Designing Response Surface Experiments for Factors with Symmetric Effects

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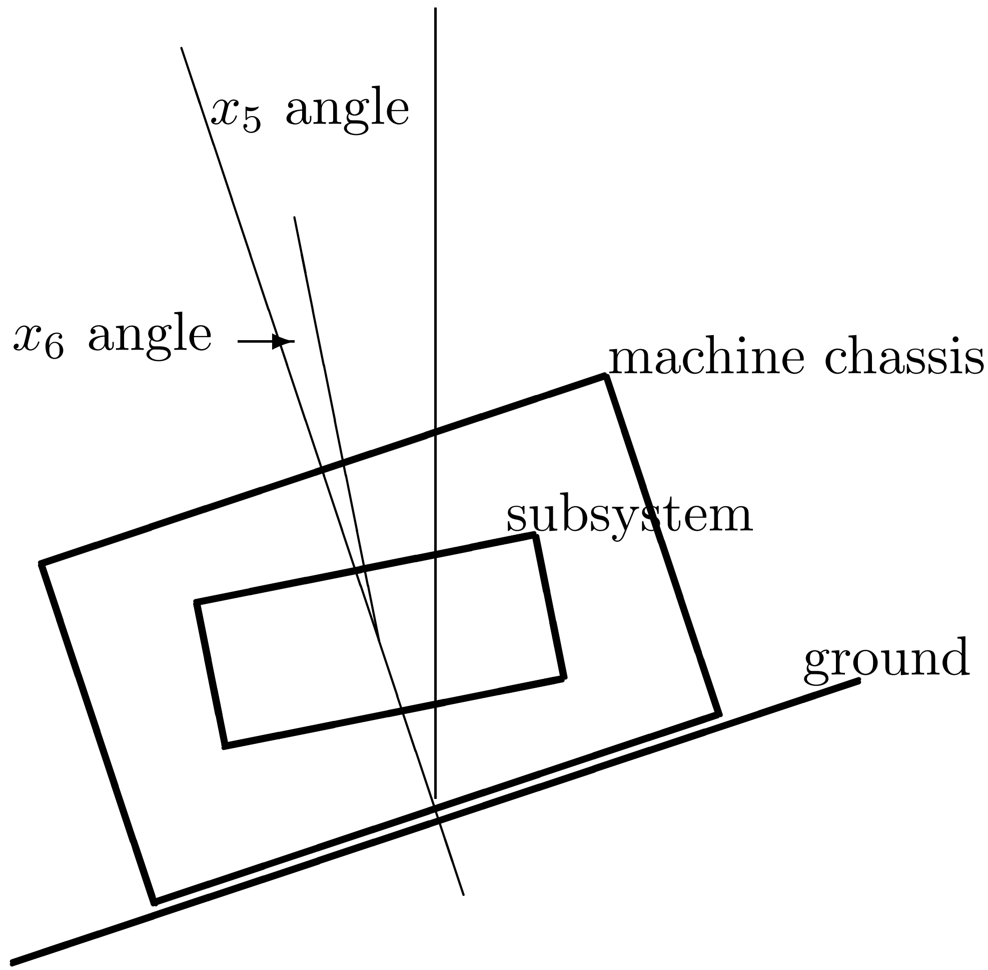
Motivating Problem: Experimentation related to the engineering design of commercial corn harvesting equipment.

- Investigation about how the efficiency of harvesting performance is influenced by six variables.
- Three of these can be described as “environmental” variables, the other three can be described as “control” variables.
- Eventual goal is to develop real-time control processes for control variables, to optimize performance for encountered values of environmental variables.

Experimental Variables and Values

Variable	Influence	Type	Domain
1	Environmental	-	positive real
2	Environmental	-	positive real
3	Control	-	positive real
4	Control	-	positive real
5	Environmental	angle	$[-\pi/2, \pi/2]$
6	Control	angle	$[-\pi/2, \pi/2]$



x_5 angle
x_6 angle
machine chassis
subsystem
ground

Pilot Experiment: Central Composite Design

($\frac{1}{2}$ fraction of 2^6 + 12 star/axial + 10 center points)

+1	+1	+1	+1	+1	+1	
-1	-1	+1	+1	+1	+1	
-1	+1	-1	+1	+1	+1	
...	...	...	...	...	...	
-1	-1	-1	-1	-1	-1	(32 runs)
+2	0	0	0	0	0	
-2	0	0	0	0	0	
0	+2	0	0	0	0	
...	...	...	...	...	...	(12 runs)
0	0	0	0	0	0	
...	...	...	...	...	...	(10 runs)

Note: Values for x_1 - x_4 are centered and scaled; values for x_5 and x_6 are scaled only (zero is “true” zero)

But:

- $(x_5, x_6) = (+,-)$ and $(-,+)$ don't make physical sense
  - angles are parameterized so that only pairs of the the same sign are operationally feasible
- Symmetry of system implies you only need one of (+,+), (-,-)
  - reversing the signs of both x_5 and x_6 simultaneously lead to a physically symmetric configuration, and the same expected response
- For the follow-up experiment, we wanted an asymmetric composite design that still puts most of the weight at the origin (in coded variables for x_1 - x_4, true zero for x_5 and x_6), and uses only the (+,+) quadrant for (x_5, x_6).
- Related: Lucas, J.M. (1974), "Optimum Composite Designs," *Technometrics* **4** pp 561-567

Template for Some Asymmetric Composite Designs

+1	+1	+1	+1	f	f	
-1	-1	+1	+1	f	f	
-1	+1	-1	+1	f	f	
...	...	...	...	...	...	
-1	-1	-1	-1	0	0	(32 runs)
0	0	0	0	a	a	
0	0	0	0	a	a	
+2	0	0	0	a	a	
-2	0	0	0	a	a	
0	+2	0	0	a	a	
...	...	...	...	...	...	
0	0	0	0	a	+2	
0	0	0	0	a	x	(14 runs)
0	0	0	0	c	c	
...	...	...	...	...	...	(8 runs)

Candidate Designs:

- 8 combinations of
  - $f = +1$ or $+2$
  - $a = 0$ (then x=1) or +1 (then x=0)
  - $c = 0$ or +1
- Denote by (f,a,c), e.g. "design 211"

Which is best? In this application (as in most), many issues – some statistical and some operational/engineering – are involved in this decision. Based on many of these, we used:

Design 210

One- and Two-Dimensional Projections

Projection for var 1:

1	16	18	16	1

Projection for var 5:

0	0	23	12	17

Projection for vars 1 2:

0	0	1	0	0
0	8	0	8	0
1	0	16	0	1
0	8	0	8	0
0	0	1	0	0

Projection for vars 1 5:

0	8	1	8	0
1	0	10	0	1
0	8	7	8	0
0	0	0	0	0
0	0	0	0	0

Projection for vars 5 6:

0	0	8	1	8
0	0	1	10	1
0	0	14	1	8
0	0	0	0	0
0	0	0	0	0

More Generally:

- The problem has other potential settings, including:
  - multiple sources of fluid flow, each $\leftarrow$ or $\rightarrow$, in a closed system
  - opposing magnetic fields, each $+$ or $-$, in a control setting
  - multiple heat pumps, each $\uparrow$ or $\downarrow$, in a common space
- Suppose we have $k = k_1 + k_2$ factors:
  - k_1 *asymmetric* factors, $A, B, C, \ldots$, or $\mathbf{x}_1$.
  - k_2 *symmetric* factors, $1, 2, 3, \ldots, k_2$, or $\mathbf{x}_2$.
- Extend the symmetry assumption to say that the expected response is not changed when *all* symmetric factors are multiplied by -1.

More about Symmetry:

- Full second-order model:

$$\eta(\mathbf{x}_1, \mathbf{x}_2) = \beta_0 + \sum_{i=1}^{k} x_i\beta_i + \sum_{i=1}^{k} x_i^2\beta_{ii} + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} x_ix_j\beta_{ij}$$

- System symmetry assumption implies:

$$\eta(\mathbf{x}_1, \mathbf{x}_2) = \eta(\mathbf{x}_1, -\mathbf{x}_2), \quad \text{all } \mathbf{x}$$

- Equivalently, for the second-order model:

$$\sum_{i=k_1+1}^{k} x_i\beta_i + \sum_{i=1}^{k_1}\sum_{j=k_1+1}^{k} x_ix_j\beta_{ij} = 0, \quad \text{all } \mathbf{x}$$

- Or, all β's in this equation = 0.
- (Data from the Pilot Study supported this in our application.)

- Parameters of the second-order model that are present under the symmetry assumption (s), and parameters that should be zero (z) under that assumption:

	-	1	2	...	k_1	k_1+1	k_1+2	...	k_1+k_2
-	β_0	**s**	**s**	...	**s**	z	z	...	z
1		**s**	**s**	...	**s**	z	z	...	z
2			**s**	...	**s**	z	z	...	z
...				....	...	...	...	...	...
k_1					**s**	z	z	...	z
k_1+1						**s**	**s**	...	**s**
k_1+2							**s**	...	**s**
...								...	**s**
k_1+k_2									**s**

- Consider designs for fitting the assumed model (**s**'s only), assuming that the assumption (z's = 0) has been validated in a pilot study.

- Central Composite Designs for the full quadratic model include:
  - Regular fractional factorial of Resolution $\geq$ V [$\leftarrow$]
  - $2k$ axial points
  - n_{cp} center points
- For the *assumed model*, the generating relation for a regular f.f. can contain:
  - words of length 5 or more, AND
  - shorter words including an odd number of symmetric factors
- Can shift projection of symmetric factors to one quadrant if desired

Examples: 2^{6-2} maximum resolution & minimum aberration

k_1	k_2	$I = \ldots$		
5	1	$ABCDE$	$AB1$	$CDE1$
4	2	$AB1$	$ACD2$	$BCD12$
3	3	$AB1$	$ABC23$	$C123$
2	4	$AB1$	$A234$	$B1234$
1	5	123	$A145$	$A2345$
0	6	123	456	123456

After selecting a composite design framework, can optimize factor levels:

- Partition the (standard notation) model matrix as

$$\mathbf{X} = (\mathbf{1}|\mathbf{X}_z|\mathbf{X}_s)$$

$$\tilde{\mathbf{X}}_z = \mathbf{X}_z(\mathbf{I} - \frac{1}{n}\mathbf{J}) \quad \tilde{\mathbf{X}}_s = \mathbf{X}_s(\mathbf{I} - \frac{1}{n}\mathbf{J}) \quad \tilde{\mathbf{X}} = (\tilde{\mathbf{X}}_z|\tilde{\mathbf{X}}_s)$$

- Think about reduced designs (above) that maximize:
  - $\phi_s = log|\tilde{\mathbf{X}}_s'\tilde{\mathbf{X}}_s|$ (fitting the assumed model)

  or full composite design that maximize:
  - $\phi_{sz} = log|\tilde{\mathbf{X}}'\tilde{\mathbf{X}}|$ (fitting the entire model)
  - $\phi_{z|s} = log|\tilde{\mathbf{X}}_z'(\mathbf{I} - \tilde{\mathbf{X}}_s(\tilde{\mathbf{X}}_s'\tilde{\mathbf{X}}_s)^{-1}\tilde{\mathbf{X}}_s)\tilde{\mathbf{X}}_z|$ (assumption test)

  and note that $\phi_{sz} = \phi_{z|s} + \phi_s$

Example (from original application)

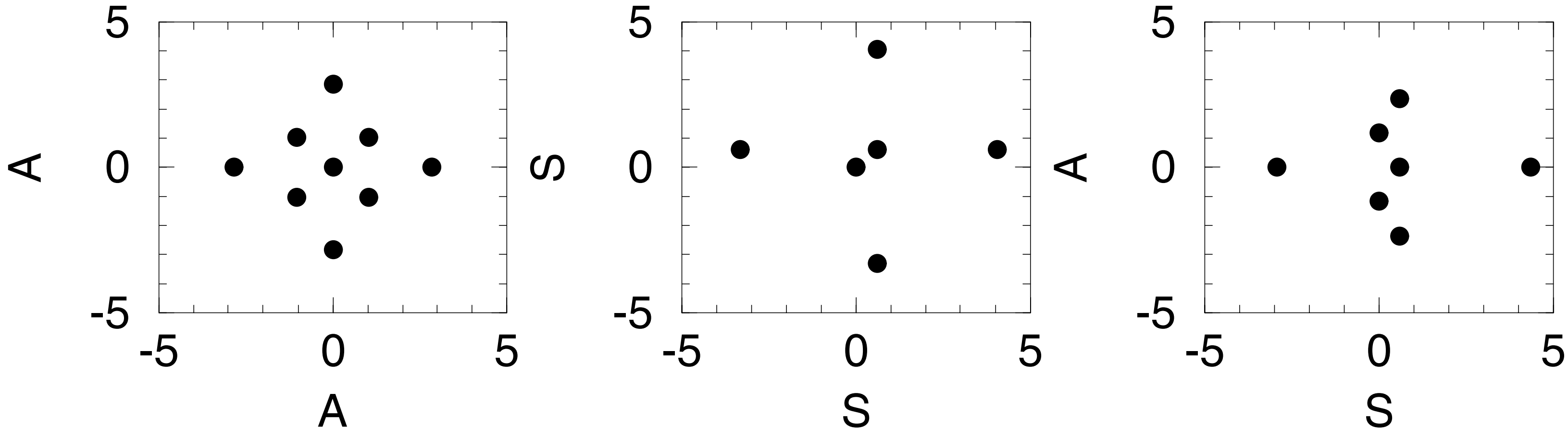
- $k_1 = 4, k_2 = 2$
- f.f.: $I = AB1 = ACD2(= BCD12)$, $n_{cp} = 5$
- optimize ϕ_s for the template:

	axial	factorial	center	factorial	axial
asymmetric factors	$-a$	$-f$	0	f	a
symmetric factors	a_L	f_L	c	f_H	a_H

subject to $\sum_{i=1}^{n} x_i^2 = n$ for each factor

↓ ↓ ↓

	axial	factorial	center	factorial	axial
asymmetric factors	-2.36	-1.17	0	1.17	2.36
symmetric factors	-2.92	0.00	0.60	0.00	4.36



5
0
-5
-5
0
5
A
A
S
S

Summary:

- Even in *empirical studies*, “system knowledge” is often available.
- Such knowledge can sometimes have important implications for *appropriate models*, and so ...
- ... it should also be considered in experimental design.
- *Joint effect symmetry*, like hierarchy, heredity, ..., is an example.