

Definitive Screening Designs

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Definitive Screening Designs

- A class of statistically designed experiments that may be used for both screening and optimization.
- Handle both quantitative and categorical factors.
- Quantitative factors are run at 3 levels, which allows the estimation of both linear and quadratic effects.
- First described by Bradley Jones and Christopher Nachtsheim in a 2011 article in the <u>Journal of</u> <u>Quality Technology</u>.



Properties

- The required number of runs is very small, usually between 1 and 3 more than twice the number of factors.
- 2. Main effects are independent of two-factor interactions.
- 3. Two-factor interactions are not perfectly confounded with other two-factor interactions, although they are correlated.
- 4. For continuous factors, all of the quadratic effects can be estimated.
- 5. Quadratic effects are orthogonal to linear main effects and only partially confounded with two-factor interactions.
- 6. For designs involving 6 through 12 factors, the full second-order model can be estimated for any 3 or less factors.



DOE Wizard

- The Statgraphics DOE Wizard provides DSDs for any combination of 4 to 16 factors.
- Both blocked and unblocked designs are available.



Example #1

- Optimization of a chemical reaction from <u>Statistics for</u> <u>Experimenters</u> by Box, Hunter and Hunter (2005).
- Response variable Y: percent reacted
- Experimental factors:
 - X1: feed rate
 - X2: amount of catalyst
 - X3: agitation rate
 - X4: temperature
 - X5: concentration



Step 1: Define Responses

Design of E	esign of Experiments Wizard - Define Responses X									
Design file	: <untitled></untitled>									
Comment:	Definitive screening desig	n for 5 factors								
Number of responses: 1 • Responses 1-16 Responses 17-32										
Response	Name	Units	Analyze		Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	reacted	%	Mean	-	Maximize 💌	0.5	3.0	Medium 💌	80	100
2	Var_2		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
3	Var_3		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
4	Var_4		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
5	Var_5		Mean	-	Maximize 💌	0.5	3.0	Medium 💌]	
6	Var_6		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
7	Var_7		Mean	-	Maximize 💌	0.5	3.0	Medium 💌	[
8	Var_8		Mean	-	Maximize 💌	0.5	3.0	Medium 💌]	
9	Var_9		Mean	-	Maximize 💌	0.5	3.0	Medium 💌	[
10	Var_10		Mean	-	Maximize 💌	0.5	3.0	Medium 💌]	
11	Var_11		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
12	Var_12		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
13	Var_13		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
14	Var_14		Mean	-	Maximize 💌	0.5	3.0	Medium 💌]	
15	Var_15		Mean	-	Maximize 💌	0.5	3.0	Medium 💌		
16	Var_16		Mean	Ŧ	Maximize 💌	0.5	3.0	Medium 💌		



Cancel

ΟK

Help

Step 2: Define Experimental Factors

Design of	Experiments Wizard -	Define Factors					×	
Design	Design file: dsd.sgx							
Comme	nt: Definitive screening (
Number	Number of controllable process factors: 5 🔄 Number of controllable mixture components: 0 📫 Number of noise factors: 0 📫							
Factor	Name	Units	Туре	Role	Low	High	Levels	
А	feed rate	liters/min	Continuous 💌	Controllable	10.0	15.0	10.0,15.0	
В	catalyst	%	Continuous 💌	Controllable	1.0	2.0	1.0,2.0	
С	agitation	rpm	Continuous 💌	Controllable	100.0	120.0	100.0,120.0	
D	temperature	degrees	Continuous 💌	Controllable	140.0	180.0	140.0,180.0	
Е	concentration	%	Continuous 💌	Controllable	3.0	6.0	3.0,6.0	
F	Factor_F		Continuous 💌		-1.0	1.0	1,2,3,4	
G	Factor_G		Continuous 💌		-1.0	1.0	1,2,3,4	
Н	Factor_H		Continuous 💌		-1.0	1.0	1,2,3,4	
I	Factor_I		Continuous 💌		-1.0	1.0	1,2,3,4	
J	Factor_J		Continuous 💌		-1.0	1.0	1,2,3,4	
К	Factor_K		Continuous 💌		-1.0	1.0	1,2,3,4	
L	Factor_L		Continuous 💌		-1.0	1.0	1,2,3,4	
М	Factor_M		Continuous 💌		-1.0	1.0	1,2,3,4	
Total	Total for controllable mixture components: 1.0 Factors A-M Factors N-Z							
	OK Back Cancel Help							



Step 3: Select Design

Design of Experiments Wizard - Select Design \times Design file: dsd.sgx Robust Parameter Design Combined array. Comment: Definitive screening design for 5 factors C Crossed array Runs Blocks Design Segment Factors Options... Process factors 5 0 0 Press the Options button. Mixture components 0 0 0 0 0 0 COMBINED 5 Designs for Continuous or Two-Level Factors Х BLOCK feed rate Design Class ature cncentration ۰ OK. liters/min ees % Screening Cancel C Response Surface Help O Multilevel Factorial Orthogonal Array. Computer Generated Ŧ • 0K Cancel Rerandomize Constraints Help



Step 3: Select Design (cont.)

omment: Del	initive scre	eening design	for 5 factors						C Combined a	irray av	
	Segme	ent	Factors	Runs	Blocks	Design					
Options	Proce:	ss factors	5	0	0	Press tł	ne Options butto	on.			
0.7	1	Screening D	esian Select	ion			•		×		
Uptions	Mixtu								~ ~		
Options	1	Name				Runs	Resolution	Error d.f.	Block Size		
		Factorial			2^5	32	V+	16	32 🔻		
	COM	Factorial			2^5	32	v+	16	32		
	DOK	Factorial	in 2 block		2^5	32	v+	15	16		1
	JUK	Factorial	in 4 block		2^5	32	V*	13	8	centration	
	_	Factorial	in 8 block		2^5	32	IV*	11	4	%	
		Factorial	in 16 blo	:ks	2^5	32	IV*	11	2		
		Half fract	tion		2^5-1	16	v	0	16		
		Irregular	fraction		2^5*3/8	12	~IV	1	12		
		Quarter f:	raction		2^5-2	8	III	0	8		
		Mixed leve	el fraction		3*2^4-1	24	~7	7	24		
		Mixed leve	-1 fraction	-	3*2^4-2	12	~TV	i	12		
		Half fract	tion in 21	locks	2^5-1	16	TV*	0	8		
		Definitiv	screenin	, design	201	12	TV	0	12		
		Blocked de	finitive	creenin	a desian	12	TV	0	7		
		Usersenec	ified desig	m	g ucsign	10			· · · · · · · · · · · · · · · · · · ·		
		☑ Display B	Blocked Desi	gns OK	Cancel		Back	Help			220.22
0											



Step 3: Select Design (cont.)

esign file: dsc	l.sgx					Robust Parameter Design	
mment: Defi	nitive screening design	for 5 factors				Combined array Constant array	
	Segment	Factors	Runs	Blocks	Design	* Clossed allay	
Options	Process factors	5	0	1	Definitive screening design		
Options Options	Mixture components	0 Defini	0 tive Screen	0 ing Design (Options	×	
BLC	COMBINED ICK feed ra liters/n	5 Cer Nun aite Nun 3 PI C C C	terpoints aber: acement Random Spaced First Last		Replicate Design Number: 0 Randomize	ure cncentration s %	
			OK		Cancel Help		



Step 3: Select Design (cont.)

Design of Experiments Wizard - Select Design Х Design file: dsd.sgx Robust Parameter Design Combined array. Comment: Definitive screening design for 5 factors C Crossed array. Segment Factors Runs Blocks Design Options... Process factors 5 16 Definitive screening design 1 Mixture components 0 0 0 0 0 0 Samples per run: 1 COMBINED 5 16 1 BLOCK feed rate catalyst. agitation temperature cncentration ۰ % % liters/min degrees rpm 1 1 15.0 1.0 100.0 180.0 4.5 1.0 180.0 6.0 2 1 10.0 110.0 15.0 1.0 120.0 140.0 6.0 3 1 4.5 1 10.0 2.0 120.0 140.0 4 12.5 5 1 1.0 100.0 140.0 3.0 12.5 2.0 120.0 180.0 6.0 6 1 12.5 1.5 4.5 7 1 110.0 160.0 1 12.5 1.5 110.0 160.0 4.5 8 9 1 10.0 1.5 100.0 140.0 6.0 15.0 1.5 120.0 3.0 10 1 180.0 1 12.5 1.5 110.0 160.0 4.5 11 12 1 12.5 1.5 110.0 160.0 4.5 13 1 10.0 1.0 120.0 160.0 3.0 14 1 10.0 2.0 100.0 180.0 3.0 1 15.0 2.0 6.0 15 100.0 160.0 15.0 2.0 110.0 140.0 3.0 16 1 ¥ 4 ► OK. Cancel Rerandomize Constraints Help



Step 4: Specify Model





Step 5: Select Runs

 Not required since the design already has the desired number of runs. This step is used for a computer generated design (such as a D-optimal design) when a subset of a large set of candidate runs needs to be selected.



Step 6: Evaluate Design

ANOVA Table

Source	D.F.
Model	10
Total Error	5
Lack-of-fit	2
Pure error	3
Total (corr.)	15



Model Coefficients

				Power at	Power at	Power at
Coefficient	Standard Error	VIF	Ri-Squared	SN = 0.5	SN = 1.0	SN = 2.0
constant	0.494152			7.01%	13.19%	37.52%
Α	0.316228	1.0	0.0	9.96%	25.18%	71.61%
В	0.316228	1.0	0.0	9.96%	25.18%	71.61%
С	0.316228	1.0	0.0	9.96%	25.18%	71.61%
D	0.316228	1.0	0.0	9.96%	25.18%	71.61%
E	0.316228	1.0	0.0	9.96%	25.18%	71.61%
AA	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
BB	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
CC	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
DD	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
EE	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%

alpha = 5.0%, sigma estimated from total error with 5 d.f.



Alias Matrix

Effect	AB	AC	AD	AE	BC	BD	BE	CD	CE	DE
constant	0.1163	-0.1163	0.1163	-0.1163	0.1163	-0.1163	0.1163	0.1163	-0.1163	0.1163
A										
В										
С										
D										
E										
AA	0.1628	-0.1628	0.1628	-0.1628	-0.8372	-1.1628	-0.8372	-0.8372	-1.1628	-0.8372
BB	0.1628	-1.1628	-0.8372	0.8372	0.1628	-0.1628	0.1628	-0.8372	0.8372	1.1628
CC	-0.8372	-0.1628	1.1628	0.8372	0.1628	0.8372	1.1628	0.1628	-0.1628	-0.8372
DD	-0.8372	0.8372	0.1628	-1.1628	1.1628	-0.1628	-0.8372	0.1628	0.8372	0.1628
EE	1.1628	0.8372	-0.8372	-0.1628	-0.8372	0.8372	0.1628	1.1628	-0.1628	0.1628



Correlation Matrix

	Α	В	С	D	E	AA	BB	CC	DD	EE
Α	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
В	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
С	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
D	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
E	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AA	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.4667	0.4667	0.4667	0.4667
BB	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	1.0000	0.4667	0.4667	0.4667
CC	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	1.0000	0.4667	0.4667
DD	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	0.4667	1.0000	0.4667
EE	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	0.4667	0.4667	1.0000











Step 7: Save Experiment





Step 8: Analyze Experiment

Design of Experiments Wizard	- Analyze Data		×
Response More	Transformation	Power	Addend
reacted	None	1.0	0
	None	1.0	0
OK	Cancel	H	Help



Pareto Chart of Effects

Standardized Pareto Chart for reacted



Collapse Design

Exclude Effects Options		\times
Include: B:catalyst BB BD BE D:temperature DD DE E:concentration EE	Exclude: A:feed rate AA AB AC AD AE BC C:agitation CC CD CE	
Ignore Block Numbers		
OK Can	cel Help	
	aphics®	



Main Effects Plot

Main Effects Plot for reacted







Interactions Plot



Interaction Plot for reacted







Mesh Plot





Step 9: Optimize Responses





Step 9: Optimize Responses (cont.)

Step 9: Optimize the responses

Response Values at Optimum

Response	Optimized	Prediction	Lower 95.0% Limit	Upper 95.0% Limit	Desirability
reacted	yes	100.484	96.4202	104.548	1.0

Factor Settings at Optimum

Factor	Setting
feed rate	11.1915
catalyst	1.99574
agitation	110.873
temperature	174.566
concentration	3.01764



Designs with Categorical Factors

- DSDs may also contain 2-level categorical factors.
- The next example shows a design with 4 continuous factors and 2 categorical factors.



Example #2

Comme	ent:							
Numbe	r of controllable proce	ss factors: 6	Number of controllable mix	ture components	: 0 •	Number of	noise factors: 0	
Factor	Name	Units	Туре	Role	Low	High	Levels	
А	Factor_A		Continuous 💌	Controllable	-1.0	1.0	1.2.3,4	
В	Factor_B		Continuous 💌	Controllable	-1.0	1.0	1,2,3,4	
С	Factor_C		Continuous 💌	Controllable	-1.0	1.0	1,2,3,4	
D	Factor_D		Continuous 💌	Controllable	-1.0	1.0	1.2.3.4	
Е	Factor_E		Categorical 💌	Controllable	-1.0	1.0	1,2	
F	Factor_F		Categorical 💌	Controllable	-1.0	1.0	1.2	
G	Factor_G		Continuous 💌		-1.0	1.0	1,2,3,4	
н	Factor_H		Continuous 💌		-1.0	1.0	1,2,3,4	
Ι	Factor_I		Continuous 💌		-1.0	1.0	1,2,3,4	
J	Factor_J		Continuous 💌		-1.0	1.0	1,2,3,4	
К	Factor_K		Continuous 💌		-1.0	1.0	1,2,3,4	
L	Factor_L		Continuous 💌		-1.0	1.0	1,2,3,4	
м	Factor_M	— í	Continuous 🔻		-1.0	1.0	1,2,3,4	
Tota	, I for controllable mixtu	re components: 1.0			, F	Factors A-M	Factors N-Z	



Example #2 (cont.)

Comment									Cor	mbined ar	rray	
	Com	ant	Epotoro	Duna	Plaaka	Design			C Cro	issed arra	iy	
	Seyna	Brit	Factors	nuns	DIUCKS	Design	-					
Uptions	Proce:	ss factors	6	U	U	Press th	ne Uptions butto	on.				
Options	Mixtu	Screening D	esign Select	ion						×		
Options		Name				Runs	Resolution	Error d.f.	Block	Size		
	COM	Definitiv	e screenin	g design		14	IV	0	14	-		
	COM	Factorial	in 8 bloc		2^6	64	V*	25	8			
		Factorial	in 16 bloc	-k =	2^6	64	TV*	31	4	<u>^</u>		_
BLC	ICK	Factorial	in 32 blo	ik s	2^6	64	IV*	26	2		actor_E	
	_	Half frac	tion		2^6-1	32	V+	10	32			
		Half frac	tion in 2)	locks	2^6-1	32	V*	9	16			
		Folded Pl	ackett-Burn	an	2^6*2/8	24	TV	17	24			
		Trrecular	fraction		2^6*2/8	24	a V	2	24			
		Our start of			205-20	16		-	16			
		Quarter 1	Particle		2 6-2	10	1.1	2	10			
		Flackett-	burman		2 6-3/16	12	111		12			
		Irregular	fraction		2~6*3/16	12	~1V	0	12			
		Eighth fr	action		2~6-3	8	111	0	8	_		
		Definitiv	e screenin	j design		14	IV	0	14			
		Blocked d	efinitive :	screenin	g design	16	IV	0	16			
		User-spec	ified desig	m						*		
		💌 Display B	Blocked Desi	gns								
									1			
				OK	Cancel		Back	Help				



Example #2 (cont.)

								mbined array ossed arrav	
	Segment	Factors	Runs	Blocks	Design				
Options	Process factors	6	14	1	Definiti	ve screening design			
Options	Mixture components	0	0	0					
Options		0	0	0					
	COMBINED	6	14	1	Sample	es per run: 1			
BLC	CK Factor_A	Fa	actor_B	Facto	or_C	Factor_D	Factor_E	Factor_F	
1 1	1.0	1.0		1.0		10	2	1	
2 1	-1.0	1.0		1.0		1.0	1	2	
2 1	1.0	0.0		1.0		1.0	1	1	
4 1	-1.0	-1.0		0.0		1.0	2	1	
5 1	0.0	0.0		0.0		0.0	2	2	
6 1	1.0	1.0		0.0		-1.0	1	2	
7 1	-1.0	0.0		-1.0		-1.0	2	2	
8 1	-1.0	1.0		1.0		-1.0	2	1	
9 1	0.0	0.0		0.0		0.0	1	1	
10 1	0.0	-1.0		-1.0		-1.0	1	1	
11 1	-1.0	-1.0		1.0		0.0	1	2	
12 1	1.0	1.0		-1.0		0.0	2	1	
13 1	1.0	-1.0		-1.0		1.0	1	2	
14 1	0.0	1.0		1.0		1.0	2	2	
1									



Designs with Blocking

- DSDs may be run in more than one block.
- The next example shows a design with 6 continuous factors divided into 2 blocks.



Example #3

esign file: <un omment:</un 	ititled>							_	Robust Par	rameter ined arr	Design ay	
,	Segme	ent	Factors	Runs	Blocks	Design			C Crosse	ed array		
Options	Proces	s factors	6	0	0	Press tł	e Options butto	on.				
Options	Mixtu	Screening D	esign Select	ion						×		
Options		Name				Runs	Resolution	Error d.f.	Block Si	ze		
	СОМ	Blocked d	efinitive	screenin	g design	13	IV	0	7	•		
		Factorial	in 8 bloc	ks	2^6	64	V*	35	8	^		
BLO	CK	Factorial	in 16 blo		216	64	10*	31 26	4		actor_E	-
		Half fract	tion		2^6-1	32	V+	10	32			
		Half frac	tion in 2	blocks	2^6-1	32	V*	9	16			
		Folded Pl	ackett-Bur	nan	2^6*3/8	24	IV	17	24			
		Irregular	fraction		2^6*3/8	24	~V	2	24			
		Quarter f:	raction		2^6-2	16	IV	2	16			
		Plackett-1	Burman		2^6*3/16	12	III	5	12			
		Irregular	fraction		2^6*3/16	12	~IV	0	12			
		Eighth fr	action		2^6-3	8	III	0	8			
		Definitiv	e screenin	g design		13	IV	0	13	_		
		Blocked d	efinitive	screenin	g design	13	IV	0	7			
		User-spec	ified desi	gn						~		
		🔽 Display B	Blocked Desi	gns OK	Cancel		Back	Help				
												►
	OK		Cano	el	Re	erandomize		Constraint	8		Help]
				A	0.000	1.1.1	Protect Constant					

Example #3 (cont.)

Design file:	ntitlada	2				Rahush Basaratas Davien
Comment:	naaea>					Combined array
	Segment	Factors	Runs	Blocks	Design	Clossed allay
Options	Process factors	6	0	0	Press the Options button.	
Options Options	Mixture components	0 Definit	0 ive Screenir	0 ng Design (Options	×
BLC	COMBINED	6 Cen A Num Pla C C C	terpoints ber: acement Random Spaced First Last	1	Replicate Design Number: 0 Randomize Number of blocks: 2	D Factor_E
4		-		J		
	ОК	Cano	el	Re	randomize	aints Help



Example #3 (cont.)

Commer	nt							mbined array	
Segment		Fact	ors Runs	Blocks	Design	Jsseu allay			
Optio	ons	Process factors		14	2	Blocked definitive screen	ing design		
Optic	ons			Ω	Ο				
0.4				-					
Uptic	ons		0	0	0				
	I	COMBINED	6	14	2	Samples per run: 1	_		
	BLOCK	Factor_/	4	Factor_B	Fac	tor_C Factor_D	Factor_E	Factor_F	
	-			1.0	1.0	1.0	1.0	0.0	
1	1	1.0		-1.0	1.0	-1.0	1.0	0.0	
2	<u>ו</u> ר	1.0		-1.0	-1.0	1.0	0.0	1.0	
3	1	0.0		1.0	-1.0	-10	1.0	-1.0	
4	2	-1.0		0.0	-1.0	-1.0	1.0	1.0	
6	2	0.0		0.0	0.0	0.0	0.0	0.0	
7	2	-1.0		-1.0	0.0	1.0	1.0	-1.0	
8	1	-1.0		1.0	-1.0	1.0	-1.0	0.0	
9	1	-1.0		1.0	1.0	-1.0	0.0	-1.0	
10	2	1.0		0.0	1.0	1.0	-1.0	-1.0	
11	2	-1.0		-1.0	1.0	0.0	-1.0	1.0	
	1	0.0		0.0	0.0	0.0	0.0	0.0	
12		1.0		1.0	0.0	-1.0	-1.0	1.0	
12 13	2					La co	11.0	11.0	



References

StatFolios and data files are at: <u>www.statgraphics.com/webinars</u>

Articles:

Box, G. E. P., Hunter, W. G. and Hunter, J. S. (2005). <u>Statistics for Experimenters: An</u> <u>Introduction to Design, Data Analysis, and Model Building, 2nd edition</u>. New York: John Wiley and Sons.

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