Introducing Confidence Bounds and Confidence Levels into Iterated Fractional Factorial Design Analysis

by

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Abstract

This report is further development of a methodology known as **I**terated **F**ractional **F**actorial **D**esign **A**nalysis (IFFDA). IFFDA uses experimental designs to identify the influential parameters in systems with many (hundreds or thousands) of parameters. At its previous stage of development, IFFDA gives no well-defined measure of the reliability of the results. This report includes enhancements to assign confidence levels and confidence bounds to the estimates produced by IFFDA. These enhancements can be incorporated into the application of IFFDA and the result is a more objective analysis.

Two examples are discussed. The first is small and contrived and used to illustrate the capabilities of IFFDA in previous applications. A larger system is required to demonstrate how the confidence bounds and confidence levels can be estimated and a computer model known as SYVAC3-CC3 is used. SYVAC3-CC3 was chosen because it is well known (Goodwin et al 1994 for example) and yet has enough system parameters (~3300) to be non-trivial.

Two strategies are given for incorporating confidence levels and confidence bounds into IFFDA. The first assumes that no expert knowledge of the system is available and the second incorporates expert knowledge into the analysis.

In the SYVAC3-CC3 example, the enhanced methodologies gave results that are consistent with the understanding of the system. Results are even more satisfactory when expert knowledge is incorporated into the analysis.

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Chapter 1
Introduction and Summary

1.1 Motivation for IFFDA

Iterated Fractional Factorial Design Analysis (IFFDA) was developed for sensitivity analysis of a family of computer models associated with **SY**stems **V**ariable **A**nalysis **C**ode (SYVAC) (Goodwin et al.1994 and Goodwin et al. 1996). These models are used to predict the impact of nuclear waste repositories. Sensitivity analysis of these models is challenging because:

- There are many (hundreds or thousands) of system parameters.
- Many fields of expertise are incorporated (metal corrosion, hydrogeology, chemistry, dosimetry, etc) into the models.
- For some of the system parameters, the value is uncertain and could vary by several orders of magnitude.

Generally, SYVAC models are constructed to run probabilistically. The system parameters are assigned probability density functions (PDFs) instead of single values. The parameter values are sampled randomly according to the assigned PDFs and the corresponding responses (radiological dose for example) can be estimated. By repeatedly sampling the parameter values and re-calculating the responses, a sample of system responses can be generated. From this sample, it is possible to make statistical inferences about the behaviour of the system.

For SYVAC models, IFFDA has been used to identify the system parameters where uncertainty in the values (as expressed through the assigned PDFs) leads to significant variability in the system response. An example of a direct conclusion made as a result of IFFDA is:

> When the tortuosity of the lower rock is increased from a low to a high value, the dose rate decreases by 1.7 orders of magnitude.

Indirectly, IFFDA can identify other important features of the system. For example:

> If the characteristics of a layer of rock influence the estimated dose rate, then at least under some circumstances that layer of rock is an important barrier to the flow of radioactive contaminants.

1.2 History of IFFDA

Iterated Fractional Factorial Design Analysis (IFFDA) was developed as part of the Canadian Nuclear Fuel Waste Management Program. It has been used in two assessments of the long-term impacts of a hypothetical repository for high-level nuclear waste (Goodwin et al. 1994, Goodwin et al. 1996).

Nuclear waste management has been the motivation for much of the development of sensitivity analyses for large predictive computer models (Andres 1987, Andres and Hajas 1993 and Goodwin et al. 1984 and Iman and Conover 1980). Of particular interest, are Satelli, Andres and Homma 1993 and 1995 where comparisons are made of eight methodologies.

Sensitivity analysis of large predictive computer models has received some attention outside the field of nuclear waste management. Kliejnen 1992 for example proposes an approach that has similarities to IFFDA.

Though many approaches have been devised for the sensitivity analysis of large predictive computer models, IFFDA has the distinction that it is the only one that has been applied to systems with hundreds and thousands of parameters in a real application. IFFDA has the following advantages that make it well suited to the task:

1. Able to deal with a large number of system parameters (hundreds or thousands).

2. Minimal assumptions about the behaviour of the system when the design is applied.

3. For the applications that have been made so far, the number of simulations required for the analysis is manageable (hundreds).

Previous applications of IFFDA were successful in identifying the main and quadratic effects as well as interactions in SYVAC models. However those applications relied on expert knowledge of the system and on other statistical methods to establish confidence in the results. This paper enhances IFFDA so that confidence coefficients and confidence bounds are generated for the estimated effects. The confidence coefficients can be incorporated into the application of IFFDA.

1.3 A Brief Summary Of The Methodology

IFFDA is the implementation of an experimental design and the analysis of the resulting system responses. Experimental designs are usually applied to physical systems but this report will consider their application to two mathematical functions.

1.3.1 The Design

As the name suggests, IFFDA is closely related to fractional factorial designs (Montgomery,1991). In fact, IFFDA uses a fractional factorial design as a sub-design. The same sub-design is repeated many times.

In the sub-design, *experimental factors* (as opposed to the system parameters) are toggled between LOW and HIGH as they would be in a standard fractional factorial design. Each experimental factor controls a random group of system parameters.

Consequently, many system effects will be aliased in an iteration of the sub-design. However, the assignment of system parameters to experimental factors is different for each iteration; thus the alias structure of the system effects is also different.

1.3.2 Estimating Main Effects And Interactions

A simplistic approach is used to estimate main effects and interactions for the system parameters. These values are the averages of the estimable effects of the experimental factors that contain them.

The estimated value of the system effects are subject to error due to aliasing, but the aliasing structure changes with each iteration of the sub-design. Given enough iterations, the error due to aliasing will "average down" to an acceptable level.

1.3.3 Confidence Coefficients and Confidence Bounds For Main Effects And Interactions

As discussed in Section 1.3.2, the estimated value of a system effect is the average of estimable effects. If the estimable effects have a Normal distribution (as appears to be the case in one of the examples), then the mean of a random set of these effects can be converted to a variable having a Student-t distribution. Standard statistical procedures are available to assign confidence coefficients and confidence bounds to these estimates.

1.3.4 Refining The Estimated Values Of Main Effects And Interactions

The estimated system effects are subject to error due to aliasing that occurs within the iterations of the sub-design. However, there is a step-wise approach to reducing this error.

The system effects are estimated from the effects that can be estimated from individual iterations of the sub-design. Conversely, the effects that can be estimated are approximately a sum of many system effects. If there is a good estimate of a system effect, the appropriate estimable effects can be adjusted to remove the estimated effect. When the other system effects are recalculated from the adjusted estimable effects, the error due to aliasing with the removed system effect will approximately disappear.

1.3.5 Estimating Quadratic Effects

The quadratic effect of a system parameter is illustrated in Figure 1.3.5.1. A convenient definition is:

> Mean of the response where the system parameter is held MEDIUM minus the mean of the responses for the iterations where the system parameter toggles between LOW and HIGH.

1.3.6 Confidence Coefficients And Confidence Bounds For Quadratic Effects

Estimates of quadratic effects are calculated from the means of the system responses for each iteration of the sub-design. If the estimated quadratic effects are random combinations of iteration means, then they can be transformed to variables with a Student-t distribution. Standard statistical procedures are available to assign confidence coefficients and confidence bounds to the associated t-variates.

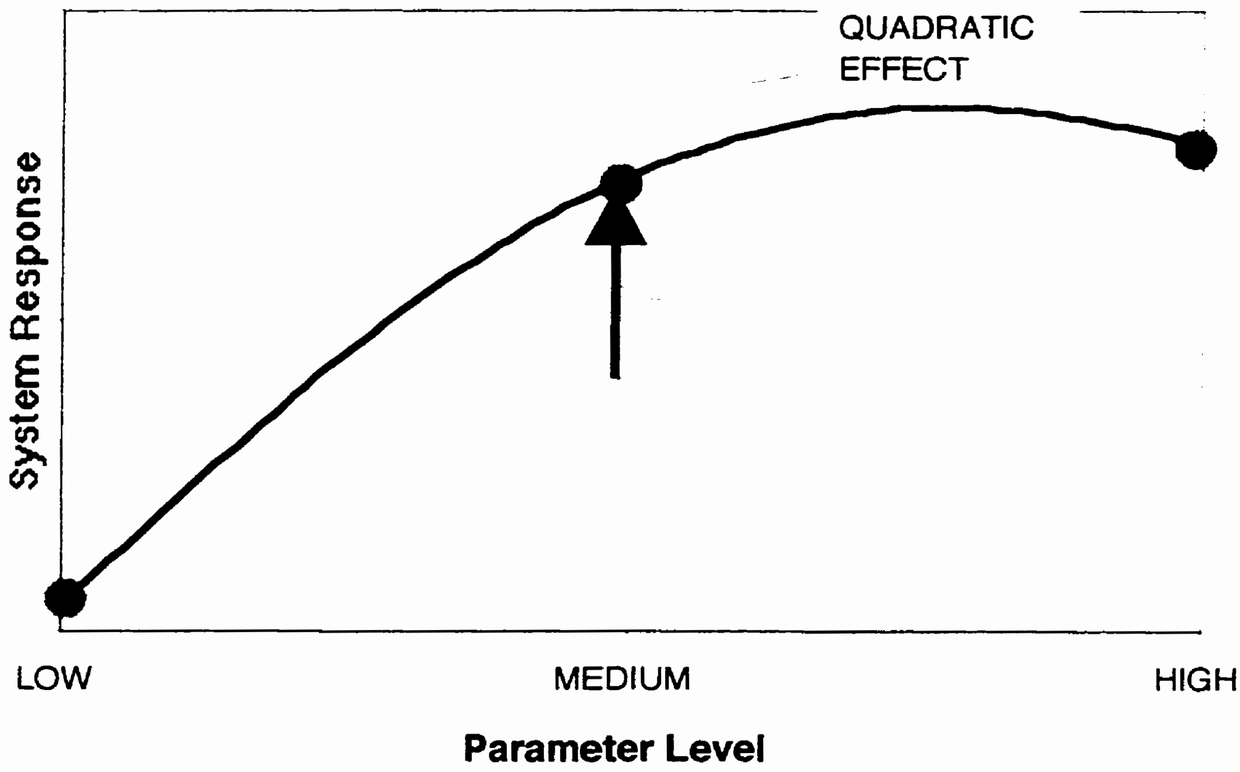

Figure 1.3.5.1: **Illustration Of A Quadratic Effect**

1.3.7 Refining The Estimated Values Of Quadratic Effects

The estimated quadratic effects can be refined in much the same way main effects and interactions were refined.

When system parameters are held MEDIUM in the same iteration of the sub-design, their quadratic effects will be confounded for that iteration. However, if there is a good estimate of one quadratic effect, the appropriate iteration averages can be adjusted to take away its influence from the estimated value of other quadratic effects.

1.4 Examples To Be Discussed

Experimental designs are more typically applied directly to physical systems such as a biological or manufacturing process. However, as discussed in Section 1.1, IFFDA was developed to identify the important features in large, complex computer models. Consequently, one of the examples chosen for this report is a large computer model. The other example is a very simple mathematical function used to demonstrate some of the calculations.

The major impact of applying an experimental design to a computer model instead of a physical system is that there is no natural variability in the system.

1.4.1 Small Example

The first example is small and contrived. It is presented to demonstrate how the system effects are estimated and how those estimates can be refined. In a real situation, other methods would be more appropriate for investigating this system.

The system is a simple mathematical function of four *system* parameters:

$$y(x_1, x_2, x_3, x_4) = 2 * x_1 + x_2 + x_3^2 + x_2 * x_3$$

Each variable has three possible values; LOW, MEDIUM and HIGH are defined to be –1, 0 and 1 respectively.

Ideally, the effects that IFFDA will find are:

- x_1 and x_2 have main effects of 4 and 2 respectively.
- The interaction between x_2 and x_3 has a value of 2
- x_3 has a quadratic effect of -1

1.4.2 SYVAC3-CC3 Example

In this report, IFFDA will also be applied to a computer model known as SYVAC3-CC3 (see Goodwin et.al 1994). SYVAC3-CC3 was developed to estimate the impacts of a hypothetical nuclear waste repository. It is used in this report to demonstrate how confidence limits and confidence bounds can be incorporated into IFFDA.

SYVAC3-CC3 has approximately 3300 system parameters. These are variables in the computer model that the user can control independently. Each of the system parameters is assigned an appropriate probability density function (PDF) so that the model can be run stochastically.

These PDFs are also convenient for defining the parameter levels used in experimental designs. In the SYVAC3-CC3 example, LOW, MEDIUM and HIGH are defined as equally probable ranges of values as determined from the PDFs.

Table 1.4.2.1 describes some of the system parameters in SYVAC3-CC3. In the sample calculations, the system parameters are referenced by the *parameter number*, p, which is an arbitrary index.

The user must choose a suitable system response for the analysis. In the sample calculations, the objective function is the $\log_{10}$ of the maximum radiological dose to 100 000 years after the closure of the repository.

There are two reasons for choosing SYVAC3-CC3 for the sample calculations:

- SYVAC3-CC3 has enough system parameters to be non-trivial.

- SYVAC3-CC3 has been studied extensively (Goodwin et al 1984 for example) and new features of IFFDA can be evaluated with respect to expert knowledge of the system.

Parameter Number(p)	Parameter Description
104	Buffer anion correlation parameter
2239	Tortuosity of the lower rock zone
2355	Aquatic mass loading coefficient for the lake for iodine
2443	Source of domestic water (lake or well)
2803	Retardation factor for iodine in compacted lake sediment
2825	Iodine plant/soil concentration ratio
2826	Gaseous evasion rate of iodine from soil

Table 1.4.2.1: Some SYVAC3-CC3 Parameters Discussed In This Report.

Chapter 2

Experimental Designs In The Example Applications

There is flexibility in the choice of the sub-design. In Andres(1996) and Andres and Hajas (1993), the only restriction on the sub-design is that it is Resolution IV fractional factorial. In this report, the SYVAC3-CC3 example takes advantage of some specific characteristics of the sub-design.

It is easy to speculate how many of the ideas in IFFDA could be generalized to accommodate other sub-designs. However, many important features are inherited from the fractional factorial sub-designs; most notably the ability to express results as main effects and interactions.

2.1 Small Example

For the small example, the experimental design consists of six iterations of a sub-design. The sub-design is a 2^{4-1} fractional factorial design(Montgomery 1991). In each iteration, four *experimental factors* are toggled between LOW and HIGH in eight experiments. In common notation, the defining contrast is I=ABCD (Montgomery 1991).

It should be noted that these experimental factors are different than the system parameters. An experimental factor represents a random combination of system parameters. The assignment of system parameters to experimental factors is different for each iteration of the sub-design. Table 2.1.1 shows how these assignments were made for the small example. The system parameters are represented by columns and iterations by rows.

Iteration	System Parameters 1	2	3	4
1	0	0	0	3
2	-2	-3	0	-4
3	1	1	1	-2
4	-4	1	3	0
5	0	0	-4	0
6	-3	3	-3	-3

Table 2.1.1 Assignment Of System Parameters To Experimental Factors For The Small Example

In an iteration, a system parameter does one of three things:

- Toggle between LOW and HIGH with an experimental factor (positive value in Table 2.1.1)

  For example, in iteration number one, system parameter number four toggles in the *same* direction as experimental factor number three.

- Toggle between LOW and HIGH in the opposite direction to an experimental factor (negative value in Table 2.1.1)

  For example, in iteration number two, system parameter number one toggles in the opposite direction as experimental factor number two.

- Remain at MEDIUM and not be included in the sub-design(zero value in Table 2.1.1)

  For example, in iteration number one, system parameter number one is held at MEDIUM.

Each system parameter is randomly assigned to experimental factors with the restriction that in one third of the iterations, it is held MEDIUM and not included in the sub-design. There is an equal probability that a system parameter will be assigned to toggle with or against an experimental factor.

Table 2.1.2 shows how the system parameters are set for each of the 48 experiments. The experimental factors are subjected to the 2^{4-1} sub-design and the system parameters follow the experimental factors they were assigned in Table 2.1.1.

In the small example, there are seven effects that can be estimated for each iteration. These *estimable effects* can be expressed in terms of the experimental factors. They are:

$E_{i,1}+E_{i,234}$	$E_{i,12}+E_{i,34}$
$E_{i,2}+E_{i,134}$	$E_{i,13}+E_{i,24}$
$E_{i,3}+E_{i,124}$	$E_{i,14}+E_{i,23}$
$E_{i,4}+E_{i,123}$	

where $E_{i,e}$ is the effect of experimental factor number e in the ith iteration of the sub-design and E_{i,e_1e_2} is the interaction between experimental factors e_1 and e_2.

Table 2.1.1 can then be used to express these estimable effects in terms of the system effects. Using iteration 3 as an example:

- System parameters one, two and three are assigned to experimental factor number one. Therefore:

  $E_{3.1}=S_1+S_2+S_3$

  where S_p is the main effect of system parameter number p.

- There are no system parameters assigned to experimental factors numbered three and four. Therefore $E_{3.234}$ does not represent interaction of system parameters and $E_{3.234}=0$.

- $E_{3.1}+E_{3.234}$ can be estimated and

  $E_{3.1}+E_{3.234}=S_1+S_2+S_3$

Table 2.1.3 shows all the estimable effects in the small example. The effects are listed according to the experimental effects they represent. The numerical values are calculated according to standard methods (Montgomery 1991).

Iteration	Experimental Factors 1	2	3	4	System Parameters 1	2	3	4	System Response y
1					*0*	*0*	*0*	*3*	
	-1	-1	-1	-1	0	0	0	-1	0
	1	-1	-1	1	0	0	0	-1	0
	-1	1	-1	1	0	0	0	-1	0
	1	1	-1	-1	0	0	0	-1	0
	-1	-1	1	1	0	0	0	1	0
	1	-1	1	-1	0	0	0	1	0
	-1	1	1	-1	0	0	0	1	0
	1	1	1	1	0	0	0	1	0
2					*-2*	*-3*	*0*	*-4*	
	-1	-1	-1	-1	1	1	0	1	3
	1	-1	-1	1	1	1	0	-1	3
	-1	1	-1	1	-1	1	0	-1	-1
	1	1	-1	-1	-1	1	0	1	-1
	-1	-1	1	1	1	-1	0	-1	1
	1	-1	1	-1	1	-1	0	1	1
	-1	1	1	-1	-1	-1	0	1	-3
	1	1	1	1	-1	-1	0	-1	-3
3					*1*	*1*	*1*	*-2*	
	-1	-1	-1	-1	-1	-1	-1	1	-1
	1	-1	-1	1	1	1	1	1	5
	-1	1	-1	1	-1	-1	-1	-1	-1
	1	1	-1	-1	1	1	1	-1	5
	-1	-1	1	1	-1	-1	-1	1	-1
	1	-1	1	-1	1	1	1	1	5
	-1	1	1	-1	-1	-1	-1	-1	-1
	1	1	1	1	1	1	1	-1	5
4					*-4*	*1*	*3*	*0*	
	-1	-1	-1	-1	1	-1	-1	0	3
	1	-1	-1	1	-1	1	-1	0	-1
	-1	1	-1	1	-1	-1	-1	0	-1
	1	1	-1	-1	1	1	-1	0	3
	-1	-1	1	1	-1	-1	1	0	-3
	1	-1	1	-1	1	1	1	0	5
	-1	1	1	-1	1	-1	1	0	1
	1	1	1	1	-1	1	1	0	1
5					0	0	-4	0	
	-1	-1	-1	-1	0	0	1	0	1
	1	-1	-1	1	0	0	-1	0	1
	-1	1	-1	1	0	0	-1	0	1
	1	1	-1	-1	0	0	1	0	1
	-1	-1	1	1	0	0	-1	0	1
	1	-1	1	-1	0	0	1	0	1
	-1	1	1	-1	0	0	1	0	1
	1	1	1	1	0	0	-1	0	1
6					*-3*	*3*	*-3*	*-3*	
	-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

Table 2.1.2 **Experimental Factors, System Parameters and System Responses for the Small Example.**

Iteration (i)		Estimable Effect $E_{I.1}+E_{I.234}$	$E_{I.2}+E_{I.134}$	$E_{I.3}+E_{I.124}$	$E_{I.4}+E_{I.123}$	$E_{I.12}+E_{I.34}$	$E_{I.13}+E_{I.24}$	$E_{I.14}+E_{I.23}$
1	Numerical Value	0	0	0	0	0	0	0
	System Effects			S_4				
2	Numerical Value	0	-4	-2	0	0	0	0
	System Effects	$-S_{124}$	$-S_1$	$-S_2$	$-S_4$	S_{24}	S_{14}	S_{12}
3	Numerical Value	6	0	0	0	0	0	0
	System Effects	$S_1+S_2+S_3$	$-S_4$			$-S_{14}-S_{24}-S_{34}$		
4	Numerical Value	2	0	0	-4	0	2	0
	System Effects	S_2	$-S_{123}$	S_3	$-S_1$	$-S_{13}$	S_{23}	$-S_{12}$
5	Numerical Value	0	0	0	0	0	0	0
	System Effects				$-S_3$			
6	Numerical Value	0	0	-2	0	0	0	0
	System Effects			$-S_1+S_2-S_3-S_4$				

Table 2.1.3 Estimable Effects For The Small Example. Initial Estimates.

2.2 SYVAC3-CC3 Example

The design used for the SYVAC3-CC3 example is similar to the small example except that it is done on a larger scale. The sub-design is a 2^{8-4} fractional factorial design and it is iterated 30 times. There are approximately 3300 system parameters.

The larger sub-design means that interactions of up to order seven will exist. There are fifteen estimable effects for each iteration of the sub-design.

The large number of system parameters means that more system effects are aliased with each estimable effect. For example, the number of main system effects aliased with a single main experimental effect is $\sim 3300/8*(2/3)= 275$.

Table 2.2.1 shows how some of the system parameters were assigned to experimental factors for the sample calculations. In the table, the rows represent iterations of the sub-design and the columns represent system parameters.

As with the small design, the iterated fractional factorial design has introduced aliasing into the analysis. For example, in the first iteration of the sub-design, system parameters 2239 and 2443 are both assigned to the same experimental factor and will be aliased for those 16 simulations. However, the aliasing between system parameters is different in each iteration.

The SYVAC3-CC3 example takes advantage of another characteristic of the sub-design. Even-ordered interactions are only aliased with other even-ordered interactions while odd-ordered interactions (including main effects) are only aliased with other odd-ordered interactions. Consequently, there are two distinct groups of estimable effects.

It should be noted that this design is slightly different than those used in Goodwin et al 1994 and therefore results will also be slightly different.

Iteration (i)	Parameter Number (p) 2239	2443	2355	2803	104	2825	2826	1126
1	-4	-4	0	8	-1	0	-5	3
2	-8	3	8	0	0	5	0	0
3	-1	5	-4	0	5	7	0	2
4	0	5	0	-6	0	5	8	0
5	0	0	0	0	-4	7	0	-6
6	3	0	0	7	6	6	-8	-6
7	0	8	7	5	-7	3	0	0
8	-1	-4	-4	2	-7	-3	-2	0
9	-3	-2	8	0	0	0	6	0
10	0	1	8	-8	-5	0	-1	2
11	-1	0	-3	2	0	0	-6	-4
12	0	7	2	5	0	0	8	-1
13	-2	-2	0	-3	5	5	0	2
14	5	0	3	0	3	-4	-1	-5
15	-2	0	-3	-5	-7	-4	-3	-6
16	0	4	-2	0	2	4	0	-2
17	-6	6	-5	-5	-2	2	1	-4
18	0	0	-2	-5	-1	5	0	-3
19	4	0	-6	0	2	-6	0	4
20	-7	-6	3	1	-6	0	7	0
21	0	4	8	2	2	-4	4	0
22	-8	1	7	2	0	0	0	0
23	6	0	0	5	-8	-4	-5	-4
24	0	0	-8	0	5	3	3	5
25	5	0	0	-8	-3	-7	-1	-2
26	5	2	0	-1	0	1	-2	0
27	4	-2	-5	6	-2	0	-3	-8
28	3	-2	0	0	0	0	6	0
29	7	-5	-2	0	0	-8	6	3
30	0	-5	0	7	0	0	0	2

Table 2.2.1: Assignment Of Some SYVAC3-CC3 Parameters To Experimental Factors.

Chapter 3
Estimating Effects In The Small Example

3.1 Estimating Main Effects And Interactions

Once the system responses are generated, the estimable effects are readily calculated (Table 2.1.3 for example). From the information given in Table 2.1.3, there are various ways the system effects could be calculated, but a method has been devised that can easily be extended to larger systems. The small example will be used to demonstrate how this method works.

Table 2.1.3 does not give a direct estimate of S_1. However, it does identify estimable effects that are aliased with S_1. For example, in iteration number three one of the estimable effects is $S_1+S_2+S_3=6$.

The method that will be used to estimate S_1 is to take the average of all the estimable effects where S_1 makes a contribution. From Table 2.1.1 or 2.1.3, the estimated value of S_1 is the average of:

- $-(-S_1)$ *iteration number 2*
- $+(S_1+S_2+S_3)$ *iteration number 3*
- $-(-S_1)$ *iteration number 4*
- $-(-S_1+S_2-S_3-S_4)$ *iteration number 5*

Negative signs are used where the system parameter toggles in the opposite direction to the experimental factor.

Obviously, there is potential error due to the aliasing of system parameters. However since there is an equal probability of any two system parameters toggling in the same or opposite directions, the expected value of error due to aliasing is zero. The error due to aliasing will become closer to zero as the number of iterations of the sub-design is increased.

Table 3.1.1 shows the first estimate of the system effects for the small example. Some important considerations about interactions are illustrated in Table 3.1.1.

- The number of estimable effects that can be used to estimate system interactions is variable.

- Generally, for higher order interactions there are fewer estimable effects that can be used to estimate the system interactions.

- It is impossible to estimate some of the system interactions because they are not aliased with any of the estimable effects.

Table 3.1.1 shows more information than is actually required to estimate the system effects. It is not necessary to explicitly deal with the aliasing between system effects. It is only necessary to identify the estimable effects that are aliased with a system effect. Such information can be generated from Table 2.1.1. For example:

- Table 2.1.1 tells us that in iteration number three, the first system parameter is aliased with the first experimental factor. In the averaging process to estimate S_1, we need to use the estimable effect that is aliased with $E_{3,1}$. Even though it is informative to know that $E_{3,1}+E_{3,234}=S_1+S_2+S_3$, it is only necessary to know that $E_{3,1}$ and S_1 are aliased and to be able to calculate the estimable effect that is aliased with $E_{3,1}$.

System Effect	Estimable Effects Used in the Calculation		Estimated Value
S_1	• $-(-S_1)$	iteration # 2	4
	• $+(S_1+S_2+S_3)$	iteration # 3	
	• $-(-S_1)$	iteration # 4	
	• $-(-S_1+S_2-S_3-S_4)$	iteration # 6	
S_2	• $-(-S_2)$	iteration # 2	2
	• $+(S_1+S_2+S_3)$	*iteration # 3*	
	• $+(S_2)$	*iteration # 4*	
	• $+(-S_1+S_2-S_3-S_4)$	*iteration # 6*	
S_3	• $+(S_1+S_2+S_3)$	*iteration # 3*	2
	• $+(S_3)$	*iteration # 4*	
	• $-(-S_3)$	*iteration # 5*	
	• $-(-S_1+S_2-S_3-S_4)$	*iteration # 6*	
S_4	• $+(S_4)$	*iteration # 1*	0.5
	• $-(-S_4)$	*iteration # 2*	
	• $-(-S_4)$	*iteration # 3*	
	• $-(-S_1+S_2-S_3-S_4)$	*iteration # 6*	
S_{12}	• $+(S_{12})$	*iteration # 2*	0
	• $-(-S_{12})$	*iteration # 4*	
S_{13}	• $-(-S_{13})$	*iteration # 4*	0
S_{14}	• $+(S_{14})$	*iteration # 2*	0
	• $-(S_{14}+S_{24}-S_{34})$	*iteration # 3*	
S_{23}	• $+(S_{23})$	*iteration # 4*	2
S_{24}	• $+(S_{24})$	*iteration # 2*	0
	• $+(S_{14}+S_{24}-S_{34})$	*iteration # 3*	
S_{34}	• $-(S_{14}+S_{24}-S_{34})$	*iteration # 3*	0
S_{123}	• $-(-S_{123})$	*iteration # 4*	0
S_{124}	• $-(-S_{124})$	*iteration # 2*	0
S_{134}	• none available		
S_{234}	• none available		

Table 3.1.1 The Calculation Of Main Effects And Interactions For The Small Example.

Table 3.1.2 shows the information that is necessary to estimate main effects and interactions without explicitly dealing with the aliasing amongst system parameters. This streamlined approach is readily applied to larger systems and larger experimental designs.

As mentioned, the system effects that are estimated so far are a first approximation. It is possible to revise the estimated values to reduce the error due to aliasing. The results will be refined in Section 3.3.

3.2 Estimated Quadratic Effects

Quadratic effects are defined as shown in Figure 1.3.5.1. As a simple approximation:

- If there is no quadratic effect, the average response where a parameter is held MEDIUM is equal to the average responses where the parameter toggles between LOW or HIGH.

  The difference between these two averages is used to estimate the quadratic effect.

For the actual calculations, it will be convenient to use the average responses for the iterations of the sub-design rather than the results from individual experiments. A_i is used to represent the average response from iteration i of the sub-design. Table 2.1.1 can be used to determine in which iterations the system parameter is MEDIUM and in which iterations it toggles between LOW and HIGH. Table 3.2.1 shows the iteration averages for the small example and Table 3.2.2 shows how the iteration averages are used to estimate the quadratic effects.

System Effect	Aliased Experimental Effects						Estimated Value
	Iteration						
	1	2	3	4	5	6	
S_1		$-E_{2.2}$	$E_{3.1}$	$-E_{4.4}$		$-E_{6.3}$	4.0
S_2		$-E_{2.3}$	$E_{3.1}$	$E_{4.1}$		$E_{6.3}$	2.0
S_3			$E_{3.1}$	$E_{4.3}$	$-E_{5.4}$	$-E_{6.3}$	2.0
S_4	$E_{1.3}$	$-E_{2.4}$	$-E_{3.2}$			$-E_{6.3}$	0.5
S_{12}		$E_{2.23}$		$-E_{4.14}$			0.0
S_{13}				$-E_{4.34}$			0.0
S_{14}		$E_{2.24}$	$-E_{3.12}$				0.0
S_{23}				$E_{4.13}$			2.0
S_{24}		$E_{2.34}$	$-E_{3.12}$				0.0
S_{34}			$-E_{3.12}$				0.0
S_{123}				$-E_{4.134}$			0.0
S_{124}		$-E_{2.234}$					0.0
S_{134}							not available
S_{234}							not available

Table 3.1.2 System Effects As Estimated By The Streamlined Approach For The Small Example. Original Estimates.

3.3 Refining Estimates of Main Effects And Interactions

A step-wise approach is used refine the estimated main effects and interactions.

According to Tables 3.1.1 and 3.1.2, one of the largest system effects is S_1 and consequently S_1 will be one of the largest sources of error due to aliasing. Given an estimate of S_1, it is possible to reduce the error it induces in estimates of the other system effects.

Iteration(i)	1	2	3	4	5	6
Iteration Average(A_i)	0	0	2	1	1	0

Table 3.2.1 Iteration Averages For The Small Example.

System Parameter	Iterations Where The Parameter Is Held MEDIUM		Iterations Where The Parameter Is HIGH and LOW		Estimated Quadratic Effect
(p)	i	Mean Response	i	Mean Response	($\dot{Q}_p$)
1	1,5	0.50	2,3,4,6	0.75	-0.25
2	1,5	0.50	2,3,4,6	0.75	-0.25
3	1,2	0.00	3,4,5,6	1.00	-1.00
4	4,5	1.00	1,2,3,6	0.50	+0.50

Table 3.2.2: Estimated Quadratic Effects For The Small Example. Original Estimates.

For example, according to Table 2.1.3:

$$E_{3.1}+E_{3.234} = S_1+S_2+S_3 = 6.0$$

To remove the disruptive influence of S_1, a very simplistic approximation can be made for the third iteration:

$$(E_{3.1}+E_{3.234})-S_1=6.0-S_1$$

$$(S_1+S_2+S_3)-S_1 = 6.0-S_1$$

$$S_2+S_3=6.0-4.0=2.0$$

Information from Table 2.1.1 can be used to determine the other estimable effects to adjust with respect to S_1. Table 3.1.2 can be transformed into Table 3.3.1 by reducing the error due to aliasing with S_1. Note that the refinement is only applied to system effects other than S_1.

Table 3.3.1 suggests the next step in the refinement. S_2 is the next major source of error due to aliasing and its influence should be removed from the estimable effects. The result is Table 3.3.2.

Table 3.3.2 represents as much refinement as can be made to the estimated main system effects. They are all fall into one of three categories:

- Their influence has been removed from the estimable effects. (S_1 and S_2).

- Their estimated value is small and unlikely to lead to error in the estimated values of the other system effects. (S_3, S_4, ...).

- They are not aliased with any other system effects except for those that no longer influence the estimable effects.

A comparison of Table 3.3.2 and the results that were predicted in Section 1.4.1 demonstrates that the step-wise refinement has performed well for main effects and interactions.

System Effect	Aliased Experimental factors Iteration 1	2	3	4	5	6	Estimated Value
S_1		$-E_{2.2}$	$E_{3.1}$	$-E_{4.4}$		$-E_{6.3}$	4.0
S_2		$-E_{2.3}$	$E_{3.1}-\hat{S}_1$	$E_{4.1}$		$E_{6.3}+\hat{S}_1$	2.0
S_3			$E_{3.1}-\hat{S}_1$	$E_{4.3}$	$-E_{5.4}$	$-E_{6.3}-\hat{S}_1$	0.0
S_4	$E_{1.3}$	$-E_{2.4}$	$-E_{3.2}$			$-E_{6.3}-\hat{S}_1$	-0.5
S_{12}		$E_{2.23}$		$-E_{4.14}$			0.0
S_{13}				$-E_{4.34}$			0.0
S_{14}		$E_{2.24}$	$-E_{3.12}$				0.0
S_{23}				$E_{4.13}$			2.0
S_{24}		$E_{2.34}$	$-E_{3.12}$				0.0
S_{34}			$-E_{3.12}$				0.0
S_{123}				$-E_{4.134}$			0.0
S_{124}		$-E_{2.234}$					0.0
S_{134}							
S_{234}							

Table 3.3.1 Estimated Main Effects And Interactions For The Small Example After One Refinement Of The Results.

System Effect	Aliased Experimental Factors						
	Iteration						
	1	2	3	4	5	6	Estimated Value
S_1		$-E_{2.2}$	$E_{3.1}$	$-E_{4.4}$		$-E_{6.3}$	**4.0**
S_2		$-E_{2.3}$	$E_{3.1}-\hat{S}_1$	$E_{4.1}$		$E_{6.3}+\hat{S}_1$	**2.0**
S_3			$E_{3.1}-\hat{S}_1-\hat{S}_2$	$E_{4.3}$	$-E_{5.4}$	$-E_{6.3}-\hat{S}_1+\hat{S}_2$	0.0
S_4	$E_{1.3}$	$-E_{2.4}$	$-E_{3.2}$			$-E_{6.3}-\hat{S}_1+\hat{S}_2$	0.0
S_{12}		$E_{2.23}$		$-E_{4.14}$			0.0
S_{13}				$-E_{4.34}$			0.0
S_{14}		$E_{2.24}$	$-E_{3.12}$				0.0
S_{23}				$E_{4.13}$			2.0
S_{24}		$E_{2.34}$	$-E_{3.12}$				0.0
S_{34}			$-E_{3.12}$				0.0
S_{123}				$-E_{4.134}$			0.0
S_{124}		$-E_{2.234}$					0.0
S_{134}							
S_{234}							

Table 3.3.2 Estimated Main Effects And Interactions For The Small Example After Two Refinements Of The Results.

3.4 Refining Estimates of Quadratic Effects

Just as the estimates of the main effects were refined by adjusting the estimable effects, the estimates of the quadratic effects can be refined by adjusting the iteration averages. From Table 3.2.2, it appears the largest quadratic effect is Q_3. The average response for iterations 1 and 2 can be adjusted to remove the estimated influence of Q_3. Tables 3.4.1 and 3.4.2 show the result of the adjustment. The row for Q_3 is shaded because it shows results from a previous estimate.

Iteration(i)	1	2	3	4	5	6
Iteration Average(A_i)	$0-\hat{Q}_3=$ 1	$0-\hat{Q}_3=$ 1	2	1	1	0

Table 3.4.1 Iteration Averages For The Small Example After One Refinement.

System Parameter (p)	Iterations Where The Parameter Is Held MEDIUM		Iterations Where The Parameter Is HIGH and LOW		Estimated Quadratic Effect ($\hat{Q}_p$)
	i	Mean Response	i	Mean Response	
1	1,5	1.00	2,3,4,6	1.00	0.00
2	1,5	1.00	2,3,4,6	1.00	0.00
3	1,2	**0.00**	**3,4,5,6**	**1.00**	**-1.00**
4	4,5	1.00	1,2,3,6	1.00	0.00

Table 3.4.2 Estimated Quadratic Effects For The Small Example After One Refinement.

Chapter 4

Confidence Coefficients And Confidence Bounds In The SYVAC3-CC3 Example

4.1 The Estimated Effects

The calculations made for the small example are very transferable to the SYVAC3-CC3 example. However, the sheer number of effects prevents the luxury of a complete description of the aliasing structure as was done in Table 2.1.3. Fortunately, calculations such as those in Table 3.1.2 are possible. Also, even for a system as large as SYVAC3-CC3 it is practical to estimate all the main effects and all the quadratic effects.

Table 4.1.1 shows the largest estimated main effects and Table 4.1.2 shows the largest estimated quadratic effects as determined from the initial estimates.

Of concern are the columns labeled "Actual Effect". The information in these columns is based on expert knowledge of SYVAC3-CC3. According to expert knowledge, many of the system parameters (number 1927 for example) can have no influence on the measured response of the system but the S_p and Q_p columns suggest some of these parameters do have effects.

In Tables 4.1.1 and 4.1.2, $CL_1(\hat{S}_p)$, $CL_2(\hat{S}_p)$, $CLQ_1(\hat{Q}_p)$ and $CQL_2(\hat{Q}_p)$ represent confidence coefficients and $CB(\hat{S}_p)$ and $CBQ(\hat{Q}_p)$ are confidence bounds. Sections 4.2 and 4.3 will discuss confidence coefficients and confidence bounds.

The estimated effects can be revised as was done in Sections 3.3 and 3.4.

4.2 Main Effects and Interactions

For the SYVAC3-CC3 example, it is possible to assign confidence bounds and confidence coefficients for the system effects. These assignments are based upon the assumption that the estimable effects have a Normal distribution. Normal distributions are not unexpected since a estimable effect is approximately the sum of a random set of system effects and the Central Limit Theorem is likely to take effect. As will be shown, this assumption can be easily supported through probit plots.

To look at the distribution of the estimable effects, there is a useful property of the sub-design used in the SYVAC3-CC3 example :

> The estimable effects can be divided into two mutually exclusive sets; one is aliased with odd-ordered interactions (including main effects) and the other is aliased with even-ordered interactions.
>
> This property is a result of the aliasing structure used in the sub-design which in common notation (Montgomery 1991) can be expressed as:
>
> I=ABCD=ABEF=ABGH=ACEG

p	$\hat{S}_p$	$CL_1(\hat{S}_p)$	$CL_2(\hat{S}_p)$	$CB(\hat{S}_p)$	Actual Effect
2239	-1.725	1.000	1.000	0.334	yes
2443	1.447	1.000	1.000	0.358	yes
2355	0.818	1.000	0.412	0.392	yes
1927	0.753	0.999	0.114	0.395	no
1335	-0.741	0.999	0.077	0.395	no
2633	-0.666	0.998	0.001	0.397	no
336	-0.665	0.998	0.001	0.398	no
1259	-0.643	0.997	0.000	0.398	no
2992	0.641	0.997	0.000	0.398	no
1996	-0.634	0.997	0.000	0.399	no
1	0.630	0.997	0.000	0.399	no
2973	0.620	0.996	0.000	0.399	no
2803	0.608	0.996	0.000	0.399	yes
1514	-0.596	0.995	0.000	0.400	no
593	0.560	0.992	0.000	0.400	no
2553	0.559	0.992	0.000	0.400	no
2448	0.555	0.991	0.000	0.401	no
1272	-0.555	0.991	0.000	0.401	no
545	-0.553	0.991	0.000	0.401	no
104	0.551	0.991	0.000	0.401	yes
1147	-0.548	0.991	0.000	0.401	no
693	0.543	0.990	0.000	0.401	no
36	-0.541	0.990	0.000	0.401	no
2420	-0.531	0.988	0.000	0.401	no
405	0.523	0.987	0.000	0.401	no
2472	0.520	0.987	0.000	0.402	no
1789	0.514	0.986	0.000	0.402	no
686	0.512	0.986	0.000	0.401	no
2782	0.511	0.985	0.000	0.402	no
868	-0.510	0.985	0.000	0.402	no

Table 4.1.1: The Largest Main Effects For SYVAC3-CC3. Original Estimates.

p	$\hat{Q}_p$	$CLQ_1(\hat{Q}_p)$	$CLQ_2(\hat{Q}_p)$	$CBQ(\hat{Q}_p)$	Actual Effect
1419	-0.300	0.997	0.000	0.275	no
396	-0.286	0.995	0.000	0.268	no
2315	-0.272	0.993	0.000	0.262	yes
1060	0.260	0.991	0.000	0.257	no
1550	0.255	0.990	0.000	0.255	no
1428	-0.252	0.989	0.000	0.254	no
2271	-0.252	0.989	0.000	0.254	no
2835	0.251	0.989	0.000	0.253	no
610	-0.249	0.988	0.000	0.252	no
2707	-0.248	0.988	0.000	0.252	no
2354	-0.245	0.987	0.000	0.250	no
3072	-0.245	0.987	0.000	0.250	no
24	0.239	0.985	0.000	0.248	no
2737	-0.238	0.984	0.000	0.247	no
1209	-0.234	0.982	0.000	0.246	no
1375	-0.234	0.982	0.000	0.246	no
2031	-0.234	0.982	0.000	0.246	no
3211	0.233	0.982	0.000	0.246	no
2428	-0.232	0.981	0.000	0.245	no
301	-0.226	0.978	0.000	0.242	no
581	0.226	0.978	0.000	0.242	no
1186	0.226	0.978	0.000	0.242	no
1138	-0.226	0.978	0.000	0.242	no
2243	-0.224	0.978	0.000	0.242	yes
2895	0.224	0.977	0.000	0.242	no
1239	-0.223	0.977	0.000	0.241	no
1170	0.222	0.976	0.000	0.241	no
2780	-0.221	0.975	0.000	0.240	no
1791	-0.220	0.975	0.000	0.240	no
2419	0.220	0.975	0.000	0.240	no
3021	0.220	0.975	0.000	0.240	no
1682	-0.219	0.974	0.000	0.240	no
927	0.218	0.974	0.000	0.240	no

Table 4.1.2: The Largest Estimated Quadratic Effects For SYVAC3-CC3 . Original Estimates.

Figure 4.2.1 consists of a probit plot for both of the groups of the estimable effects. Both appear to have an approximately Normal distribution.

Either of these two groups is expected to have a mean of zero. In the assignment of system parameters to experimental factors, there is an equal probability of a system parameter and an experimental factor moving in the same or opposite direction and consequently there is an equal probability that a system effect will be added to or subtracted from a estimable effect.

The standard deviations of these two groups, $STDEV_{E(odd)}$ and $STDEV_{E(even)}$ are readily estimated from the samples of values.

There is now enough information to predict the distribution of the estimated main effects and interactions of the system parameters. If these effects are simply averages of random estimable effects, the expected distribution is:

$$\frac{\hat{S}\sqrt{N}}{STDEV_{E(odd/even)}} \sim t_{N-1}$$

where:

- $\hat{S}$ is the main effect or interaction
- N is the number of iterations used to calculate $\hat{S}$
- $STDEV_{E(odd/even)}$ is $STDEV_{E(even)}$ or $STDEV_{E(odd)}$ depending on the order of the interaction
- t_{N-1} is the students t-variate with N-1 degrees of freedom

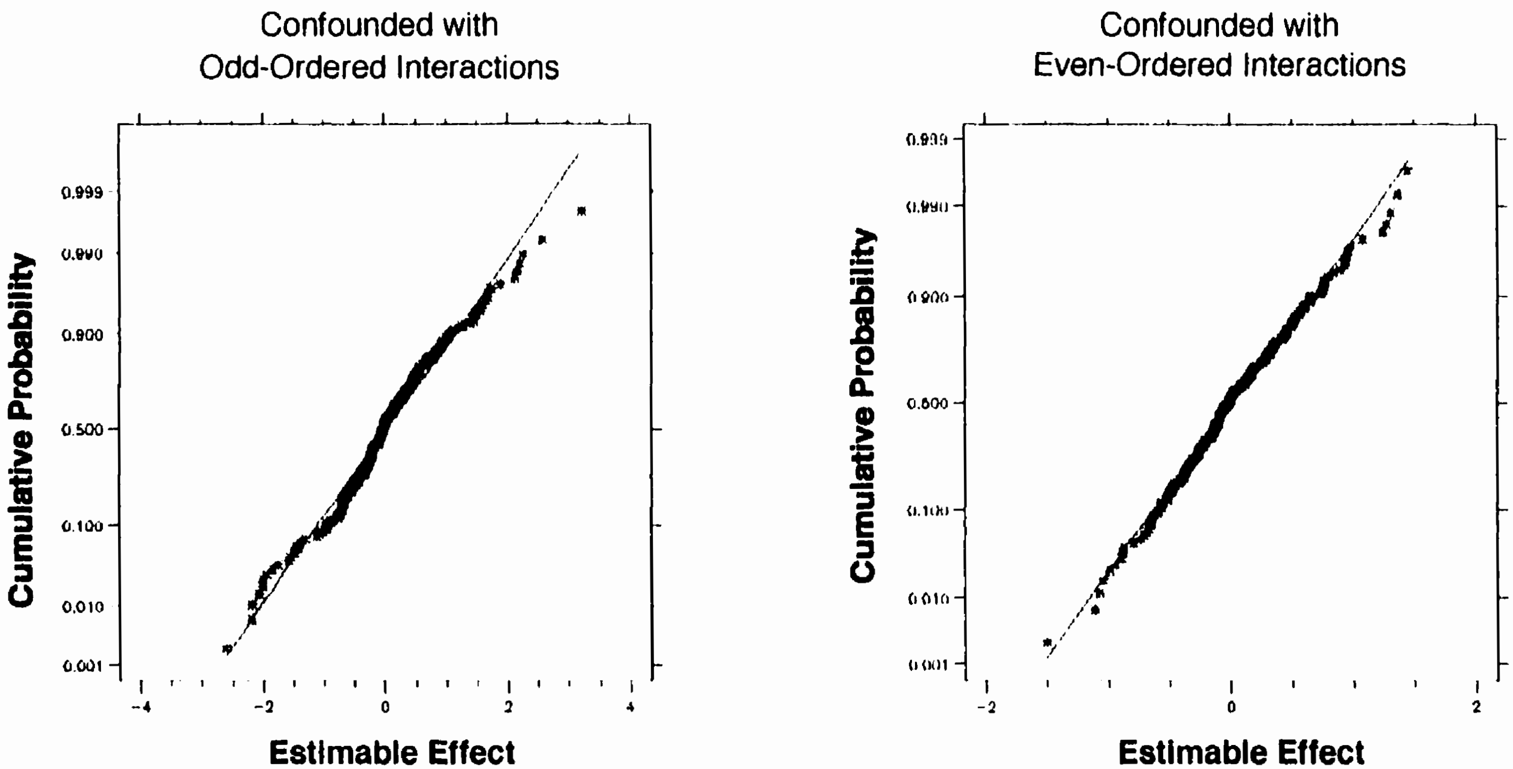

Figure 4.2.1: Distribution Of Estimable Effects.

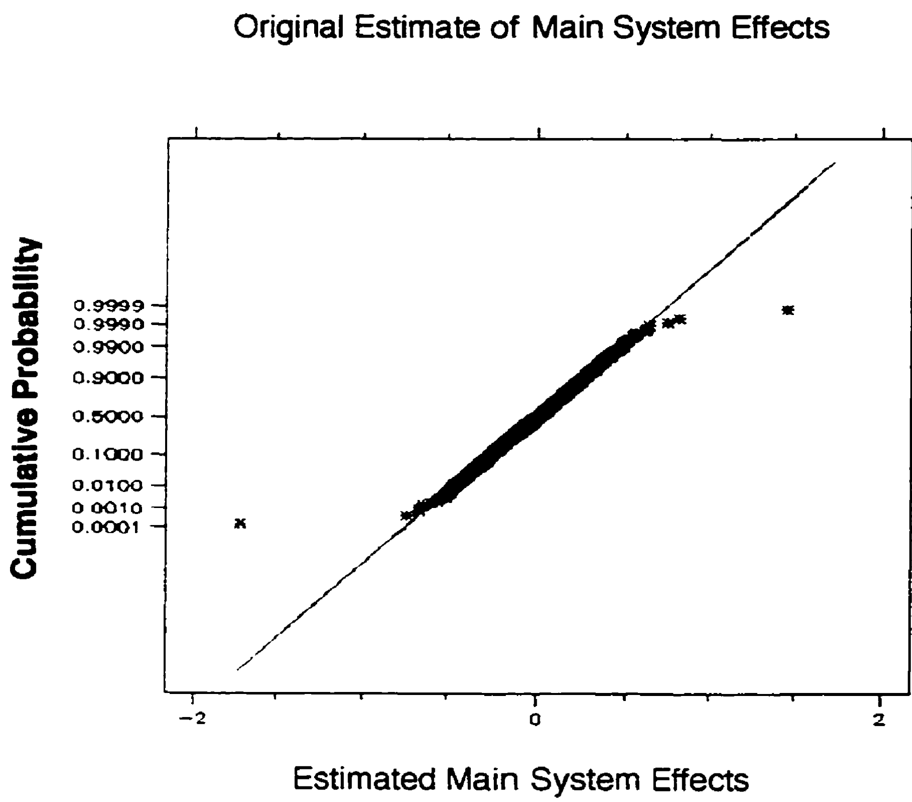

Figure 4.2.2: Distribution of Estimated Main System Effects.

Figure 4.2.2 is used to determine if the estimated main system effects are distributed as though they are merely random combinations of estimable effects. The figure is similar to a probit plot except that the transformation applied to the y-axis is based upon a t-distribution instead of a Normal distribution. Each point on the plot represents the original estimate of the value of a main system effect. The same number of iterations (two-thirds of the total) is used to estimate each of the main system effects.

According to Figure 4.2.2, the predicted distribution was a good approximation for all but two of the main system effects. These two effects have magnitudes that are much larger than would be expected given the sample size and the predicted distribution. The figure gives us confidence that these two main system effects are not occurring randomly and instead represent actual effects that occur in the system.

It is also possible to calculate confidence coefficients for the estimated system effects. A suitable null hypothesis is:

Ho: The system effect (main or interaction) is zero. S=0

Two variations on the confidence coefficient are necessary; one is useful for single effects and the other is useful for screening a large number of estimates for statistical significance.

To test individual estimates, very standard methods are available. A t-variate corresponding to the estimated effect is calculated and a p-value is generated. Corresponding confidence coefficients are assigned and listed in the table as $CL_1(\hat{S}_p)$.

Table 4.1.1 also demonstrates why $CL_1(\hat{S})$ is inappropriate for screening a large number of effects for statistical significance. To produce the table, approximately 3300 main linear effects were screened. The expected number of estimated main system effects to be declared 99% significant on a purely spurious basis is *(1%*3300)*~33. In Table 4.1.1, there are many system parameters known to have no influence on the system response (expert judgement) and yet by $CL_1(\hat{S})$ they appear significant. It is useful to have a confidence coefficient that considers the number of estimates that are tested.

$$CL_2(\hat{S}) = CL_1(\hat{S})^{N_{test}}$$

where

- N_{test} is the number of effects tested for statistical significance

is such a value. Under the predicted distribution, it is a first-order approximation to the probability that all members of the sample are smaller than the tested estimate.

$CL_2(\hat{S})$ values are also included in Table 4.1.1. Under this coefficient, only two system effects achieve a 99% level of confidence. These two effects are consistent with expert knowledge of SYVAC3-CC3. However, according to expert knowledge, some of the other parameters in Table 4.1.1 should also have significant main effects.

The $CL_2(\hat{S})$ values are more consistent with knowledge of SYVAC3-CC3 than the $CL_1(\hat{S})$ values but they are still not entirely satisfactory. However, as the estimable effects are modified to refine the estimated effects, the confidence coefficients and confidence bounds are also recalculated and the results are expected to improve.

How accurate are the estimates of S? We can find $CB(\hat{S})$ such that $\hat{S} \pm CB(\hat{S})$ forms the 95% confidence bound. We assume:

$$\frac{Err(\hat{S}) \cdot \sqrt{N}}{STDEV_{E(\hat{S})}} \sim t_{N-1}$$

where

- $\hat{S}$ is the estimated system effect
- $Err(\hat{S})$ is the error made in estimating S
- N is the number of iterations used to estimate S
- t is a variate with a Student-t distribution

- $STDEV_{E(\hat{S})}$ is an estimate of the standard deviation of the measurable effects after the estimated influence of S has been removed.

$STDEV_{E(\hat{S})}$ is closely related to $STDEV_{E(odd)}$ or $STDEV_{E(even)}$ depending on the order of S. For example, $STDEV_{E(\hat{S}_{2239})}$ is the same as $STDEV_{E(odd)}$ except that:

- $E_{1,4} + \hat{S}_{2239}$ is used instead of $E_{1,4}$
- $E_{2,8} + \hat{S}_{2239}$ is used instead of $E_{2,8}$
- $E_{6,3} - \hat{S}_{2239}$ is used instead of $E_{6,3}$
- etc.

Confidence bounds are shown for the main system effects in Table 4.1.1. Since the major source of error is aliasing, it is not surprising that the narrowest confidence bounds are associated with the largest effects.

As with the small example, the SYVAC3-CC3 results can be refined by adjusting the estimable effects for the estimated influence of a system effect. Not only can the effects be re-calculated, but so can the confidence coefficients and confidence bounds.

Table 4.2.1 shows the main effects when the estimated error due to aliasing with S_{2239} is removed.

p	$\hat{S}_p$	$CL_1(\hat{S}_p)$	$CL_2(\hat{S}_p)$	$CB(\hat{S}_p)$	Actual Effect
2239	-1.725	1.000	1.000	0.334	yes
2443	1.533	1.000	1.000	0.262	yes
2355	0.732	1.000	0.732	0.319	yes
2803	0.608	0.999	0.080	0.324	yes
2992	0.555	0.998	0.002	0.326	no
104	0.551	0.998	0.002	0.326	yes
2712	0.511	0.996	0.000	0.327	no
2026	0.499	0.996	0.000	0.327	no
2796	0.495	0.995	0.000	0.327	no
328	0.475	0.994	0.000	0.328	no
2856	0.472	0.993	0.000	0.328	no
2448	0.469	0.993	0.000	0.328	no
1272	-0.469	0.993	0.000	0.328	no
2793	0.467	0.993	0.000	0.328	no
376	0.464	0.993	0.000	0.328	no
2826	-0.460	0.992	0.000	0.328	yes
1	0.457	0.992	0.000	0.329	no
2588	0.446	0.990	0.000	0.329	no
1152	-0.438	0.989	0.000	0.329	no
405	0.436	0.989	0.000	0.329	no
1612	-0.434	0.988	0.000	0.329	no
3290	-0.431	0.988	0.000	0.329	no
2210	-0.429	0.987	0.000	0.329	no
2626	0.429	0.987	0.000	0.329	yes
686	0.426	0.987	0.000	0.329	no
2128	-0.425	0.987	0.000	0.329	no
868	-0.424	0.986	0.000	0.329	no
1002	-0.424	0.986	0.000	0.329	no
1039	-0.421	0.986	0.000	0.329	no
2825	0.420	0.985	0.000	0.329	yes
2264	0.420	0.985	0.000	0.329	no
2318	0.417	0.985	0.000	0.329	no
2358	-0.412	0.984	0.000	0.330	no
1943	0.412	0.984	0.000	0.329	no

Table 4.2.1: The Largest Estimated Main Effects For SYVAC3-CC3 After One Revision.

p	$\hat{S}_p$	$CL_1(\hat{S}_p)$	$CL_2(\hat{S}_p)$	$CB(\hat{S}_p)$	Actual Effect
2239	**-1.725**	**1.000**	**1.000**	**0.334**	**yes**
2443	**1.533**	**1.000**	**1.000**	**0.262**	**yes**
2355	**0.655**	**1.000**	**0.951**	**0.247**	**yes**
2803	0.608	1.000	0.941	0.232	yes
1461	0.414	0.999	0.044	0.225	no
772	-0.375	0.998	0.000	0.227	no
2825	0.371	0.997	0.000	0.227	yes
994	0.357	0.996	0.000	0.227	no
2826	-0.356	0.996	0.000	0.227	yes
2712	0.343	0.995	0.000	0.228	no
973	-0.332	0.994	0.000	0.228	no
603	0.331	0.994	0.000	0.228	no
842	-0.330	0.994	0.000	0.228	no
104	0.324	0.993	0.000	0.228	yes
1480	-0.311	0.990	0.000	0.229	no
2613	-0.307	0.989	0.000	0.229	no
1956	0.303	0.989	0.000	0.229	no
756	0.301	0.988	0.000	0.229	no
1126	0.298	0.987	0.000	0.229	yes
2910	-0.296	0.987	0.000	0.229	no
2413	0.296	0.987	0.000	0.229	no
2307	0.294	0.986	0.000	0.229	no
1726	0.293	0.986	0.000	0.229	no
639	-0.292	0.986	0.000	0.229	no
1205	0.292	0.986	0.000	0.229	no
2638	-0.290	0.985	0.000	0.229	no
2992	0.289	0.985	0.000	0.229	no
1024	-0.289	0.985	0.000	0.229	no
2313	0.288	0.984	0.000	0.229	no
2115	-0.285	0.983	0.000	0.229	no
1222	-0.285	0.983	0.000	0.229	no
2108	0.284	0.983	0.000	0.229	no
105	0.283	0.983	0.000	0.229	no
1943	0.412	0.984	0.000	0.229	no

Table 4.2.2: The Largest Estimated Main Effects For SYVAC3-CC3 After Three Revisions.

Table 4.2.1 suggests that the next refinement to make is to adjust the estimable effects to remove the estimated error due to aliasing with S_{2443}. And of course the step-wise refinement can continue. Table 4.2.2 shows the results after three refinements are made.

After three refinements of the results, there are no more main effects that are statistically significant (confidence coefficient greater than 95%) according to $CL_2(\hat{S})$ However, the information in Table 4.2.2 suggests some non-zero main effects are not significant according to $CL_2(\hat{S})$. According to expert knowledge, $S_{2803}, S_{2826}, S_{2825}, S_{104}$ and S_{1126} could be non-zero. According to $CL_1(\hat{S})$, their estimated effects are statistically significant but so is $\hat{S}_{1461}$, which is known to have no actual effect. Chapter 5 will discuss how expert knowledge can be incorporated into the application of IFFDA.

When confidence coefficients and confidence bounds are calculated for interactions, the only special concern is that a variable number of iterations of the sub-design are used to estimate the interactions.

4.3 Quadratic Effects

Confidence coefficients and confidence bounds can also be calculated for the quadratic effects. The methods are very analogous to those used for main effects and interactions.

Quadratic effects are estimated from the mean responses as calculated for the iterations of the sub-design(Section 3.2). The Central Limit Theorem suggests that the iteration means could have a Normal distribution. Figure 4.3.1 is a probit plot of the iteration means for the SYVAC3-CC3 example and shows that the distribution is at least approximately Normal.

If the estimated quadratic effects are created from random combinations of iteration averages, then they are expected to be transformable to a Student-t distribution.

$$\frac{\hat{Q}_p * \sqrt{\frac{N_{nz} \cdot (N_{iter} - N_{nz})}{N_{iter}}}}{STDEV_A} \sim t_{N_{iter}-2}$$

where

- $\hat{Q}_p$ is the estimated quadratic effect of parameter p
- N_{nz} is the number of iterations where parameter p is included in the sub-design
- N_{iter} is the number of iterations of the sub-design
- $STDEV_A$ is the standard deviation of the iteration means
- $t_{N_{iter}-2}$ is the Student-t distribution with N_{iter} - 2 degrees of freedom. There are N_{iter} - 2 degrees of freedom because two values are required to estimate a difference,

Figure 4.3.2 is a graphical test of whether the estimated quadratic effects have the predicted distribution. It is similar to a probit plot except that the transformation on the y-axis is based upon a Student-t distribution instead of a Normal distribution. Very low and very high $\hat{Q}_p$ values do not occur as frequently as predicted. However, the predicted distribution is close and will be assumed for the rest of the calculations.

A suitable null hypothesis is:

Ho: The quadratic effect is zero. Q_p=0

As for the main effects, two variations of a confidence coefficient will be used. $CLQ_1(\hat{Q}_p)$ uses standard p-values and is suitable for testing individual quadratic effects. $CLQ_2(\hat{Q}_p)$ is suitable for screening a large number of quadratic effects for statistical significance. The relationship between the two coefficients is:

$$CLQ_2(\hat{Q}) = CLQ_1(\hat{Q})^{N_{test}}$$

where

- N_{test} is the number of effects tested for statistical significance

Table 4.1.2 includes the confidence coefficients for the largest quadratic effects in the SYVAC3-CC3 example. None of the quadratic effects are statistically significant under $CLQ_2(\hat{Q}_p)$. However, this is not to say there are no actual quadratic effects. As shown with the linear effects, confidence coefficients such as $CL_2(\hat{S})$ and $CLQ_2(\hat{Q}_p)$ are very restrictive due to the large sample sizes. If a justification can be found to use $CLQ_1(\hat{Q}_p)$ for some of the parameters, the estimated effects may be significant.

It is convenient to apply $CLQ_1(\hat{Q}_p)$ to sets of one hundred system parameters. For a set of one hundred $CLQ_1(\hat{Q}_p)$ values, the expected number of effects to falsely appear significant ($CLQ_1(\hat{Q}_p)$>99%) is manageable (~1).

The obvious parameters to test for significant quadratic effects are those with the largest linear effects. Two assumptions are required to justify this choice:

- The system parameters with the largest quadratic effects also have the largest linear effects.

- The error in the estimated quadratic effects occur independently of the error in estimating the linear effects.

Therefore we can test the 100 system parameters with the largest linear effects to see if their quadratic effects are significant. Of these 100 quadratic effects, Table 4.3.1 shows the largest ones. Even if the quadratic effects are tested individually, no statistical significance (99% confidence coefficient) can be attributed to any of these 100 quadratic effects. As was the case for the main effects, the user has the option of spending more resources to further investigate the quadratic effects of any suspicious parameters.

The confidence bounds for the quadratic effects, $CBQ(\hat{Q}_p)$ can of course be calculated. The methodology is very similar to that used for the linear effects. We use the assumption that:

$$\frac{ERR(\hat{Q}_p)\cdot\sqrt{\dfrac{N_{nz}\cdot(N_{iter}-N_{nz})}{N_{iter}}}}{STDEV_{A(p)}} \sim t_{N_{iter}-2}$$

where:

- $ERR(\hat{Q}_p)$ is the error in the estimate of Q_p
- $t_{N_{iter}-2}$ is the Student-t distribution with $N_{iter}-2$ degrees of freedom
- $STDEV_{A(p)}$ is the standard deviation of all A_i values without the estimated influence of Q_p

$STDEV_A$ is transformed into $STDEV_{A'(p)}$ by modifying A_i values that are affected by Q_p. Using parameter number 2239 from the example:

- $A_4 - \hat{Q}_{2239}$ will be used instead of A_4
- $A_4 - \hat{Q}_{2239}$ will be used instead of A_5
- etc

The estimated 95% confidence bounds are included in Table 4.1.2

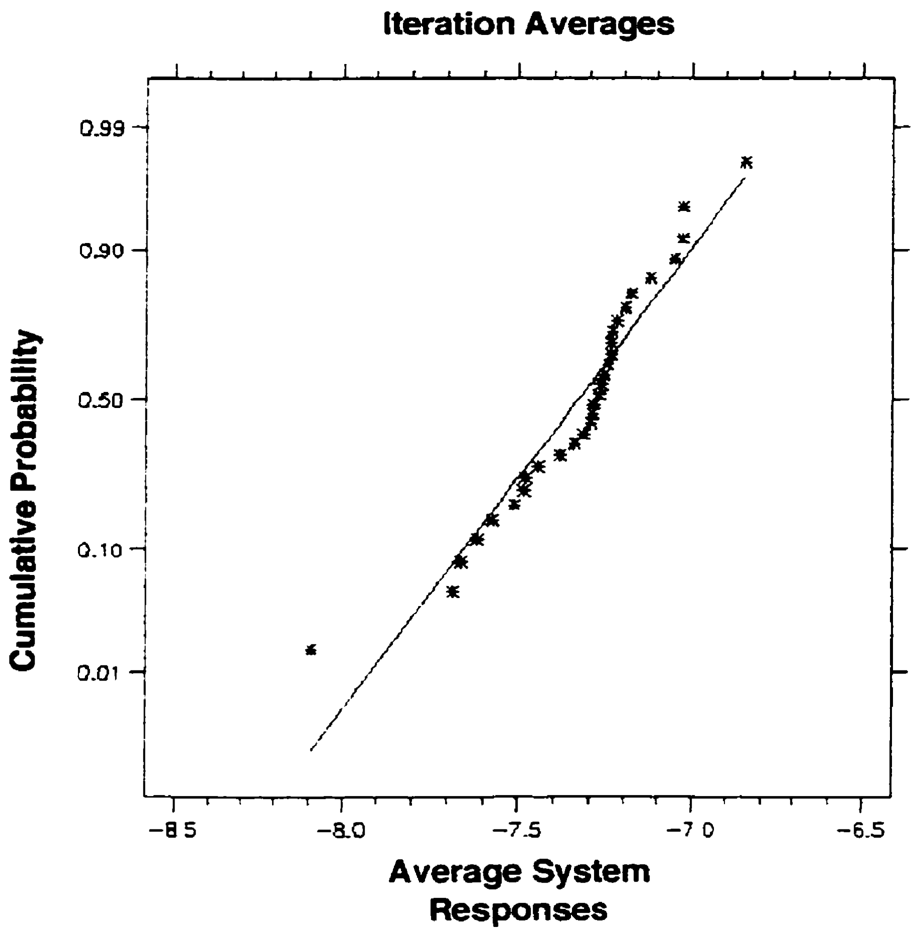

Figure 4.3.1: Distribution Of Average Responses From Iterations Of The Sub-Design.

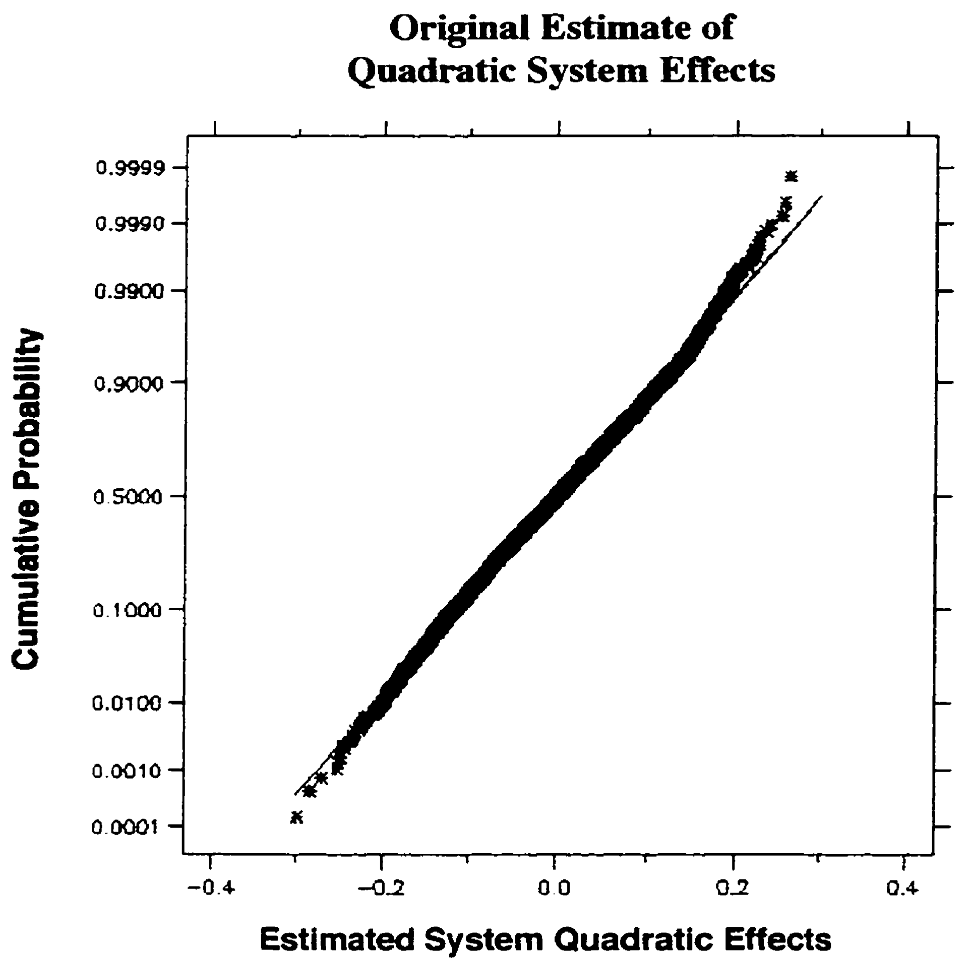

Figure 4.3.2: Distribution Of Estimated System Quadratic Effects.

p	$\hat{Q}_p$	$CLQ_1(\hat{Q}_p)$	$CLQ_2(\hat{Q}_p)$	$CBQ(\hat{Q}_p)$	Actual Effect
2796	0.199	0.959	0.000	0.232	no
1267	0.188	0.947	0.000	0.228	no
2673	0.186	0.944	0.000	0.227	no
2646	-0.181	0.938	0.000	0.225	no
768	-0.175	0.929	0.000	0.223	no
2239	0.151	0.883	0.000	0.216	yes
1592	0.148	0.877	0.000	0.215	no
2355	-0.148	0.876	0.000	0.215	yes
662	0.146	0.871	0.000	0.214	no
546	-0.142	0.860	0.000	0.213	no
1126	0.138	0.851	0.000	0.212	yes
405	-0.138	0.851	0.000	0.212	no
2803	0.131	0.828	0.000	0.210	yes
708	-0.131	0.828	0.000	0.210	no
1927	0.129	0.823	0.000	0.209	no
2108	0.128	0.820	0.000	0.209	no
2143	-0.118	0.785	0.000	0.207	no
935	-0.117	0.781	0.000	0.206	no
1987	-0.111	0.756	0.000	0.205	no
2857	0.108	0.743	0.000	0.204	no
772	0.108	0.741	0.000	0.204	no
104	0.104	0.726	0.000	0.203	yes
3278	-0.103	0.719	0.000	0.203	no
1024	0.098	0.696	0.000	0.202	no

Table 4.3.1: Estimated Quadratic Effects For SYVAC3-CC3 Parameters With The Largest Estimated Linear Effects (Not All Shown).

CHAPTER 5
Applying The Calculations To A Large System

Previous sections have discussed the calculations that are made as part of IFFDA. However, there are other issues that must be resolved for IFFDA to be applied to a large system such as SYVAC3-CC3.

- In what order should the system effects be removed from the estimable effects or the system averages so that the results can be refined?
- Which system effects should be reported?

The following assumptions are made to deal with these issues:

- The easiest system effects to detect are the main effects.
- Any parameter with a significant quadratic effect or involved in a significant interaction will also have a relatively large main effect.
- The error in estimating main effects, quadratic effects and interactions occur independently.

Under these assumptions it is still necessary to screen the system parameters to determine which ones may be important. As a result, some system effects will have to be subjected to the more restrictive tests of statistical significance, $CL_2(\hat{S})$ and $CLQ_2(\hat{Q})$. However, the screening will also provide the basis for identifying other system effects to test individually with the less restrictive tests of significance, $CL_1(\hat{S})$ and $CLQ_1(\hat{Q})$.

It is convenient to apply $CL_1(\hat{S})$ or $CLQ_1(\hat{Q})$ to sets of approximately one hundred estimated system effects. When a set of one hundred system effects are tested with $CL_1(\hat{S})$ or $CLQ_1(\hat{Q})$, approximately one of them will be assigned statistical significance (confidence coefficient greater than 99%) even though it isn't actually significant. If too many estimated effects are tested, then a large number of the effects will appear significant on a purely spurious basis. If too few effects are tested, then more significant effects will be missed because they were not tested.

5.1 A Purely Statistical Basis

The steps for the analysis of results of the experimental design can be summarized as follows:

1. Screen all the main effects (S_p) to determine which estimates are statistically significant (see Sections 3.1 and 3.3). The step-wise refinement of the results is applied as statistically significant estimates are identified.

2. Screen all the quadratic effects (Q_p) to determine if any estimates are statistically significant. (see Sections 3.2 and 3.4). The iteration averages are adjusted as statistically significant system estimates are identified.

3. Take the 100 system parameters with the largest main effects (significant or not) and test their quadratic effects individually. Record any $\hat{Q}_p$ values that are statistically significant when tested individually and adjust the experimental averages accordingly.

4. Select 15 system parameters to test for statistically significant second order interactions. These 15 parameters include:

   - the parameters with statistically significant main effects
   - the parameters with statistically significant quadratic effects
   - enough of the parameters with the largest non-significant main effects to bring the total number up to 15

   All 105 possible pairs of these system parameters are tested individually for statistical significance (Chapters 3 and 4). Adjust the estimable effects to acknowledge these significant effects.

5. Select 10 system parameters to test for statistically significant third order interactions. These 10 parameters include:

   - the parameters with statistically significant second order interactions
   - the parameters with statistically significant main effects
   - the parameters with statistically significant quadratic effects
   - enough of the parameters with the largest non-significant main effects to bring the total number up to 10

   All 120 possible third order interactions are tested individually for statistical significance. Adjust the estimable effects to acknowledge these significant effects.

6. Fourth, fifth,... etc interactions can be tested similarly if there are enough iterations that can be used to make the estimates.

7. The main effects should be re-scanned using the revised estimable effects. The revisions of the experimental effects may lead to more statistically significant effects. If such is the case then the rest of the analysis should also be repeated.

Table 5.1.1 shows the results of IFFDA using the above methodology. No expert knowledge of SYVAC3-CC3 is used. The confidence coefficient refers to $CL_1(\hat{S})$ or $CL_2(\hat{S})$ depending on whether the estimated effect was tested as part of a screening process or as a member of a relatively small group.

With the introduction of confidence coefficients, IFFDA can be applied on a purely statistical basis without any expert knowledge of the system.

5.2 Incorporating Expert Knowledge Of A System

Section 5.1 showed how IFFDA can be applied if expert knowledge of the system is not available. However, the results in the table are not entirely consistent with expert knowledge of SYVAC3-CC3.

In Table 5.1.1 there are two "false positives". Confidence coefficients of over 95% were calculated for interactions that are known to have no actual effect. This is understandable given that over 200 interactions were tested individually for statistical significance.

	p	Estimated Effect	Confidence Coefficient	Confidence Bound(±)	Actual Effect
Main Effects					
	2239	-1.725	1.000	0.334	yes
	2443	1.533	1.000	0.262	yes
	2355	0.655	0.951	0.247	yes
	2803	0.608	0.941	0.232	yes
Second Order Interactions					
	2355 2443	-0.669	1.000	0.286	yes
	104 2239	-0.337	0.980	0.272	yes
	973 2355	0.416	0.972	0.357	no
	104 2355	0.34	0.966	0.308	yes
Third Order Interactions					
	104 772 973	-0.607	0.964	0.606	no

Table 5.1.1: Results Of IFFDA If No Expert Knowledge Of SYVAC3-CC3 Is Available.

Also, in Table 4.2.2, $S_{2803}, S_{2826}, S_{2825}, S_{104}$ and S_{1126} could all possibly have actual linear effects(according to expert knowledge). Unfortunately, these estimates were tested as part of a screening process and the more restrictive test of significance, $CL_2(\hat{S})$, has to be used. These effects are not statistically significant under the appropriate test. To be pragmatic the user may wish to take advantage of expert knowledge and do any of the following:

- Include these parameters in the sets of interactions to test for statistical significance.
- Find some justification for testing these system effects individually for statistical significance.

- Do further analysis using more simulations to look specifically at these system effects.

- Increase the number of iterations of the sub-design and repeat IFFDA.

- Repeat the analysis with a different objective function.

The first option will be discussed here.

For SYVAC3-CC3, the influence of the majority (at least 2000) of the system parameters can be dismissed on the basis of expert knowledge. In such a situation, expert knowledge is very valuable. In fact, previous applications of IFFDA depended entirely on expert knowledge to guide the refinement of the results. For example:

> The estimated effects in Table 4.2.2 suggests that system parameter number 1461 has an influence on the estimated dose rate. However, according to expert knowledge of SYVAC3-CC3, this system parameter is assigned a constant value and cannot contribute to the variability of the dose estimate. On this basis, we have no confidence that parameter number 1461 has any sort of influence on the system response.
>
> Also, Table 4.2.2 suggests that one of the largest system effects is S_{2825}. Expert knowledge gives no simple reason why S_{2825} can't be important. In the previous applications of IFFDA, there confidence coefficients were not used and S_{2825} would warrant further analysis to determine its effect on the system.

The opportunity to incorporate expert knowledge comes in the choice of quadratic effects and interactions to test individually. Instead of just using the system parameters with the largest estimated main effects, we can be selective and give preference to those system parameters expected to have an influence on the system.

For example, when Table 4.2.2 is used to identify system parameters to check for second order interactions, the selection can be restricted to those marked "yes" in the Actual Effect column. This approach only gives eight parameters but the table could be extended to get more system parameters to test for second order interactions.

Table 5.2.1 shows the results if the estimated interactions associated with the eight parameters are tested for significance. Parameters 104, 1126, 2803 and 2826 are involved in statistically significant interactions. They can be considered important to the system even though there is no statistical reason for believing their main effects are significant.

However, we are still have not found any statistically significant estimate associated system parameter number 2825. With the amount of data that is used in the example (30 iterations of the sub-design), there is no statistically justifiable reason for saying that this system parameter has an influence on SYVAC3-CC3.

	p	Estimated Effect	Confidence Coefficient	Confidence Bound(±)	Actual Effect
Main Effects					
	2239	-1.725	1.000	0.334	yes
	2443	1.533	1.000	0.262	yes
	2355	0.655	0.951	0.247	yes
	2803	0.608	0.941	0.232	yes
	104	0.324	0.000	0.228	yes
	2826	-0.356	0.000	0.218	yes
	1126	0.314	0.000	0.214	yes
Second Order Interactions					
	2355 2443	-0.669	1.000	0.286	yes
	2239 2803	0.302	0.961	0.282	yes
	104 2239	-0.369	0.986	0.276	yes
	1126 2826	0.298	0.965	0.273	yes
Third Order Interactions					
	104 1126 2803	0.482	0.989	0.344	yes
	1126 2355 2826	-0.468	0.980	0.367	yes

Table 5.2.1: Results Of IFFDA When Expert Knowledge Of SYVAC3-CC3 Is Available.

CHAPTER 6
Conclusions

The ability to calculate confidence bounds and confidence coefficients for the results of IFFDA has been demonstrated. Sample calculations have been used to demonstrate this capability.

With confidence bounds and confidence coefficients, IFFDA can be applied without any expert knowledge of the system, but in the SYVAC3-CC3 example, IFFDA gives better results if expert knowledge of the system is incorporated into the analysis.

CHAPTER 7
Recommendations

Iterated Fractional Factorial Analysis (IFFDA) has already proven itself to be a powerful tool for the sensitivity analysis of computer models. This report illustrates how the introduction of confidence bounds and confidence coefficients enhance the value of IFFDA. Five further steps are possible to increase the effectiveness of IFFDA:

1. Investigate Variations On The Experimental Designs To Optimize Results.
2. Incorporate Better Statistical Methods To Estimate The Confidence Coefficients For The Estimated System Effects.
3. Investigate Using ANOVA To Screen The Main Effects and Interactions.
4. Investigate The Influence Of Aliased System Effects On the Estimated Quadratic Effects.
5. Incorporate The Analysis Stage Of IFFDA Into A Formal Software Package.

7.1 Investigate Variations On The Experimental Designs To Optimize Results

It is desirable to optimize the designs used in IFFDA to maximize the amount of information that can extracted from a given amount of data. Even for computer simulations, data can be expensive to generate. For a given number of simulations, the following features of the experimental designs are still adjustable:

- The definition of LOW, MEDIUM and HIGH for the system parameters.

- The choice of sub-designs
  - The sub-design in the sample calculations is a 2^{8-4} fractional factorial design. IFFDA could be generalized to accommodate any other sub-design.
  - The obvious sub-designs to consider are other two-level fractional factorial designs.

- The number of iterations of the sub-design.
  - If the sub-design is changed, the number of simulations per iteration will change and more or fewer iterations will be possible with the same total number of experiments.

7.2 Incorporate Better Statistical Methods To Estimate The Confidence Coefficients And Confidence Bounds

The statistical methods in this report use the assumption that the measurable effects and the iteration averages have an approximately Normal distribution. The approximation appears to be more valid for the estimable effects than the iteration averages (Figures 4.2.1 and 4.3.1). As a result, there is a concern that in future applications of IFFDA, the assumption of Normal distributions would not be suitable. In such a situation, some of the statistical methods used in this report would not be valid. Other statistical methods may have to be found.

For $CL_1(\hat{S})$, $CLQ_1(\hat{Q})$, $CB(\hat{S})$, and $CBQ(\hat{Q})$, a simple non-parametric is possible. A large number (thousands) of "pseudo system parameters" could be generated and assigned to experimental factors. Since the effects of these pseudo parameters would be zero, their estimated effects can be used to estimate the error which is likely to occur in the estimated effects of the actual system parameters. Confidence coefficients and confidence bounds could be generated.

Unfortunately, this approach would be impractical to replace $CL_2(\hat{S})$ and $CLQ_2(\hat{Q})$. Millions of the pseudo system parameters would be required.

7.3 Investigate Using ANOVA To Screen The Main Effects And Interactions

It may be possible to use one-way ANOVA to estimate main effects and interactions. It may also be possible to treat the iterations of the sub-design as experimental blocks. A block would represent an alias structure whereas in most experimental designs a block represents something physical (a plot of ground or a petri dish) or a period of time.

In order to revise results, responses of individual experiments would be adjusted instead of the measurable effects.

The major advantage of this approach would be that standard statistical methods could be used to analyze the results.

7.4 Investigate The Influence Of Aliased System Parameters On the Estimated Quadratic Effects

For the estimates of the quadratic effects, the iteration averages were adjusted with respect to the most significant estimated quadratic effects. However, the iterations are possibly influenced by interactions as well.

If a group of system parameters is aliased in an iteration, then their interaction will remain at a constant level instead of toggling between LOW and HIGH.

As a result, the average response for the iteration may be raised or lowered due to interactions between system parameters that are aliased together. Consequently, estimated quadratic effects will also be influenced.

This concern should be further investigated and if warranted, IFFDA should be modified to reduce the influence of interactions on the iteration averages and estimated quadratic effects.

7.5 Incorporate The Analysis Stage Of IFFDA Into A Formal Software Package

Computer software to generate the designs for IFFDA has been created. However, at this time, the development of software to perform the analysis part of IFFDA is still in a prototype phase.

When software is further developed to perform the analysis part of IFFDA, confidence coefficients and confidence bounds should be incorporated. Not only do these values put the results of IFFDA in better perspective, they also provide some objective guidance when the user is revising results to reduce error due to aliasing between system effects.

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Appendix

Glossary of Terms and Symbols

A_i

- the mean of the response for the ith iteration of the sub-design

$CB(\hat{S})$

- the confidence bounds for a main effect or interaction
- $\hat{S} \pm CB(\hat{S})$ forms the 95% confidence band

$CBQ(\hat{Q})$

- the confidence bound for $\hat{Q}$
- $\hat{Q} \pm CBQ_s(\hat{Q})$ forms the 95% confidence band

$CL_1(\hat{S})$

- the confidence coefficient for S if it is tested as an individual effect

$CL_2(\hat{S})$

- the confidence coefficient for $\hat{S}$ if it is tested as part of a screening of many effects

$CLQ_1(\hat{Q})$

- the confidence coefficient for Q if it is tested as an individual effect

$CLQ_2(\hat{Q})$

- the confidence coefficient for Q if it is tested as part of a screening of many effects

e, e1, e2,...

- indeces used to identify experimental effects

Ei,e

- effect of experimental factor e in iteration i of the sub-design

Ei,e1,e2 e3,...

- interaction of experimental factors e1, e2, e3,... in iteration i of the sub design

effects:

- the response of the system to a change in the value of a system parameter or an experimental factor
- in particular
  - if
    - x_i are parameters normalized to a range of [0,1]
    - y is the system response
    - $y \sim L_1 * x_1 + L_2 * x_2 + q * x_2 * x_2 + r * x_1 * x_2$
  - then
    - L_1, L_2 are main effects
    - $-.25 * q$ is a quadratic effect
    - $.5 * r$ is an interaction of order 2

estimable effect

- an effect that can be estimated from an experimental design
- typically, aliasing occurs in the design and the estimable effect represents a combination of many effects

experimental design

- a methodical way of setting parameter values in order to optimize the resulting information about the system
- in IFFDA, the experimental design consists of iterations of a sub-design

experimental factor

- a construct used in IFFDA
- level set according to a sub-design
- represents a different set of system parameters in each iteration of the sub-design
- its effects are assumed to be a sum of the effects of its member system parameters

i

- an index used to identify iterations of the sub-design

N_{test}

- the number of effects being tested for statistical significance

N_{nz}

- the number of iterations where a system parameter is included in the sub-design

Qp

- the quadratic effect of system parameter p

$\underline{p}$

- parameter number
- an index used to identify the system parameters

$\underline{S_p}$

- the linear effect of system parameter s

$\underline{STDEV_A}$

- the standard deviation of the Ai values

$\underline{STDEV_{E(odd/even)}}$

- the standard deviation of measured experimental effects that are aliased with odd/even ordered interactions

$\underline{STDEV_{E'(S)}}$

- the standard deviation of estimable effects without the contribution of S.

$\underline{STDEV_{A'(A)}}$

- the standard deviation of the iteration averages without the contribution of Q_p.

<u>sub-design</u>

- a relatively small and standard experimental design
- typically in IFFDA the sub-design is a 2^{8-4} fractional factorial design
- fractional factorial design

<u>system</u>

- the entity being analyzed
- in the sample calculations it is a mathematical or computer model but a system could be a manufacturing or a biological process

system parameter

- something in the system that can be controlled

IMAGE EVALUATION TEST TARGET (QA-3)

150mm

6"

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