathbf{x})' = 1 + (1,2) & \mathbf{c}(\mathbf{d}+\mathbf{x})' = 2 + (1,2) & \text{in the first rotation} \\ \mathbf{c}(\mathbf{d}+2\mathbf{x})' = (1,2) & \mathbf{c}(\mathbf{d}+2\mathbf{x})' = 1 + (1,2) & \mathbf{c}(\mathbf{d}+2\mathbf{x})' = 2 + (1,2) & \text{in the second rotation} \end{array}$$

The implication of this then is that an effect that was already orthogonal to the intercept will remain orthogonal to the intercept in the augmented design.

□

If the initial design was a regular fractional factorial experiment, all effects in the triple foldover design are either fully aliased with the intercept or the effects are orthogonal to the intercept. The augmented design then is still a regular design.

We will now show that tripling the size of a experiment's design will not necessarily produce a resolution IV design. This implies that there is no perfect generalization to the 2 level foldover technique for 3 level factors. First we will show an interesting fact about generating relations and then give an example of a resolution III design such that for any rotation vector **x**, a resolution IV design is unattainable for the triple foldover. Combining the two will show that any triple foldover augmentation of the design is also of resolution III.

CLAIM 3: A factor can only be in all generators in a generating relationship if there is only one generator, that is, if s = 1.

PROOF: Without loss of generality allow factor B to be represented in all generators. Then the second element of every generator **g** must be 1 or 2 (not 0). Take any two generators, $\mathbf{g}_1$ and $\mathbf{g}_2$. Then the possible pairs of second elements for these generators are (1,1), (1,2), and (2,2). Note there is no ordering to these pairs so (1,2) = (2,1).

Case 1: (1,1) If the elements representing factor B in both generators are 1 then one of the generalized interactions of $\mathbf{g}_1$ and of $\mathbf{g}_2$, which will also be aliased with the intercept, will be $\mathbf{g}_1 + 2\mathbf{g}_2$.

Since the second elements of both $\mathbf{g}_1$ and $\mathbf{g}_2$ are 1, the second level of this generalized interaction will be (1*1 + 2*1) = 0, implying that at least one effect in the aliasing structure will not contain B.

Case 2: (1,2) In a similar vain, one generalized interaction of $\mathbf{g}_1$ and $\mathbf{g}_2$ will be $\mathbf{g}_1 + \mathbf{g}_2$. Arbitrarily say the second element of $\mathbf{g}_2$ is 2 and the second element of $\mathbf{g}_1$ is 1. Then the second element of this generalized interaction will be (1*1 + 1*2) = 0, and this generalized interaction will not contain factor B.

Case 3: (2,2) If second elements in both generators are 2 then one generalized interaction interaction of $\mathbf{g}_1$ and $\mathbf{g}_2$, which will also be aliased with the intercept, will be $\mathbf{g}_1 + 2\mathbf{g}_2$. The second element for this second generalized interaction will be (1*2 + 2*2) = 0, and this generalized interaction will not contain factor B.

Then a single factor cannot be represented in all effects aliased with the intercept unless there is only one aliased term.

$\square$

CLAIM 4: There exist situations in which the triple foldover augmentation of a regular fraction with resolution III is not a resolution IV design.

PROOF: First assume it is always possible to apply a triple foldover to a resolution III design to obtain a resolution IV design.

Take a $3^{6\text{ - }3}$ fractional factorial design, with generating relation

$$\begin{aligned} I &\propto AB^2C \\ &\propto CD^2E \propto AB^2C^2D^2E \propto AB^2DE^2 \\ &\propto DEF^2 \propto AB^2EF \propto AB^2D^2F^2 \propto AB^2CDEF^2 \\ &\propto AB^2CD^2E^2F \propto AB^2C^2E^2F^2 \propto CE^2F^2 \propto CDF \propto AB^2C^2DF. \end{aligned}$$

Note please only three of these effects are independent generators; the rest are generalized interactions.

For a triple foldover design to become resolution IV all generators of length three must be removed from the generating relation. Assume that we have some rotation vector $\mathbf{x}$ such that this is achievable. To apply a triple foldover for a fractional factorial design is to decrease the number of fractional "splits" by 1 such that $3^{6\text{-}3}$ will become $3^{6\text{-}3+1}$. For this design then we would achieve $3^{6\text{ - }2}$ which will have 4 effects aliased with the intercept (two used as defining generators and two as the generalized interactions of those). If the resulting design is to be of resolution IV then the four possible remaining terms would be a subset from the following

$$\{AB^2C^2D^2E,\ AB^2DE^2,\ AB^2ED,\ AB^2D^2F^2,\ AB^2CDEF^2,\ AB^2CD^2E^2F,\ AB^2C^2E^2F^2\}$$

but according to Claim 3 this is impossible because factor A is in all generators. Then there is no triple foldover rotation vector that can produce an augmented design of resolution IV for this experiment.

□

There is an alternative formulation for how to augment the initial design matrix that we will refer to as the *equation system method*. The equation system method approaches the foldover as finding all solutions for **v** in **Mv**' = **L**, is a consistent linear equation system of f-1 equations and **L** taking on the values **Md**'. This will immediately give **d** as one of the solutions. There will be exactly two other solutions. The two solutions to **v** that are not **d** will be the new rows in the augmented design that correspond to **d**. It will be shown that it is possible to find a rotation vector **x** that will produce the same augmented design as this equation system method. Without going into detail on how to construct this matrix, the matrix **M** that produces the same augmented design as the rotation vector **x** = (1, 1, 2, 2, 0) in the example from Section 4 is

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 2 & 2 & 0 & 1 & 2 \end{bmatrix}.$$

For our chosen row vector **d** = (0, 0, 1, 1, 2), **Md**' = **L** = [1, 1, 1, 2]'. The two other vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ that are solutions to **Mv**' = **L** are (1, 1, 0, 0, 2) and (2, 2, 2, 2, 2), the same as was found with the rotation vector method.
We will now show that the equation system method is equivalent to the rotation vector method for any consistent system of linear equations. This allows us to only focus on the rotation vector method.

CLAIM 5: The rotational vector method for generating triple foldover designs is equivalent to the equation system method.

PROOF: For a given f-1 by f matrix **M**, with elements 0, 1, and 2, select a rotation vector **x** that is a solution to **Mx**' = **0** where **0** is a column vector of 0's with length f-1.

The equation system method requires that for every row **d** in the initial design matrix, we find three unique row vectors **v** that are solutions to

$$\mathbf{Mv}' = \mathbf{Md}'. \tag{1}$$

$\mathbf{d}$ will automatically be a solution to (1) and the other two solutions for $\mathbf{v}$ will be the corresponding rows in the augmented design matrix.

The rotation vector method adds the rotation vector $\mathbf{x}$ to each design row vector $\mathbf{d}$ once and then twice to obtain the two, new sets of vectors in the augmented design matrix for the triple foldover. Denote $\mathbf{d} + \mathbf{x}$ as $\mathbf{v}_1$ and $\mathbf{d} + \mathbf{2x}$ as $\mathbf{v}_2$

Note the relationship between $\mathbf{M}$ and $\mathbf{v}_1$ is

$$\mathbf{M}\mathbf{v_1}' = \mathbf{M}(\mathbf{x} + \mathbf{d})' = \mathbf{M}\mathbf{d}' + \mathbf{M}\mathbf{x}' = \mathbf{M}\mathbf{d}'.$$

Then $\mathbf{v}_1$ is in fact a valid solution to (1) and would be generated by the rotational vector method. Similarly

$$\mathbf{M}\mathbf{v_2}' = \mathbf{M}(\mathbf{2x} + \mathbf{d})' = \mathbf{M}\mathbf{d}' + \mathbf{2M}\mathbf{x}' = \mathbf{M}\mathbf{d}'$$

implies that $\mathbf{v}_2$ is also a valid solution to (1). Then if there exists a non-zero rotation vector $\mathbf{x}$ such that $\mathbf{M}\mathbf{x}' = \mathbf{0}$, the two methods are directly equivalent. It is possible to always find a rotation vector that satisfies this equality. Let $\mathbf{d}$ and $\mathbf{v}$ be two of the solutions to (1) such that

$$\begin{aligned} \mathbf{M}\mathbf{d}' &= \mathbf{M}\mathbf{v}' \\ \mathbf{M}\mathbf{d}' - \mathbf{M}\mathbf{v}' &= \mathbf{0} \\ \mathbf{M}(\mathbf{d} - \mathbf{v})' &= \mathbf{0} \\ \mathbf{M}\mathbf{x}' &= \mathbf{0} \end{aligned}$$

with the rotation vector $\mathbf{x} = \mathbf{d} - \mathbf{v}$. An implication of this is that there are non-unique rotation vectors that will produce the same result although these vectors are just multiples of themselves in a Galois Field.

$\square$

Finally we can discuss when a design of resolution III can be augmented to a resolution IV design using the triple foldover. The concept involves creating a matrix of coded generators of length 3 which will be referred to as a *pseudo-design matrix*, denoted as $\mathbf{G}^3$. For a fractional factorial design of resolution III there exists one or more generators of length three. Denote the number of generators of length three as k, which is the aberration of the design. Collecting these length three coded generators into a pseudo-design matrix $\mathbf{G}^3$ with no particular ordering will produce a k by f matrix with each row being a coded generator. For example let a generating relation be

$$
\begin{aligned}
I &\propto AB^2C \\
&\propto CD^2E \propto AB^2C^2D^2E \propto AB^2DE^2 \\
&\propto DEF^2 \propto AB^2EF \propto AB^2D^2F^2 \propto AB^2CDEF^2 \\
&\propto AB^2CD^2E^2F \propto AB^2C^2E^2F^2 \propto CE^2F^2 \propto CDF \propto AB^2C^2DF.
\end{aligned}
$$

The corresponding pseudo-design matrix contains one row corresponding to each three factor interaction in the generating relation:

A	B	C	D	E	F
1	2	1	0	0	0
0	0	1	2	1	0
0	0	0	1	1	2
0	0	1	0	2	2
0	0	1	1	0	1

Any effect that can can be coded with values of only 1 or 2 in the treatments represented in the pseudo-design matrix can be used as a rotation vector that will produce a resolution IV design. Occasionally there can be several options for a rotation vector $\mathbf{x}$ that can accomplish this. If there is no effect that only takes the values of 1 or 2 then whatever effect has the minimum amount of 0's present will produce the smallest aberration possible but still have a resolution III design. These effects then are the optimal rotation vectors.

A secondary criterion that can be used is aberration in the generating relation for the possible augmented designs. Once a set of possible rotation vectors are found, apply the same method as above to the fourth order interactions. This then can be applied iteratively upwards. It is possible that the resolution of the whole design can be increased to resolution V (or even higher) although the specific generating relation of the original design would be *very* unique.

This use of of a secondary criterion for evaluating possible rotation vectors is non-unique to three level factors. While the classic foldover for two level fractional factorial designs guarantee resolution IV augmented designs, it cannot decrease the aberration in the new design due to all even-ordered interactions being rotationally tolerant to the rotation vector $\mathbf{x} = (1, 1, ..., 1)$. The mechanics proposed here in allows for possibly finding rotation vectors that could produce resolution IV designs and minimize aberration below the classic foldover.

For example suppose we have a generating relation

$$
\begin{aligned}
I &= -ABCHI \\
&= -DEF = ABCDEFHI \\
&= BEFG = -BDG = ACDGHI = -ACEFGHI \\
&= ACEH = -BEI = -ACDFH = BDFI = ABCFGH = -ABCDEGH = DEGI = -FGI
\end{aligned}
$$

The classic foldover will produce in the augmented design a generating relation

$$\begin{aligned} I &= ABCDEFHI \\ &= BEFG = ACDGHI \\ &= ACEH = BDFI = ABCFGH = DEGI \end{aligned}$$

which is a resolution IV design with aberration 4. Alternatively, choosing the rotation vector $\mathbf{x} = (0, 1, 0, 1, 1, 1, 1, 0, 1)$ will create an augmented design with a generating relation

$$\begin{aligned} I &= -ABCHI \\ &= BEFG = -ACEFGHI \\ &= -ACDFH = BDFI = -ABCDEGH = DEGI \end{aligned}$$

which is a resolution IV design with aberration 3.

Unfortunately the only solution to finding these vectors appears to be brute force. While this is costly in human computation time, computing programs can find the optimal vectors in very little time. We have developed an R package which includes a function on finding the optimal rotation vector. A test case of a regular $3^{8\text{ - }4}$ design was created and using the "rbenchmark" package, 100 replications of finding the optimal vector took approximately 46 seconds. It should be noted that this would be a large experiment and requires checking 3280 candidate rotation vectors on every replication. Please see Appendix C for more information on the package for calculating the optimal rotation vectors.

5 Example

Oktem et al (2007) ran two experiments to study warpage and shrinkage of plastic injection molding. They were based on two different designs. The first was a study on injection time for the plastics. The five parameters associated with it are material flow rate (M_{FR}) at 8, 12 or 16 grams per ten minutes; injection velocity (I_V) at 130, 142.5, and 156.4 centimeters per second; mold temperature (MoT) at 50, 75, and 100 degrees Celsius; melt temperature (MeT) at 230, 265 and 400 degrees Celsius and finally packing pressure (P_p) in 8, 12, or 16 megapascals. Note that all factors have three levels and the experiment was organized as a regular fractional factorial design with 5 factors. The design matrix is presented below.

runs	M_{FR}	I_V	MoT	MeT	I_P
1	1	1	1	1	1
2	1	1	1	1	2
3	1	1	1	1	0
4	1	2	2	2	1
5	1	2	2	2	2
6	1	2	2	2	0
7	1	0	0	0	1
8	1	0	0	0	2
9	1	0	0	0	0
10	2	1	2	0	1
11	2	1	2	0	2
12	2	1	2	0	0
13	2	2	0	1	1
14	2	2	0	1	2
15	2	2	0	1	0
16	2	0	1	2	1
17	2	0	1	2	2
18	2	0	1	2	0
19	0	1	0	2	1
20	0	1	0	2	2
21	0	1	0	2	0
22	0	2	1	0	1
23	0	2	1	0	2
24	0	2	1	0	0
25	0	0	2	1	1
26	0	0	2	1	2
27	0	0	2	1	0

The generating relation for this 3^{5-2} experiment is

$$\begin{aligned} I &\propto ACD^2 \\ &\propto ABC^2 \propto AB^2D \propto BCD \end{aligned}$$

and is clearly a resolution III design with aberration 4. Due to the nature of the initial design the triple foldover augmentation cannot be of resolution IV. Note that any triple foldover with at least one rotationally intolerant generator $\mathbf{g}^*$ will produce an augmented design of minimum aberration. While there exist many choices for the rotation vector $\mathbf{x}$, only an experimenter familiar with this process would be qualified to talk of which factor is of most interest and by extension which aliasing structure for effects is most palatable. Arbitrarily then we will assume the effect A is of most interest. Our rotation vector will be $\mathbf{x} = (1, 0, 0, 0, 0)$ with a new generating relation

$$I \propto BCD. \tag{2}$$

The augmented design matrix will have the following two matrices "pasted" to the bottom of the original design matrix:

runs	M_{FR}	I_V	MoT	MeT	I_P	runs	M_{FR}	I_V	MoT	MeT	I_P
28	2	1	1	1	1	55	0	1	1	1	1
29	2	1	1	1	2	56	0	1	1	1	2
30	2	1	1	1	0	57	0	1	1	1	0
31	2	2	2	2	1	58	0	2	2	2	1
32	2	2	2	2	2	59	0	2	2	2	2
33	2	2	2	2	0	60	0	2	2	2	0
34	2	0	0	0	1	61	0	0	0	0	1
35	2	0	0	0	2	62	0	0	0	0	2
36	2	0	0	0	0	63	0	0	0	0	0
37	0	1	2	0	1	64	1	1	2	0	1
38	0	1	2	0	2	65	1	1	2	0	2
39	0	1	2	0	0	66	1	1	2	0	0
40	0	2	0	1	1	67	1	2	0	1	1
41	0	2	0	1	2	68	1	2	0	1	2
42	0	2	0	1	0	69	1	2	0	1	0
43	0	0	1	2	1	70	1	0	1	2	1
44	0	0	1	2	2	71	1	0	1	2	2
45	0	0	1	2	0	72	1	0	1	2	0
46	1	1	0	2	1	73	2	1	0	2	1
47	1	1	0	2	2	74	2	1	0	2	2
48	1	1	0	2	0	75	2	1	0	2	0
49	1	2	1	0	1	76	2	2	1	0	1
50	1	2	1	0	2	77	2	2	1	0	2
51	1	2	1	0	0	78	2	2	1	0	0
52	1	0	2	1	1	79	2	0	2	1	1
53	1	0	2	1	2	80	2	0	2	1	2
54	1	0	2	1	0	81	2	0	2	1	0

For a brief demonstration we will examine the main effect of A and B in the original design and their aliases compared to the main effect of A and B in the augmented design with their aliases. Please note the large reduction in aliases for the two main effects. Also note A is only aliased with fourth order interactions while B is aliased with a second order interaction. This type of situation is a common result when using the second type of foldover, whether the original or the triple foldover.

Original	$A \propto AC^2D \propto CD^2 \propto AB^2C \propto BC^2 \propto ABD^2 \propto B^2D \propto ABCD \propto AB^2C^2D^2$
Original	$B \propto ABCD^2 \propto AB^2CD^2 \propto AB^2C^2 \propto AC^2 \propto AD \propto ABD \propto zBC^2D^2 \propto CD$
Augmented	$A \propto ABCD \propto AB^2C^2D^2$
Augmented	$B \propto BC^2D^2 \propto CD$

A second 3^{4-2} experiment was ran in which multiple metrics were measured from each treatment with no replication. The four covariates were injection time (I_t) with levels a, b, c in seconds; packing pressure (P_P) with levels at 16, 21, 26 MPa, packing pressure time (P_PT) with levels at 4, 6, and 8 seconds, and cooling time (C_T) with levels at 12, 15, and 18 seconds. The first mentioned level was assumed to be level 1, second is level 2 and the third is level 0. The design matrix was

I_t	P_P	P_{PT}	C_T
1	1	1	1
1	2	2	2
1	0	0	0
2	1	2	0
2	2	0	1
2	0	1	2
0	1	0	2
0	2	1	0
0	0	2	1

with a generating relation

$$\begin{aligned} I &\propto ACD^2 \\ &\propto ABC^2 \propto AB^2D \propto BCD. \end{aligned}$$

A similar situation is occurring as with the first experiment in which there is no way to produce a resolution IV regular fraction design. Instead we will arbitrarily assume factor B is of most interest. This suggests the rotation vector $\mathbf{x} = (0, 1, 0, 0)$ and the augmented design had a generating relation

$$I \propto ACD^2.$$

The augmented design matrix will be

I_t	P_P	P_{PT}	C_T
1	1	1	1
1	2	2	2
1	0	0	0
2	1	2	0
2	2	0	1
2	0	1	2
0	1	0	2
0	2	1	0
0	0	2	1
1	2	1	1
1	0	2	2
1	1	0	0
2	2	2	0
2	0	0	1
2	1	1	2
0	2	0	2
0	0	1	0
0	1	2	1
1	0	1	1
1	1	2	2
1	2	0	0
2	0	2	0
2	1	0	1
2	2	1	2
0	0	0	2
0	1	1	0
0	2	2	1

Note that the factor B is not aliased with any second order interactions but only by third order interactions. Also note that the second order interactions involving B are only aliased with other second order interactions. Then for factor B the above design acts as a resolution V design.

6 Conclusion

The triple foldover for regular fractional factorial experiments with three level factors offers a useful extension of the classic foldover method for two levels. Our paradigm of using rotation vectors also unifies the two "types" of foldover methods into one framework. While the triple foldover is not as powerful as the two level foldover it will still always produce an optimum solution whether in increasing the resolution size or in minimizing aberration. Our solution does not meet Margolin's lower bound of 6*f - 3 for the minimal number of runs needed to achieve resolution IV designs but our method does produce resolution IV (where possible) of the same order with 6*f + 3 runs given the initial design was a nearly saturated first order model. It is worth noting that Margolin was unsure whether the lower bound was obtainable himself. Extending the method herein to regular fractional factorial designs with prime levels should be a simple task.

The introduction of rotationally tolerant and intolerant generators should be a rich resource in attempts to further generalize this technique. Future work could include generalizing the triple foldover to irregular experiments and for mixed level experiments. If all of these can be solved then Margolin's observation about extending the foldover should be fully closed.

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Appendices

A Notation

Some useful shorthand/common notation

- f: The number of factors in an experiment
- s: The number of generators defining relation in the regular fractional factorial experiment. For example 3^{f-s} would imply we have s generators originally chosen to "cut" the design plus their generalized interactions.
- $\mathbf{q}$: These are the generators used to denote the effects chosen to create the original fraction. It is a set of vectors, each of length f, each element being the power of the corresponding factor. For example, (0, 1, 2, 0) denotes BC^2. Denote a given element as q_j for j $\in$ 1, 2, ..., s.
- $\mathbf{g}$: These are all generators that are aliased with the intercept including $\mathbf{q}$ and the generalized interactions.
- $\mathbf{D}$: This is used to denote some design matrix
- $\mathbf{d}$: This is used to denote some row vector of length f from the design matrix. The elements are 0, 1, or 2 denoting the level of the corresponding factor.
- $\mathbf{x}$: This is the "rotational vector" which is a vector of length f that specfies how the design matrix should be "rotated" to provide the augmented design matrix (specifically for any $\mathbf{d}$, the first rotated design matrix will have new levels for this row as $\mathbf{d} + \mathbf{x}$ mod 3 and the second rotated design matrix will have new levels for this row as $\mathbf{d} + 2\mathbf{x}$ mod 3
- ROTATIONALLY INTOLERANT: An f-element vector $\mathbf{v}$ is *rotationally intolerant* (RI) with respect to a rotation vector $\mathbf{x}$ if $\mathbf{v}'\mathbf{x} \neq 0$. If $\mathbf{v}'\mathbf{x} = 0$, $\mathbf{v}$ is *rotationally tolerant* (RT).
- g^*: The star is used to indicate that a particular generator is rotationally intolerant (RI).

B Rotationally Tolerant Results

The following are some general results that showcase the relationships of rotationally tolerant and intolerant generators. For a regular fractional factorial design, 3^{f-s} with s $\geq$ 2 and any two defining generators within the defining relation $\mathbf{q}$, $\mathbf{q}_1$ and $\mathbf{q}_2$, the two generalized interactions can be represented by $\mathbf{q}_1 + \mathbf{q}_2$ mod 3 and $\mathbf{q}_1 + 2\mathbf{q}_2$ mod 3. It doesn't matter which you make as $\mathbf{q}_1$ and $\mathbf{q}_2$ due to the unique properties of a Galois Field. For a rotation vector $\mathbf{x}$ if

- $\mathbf{q}_1\mathbf{x}' \neq 0$ and $\mathbf{q}_2\mathbf{x}' \neq 0$, then exactly one interaction of the two, $g_{2,i}$, i $\in$ {1,2}, will be such that $g_{2,i}'\mathbf{x} = 0$.

> PROOF: Since both $\mathbf{q}_1$ and$\mathbf{q}_2$ are rotationally intolerant then $\mathbf{q}_1\mathbf{x}'$ and $\mathbf{q}_2\mathbf{x}'$ will be 1 or 2. If their levels are {1, 2} or {2, 1} then the first mentioned generalized interaction will be 0 with respect to a rotation vector, i.e. rotationally tolerant. If

their levels are {1, 1} or {2, 2} then the second mentioned generalized interaction will be 0 with respect to a rotation vector, i.e. rotationally tolerant. Also note that the other generalized interaction will still be rotationally intolerant.

- $\mathbf{q}_1\mathbf{x}' \neq 0$ or $\mathbf{q}_2\mathbf{x}' \neq 0$, but not both, then both interactions of the two, $g_{2,i}$, i $\in$ {1,2}, will be such that $g_{2,i}\prime\mathbf{x} \neq 0$.

  PROOF: Arbitrarily say $\mathbf{q}_2$ is the rotationally intolerant generator. Then $\mathbf{q}_2\mathbf{x}'$ will be 1 or 2 while $\mathbf{q}_1\mathbf{x}'$ will be 0. Then clearly $\mathbf{q}_1\mathbf{x}' + \mathbf{q}_2\mathbf{x}' = 0 + \mathbf{q}_2\mathbf{x}'$ will be 1 or 2. Alternatively $\mathbf{q}_1\mathbf{x}' + 2\mathbf{q}_2\mathbf{x}' = 0 + 2\mathbf{q}_1\mathbf{x}'$ will be 2 or 4 mod 3 = 1. So both generalized interactions will be rotationally intolerant.

- $\mathbf{q}_1\mathbf{x}' = 0$ and $\mathbf{q}_2\mathbf{x}' = 0$ then neither interaction, $g_{2,i}$, i $\in$ {1,2},will be such that $g_{2,i}\prime\mathbf{x} \neq 0$

  PROOF: Since $\mathbf{q}_1\mathbf{x}' = 0$ and $\mathbf{q}_2\mathbf{x}' = 0$ the generalized interactions will be $\mathbf{q}_1\mathbf{x}' + \mathbf{q}_2\mathbf{x}' = 0 + 0 = 0$ and $\mathbf{q}_1\mathbf{x}' + 2\,\mathbf{q}_2\mathbf{x}' = 0 + 2*0 = 0$. So both generalized interactions are rotationally tolerant.

C R Package

The R package developed is entitled "TripleFold" and is available for download at "https://github.com/vinny-paris/TripleFold.git". The package has three main functions which we will discuss. To begin with the package assumes you have already built a coded three level design matrix. For example the design matrix could be similar to

```
> design
     [,1] [,2] [,3] [,4]
 [1,]    0    0    0    0
 [2,]    1    0    1    1
 [3,]    2    0    2    2
 [4,]    0    1    2    1
 [5,]    1    1    0    2
 [6,]    2    1    1    0
 [7,]    0    2    1    2
 [8,]    1    2    2    0
 [9,]    2    2    0    1
```

1. what_frac()

   The goal of this function is to identify the generating relation in a given design matrix. This in turn will help make informed statements about non-unique estimation and how different effects are aliased without having to build the alias structure by hand.

```
> what_frac(design)
      Aliased with the Intercept
[1,] "A_C_D"
[2,] "A_B_D2"
[3,] "A_B2_C2"
[4,] "B_C2_D"
```

2. opt_rotation() This function offers a list of the rotation vectors that will augment the orig-

   inal design **D** and increase it to resolution IV or will minimize the aberration. It takes in a design matrix and returns a list of two things: a data frame with each row being a proposed rotation vector and the pseudo-design matrix G^3.

```
> opt_rotation(design)
$`Minimum Aberration Achieved`
      col col col col
 [1,]   1   0   0   0
 [2,]   1   0   0   1
 [3,]   1   0   0   2
        .
        .
        .
        .
[35,]   0   0   1   2
[36,]   0   0   0   1

$`psuedo-design matrix`
     [,1] [,2] [,3] [,4]
[1,]    1    0    1    1
[2,]    1    1    0    2
[3,]    1    2    2    0
[4,]    0    1    2    1
```

3. triple_fold()

   This is the function that explicitly tells you what your new augmented design matrix will be. It takes in the original design matrix **D** and a vector that is the chosen rotation vector **x**. It will return a list of the new generating relation and the new design matrix.

```
> triple_fold(design, c(1,0,0,0))
$Aliased_with_Fraction
     [,1]
[1,] "B_C2_D"

$Design_Matrix
      [,1] [,2] [,3] [,4]
 [1,]    0    0    0    0
 [2,]    1    0    1    1
         .
         .
         .
         .
[26,]    0    2    2    0
[27,]    1    2    0    1
```