Introduction to Screening Designs

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Outline

- What is the experiment?
- Objectives of experimental problem
- Screning designs
- Placket-Burman designs
- DSD-based Screening designs
- Supersaturated designs (SSD)
- Thermostats experiment
- Pharmaceutical experiment and saturated designs
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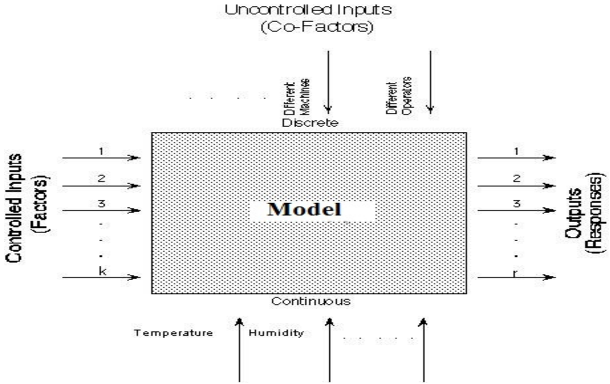
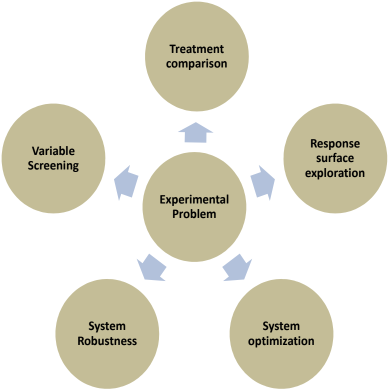
What is the experiment?



Steps for Experimental Design Selection?

1. Statement of the objective.
2. Input Factors: Type (Quantitative or Qualitative), levels , constraint.
3. Response: Value, limits.
4. Model: Which effects should be included? main effects, interaction effects, quadratic effects.
    - First-order model: $y = \beta_0 + \beta_1 x_1 + \cdots + \beta_m x_m + \epsilon$
    - Pure-quadratic model: $y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_i x_i^2 + \epsilon$
    - Second-order model: $$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij} x_i x_j + \sum_{i=1}^{m} \beta_i x_i^2 + \epsilon$$
5. Run selection: total number of runs, center point, replication, order of runs.
6. Choose the Design.

Objectives of experimental problem?



Experimental Problem

Treatment comparison

Response surface exploration

System optimization

System Robustness

Variable Screening

Screening design

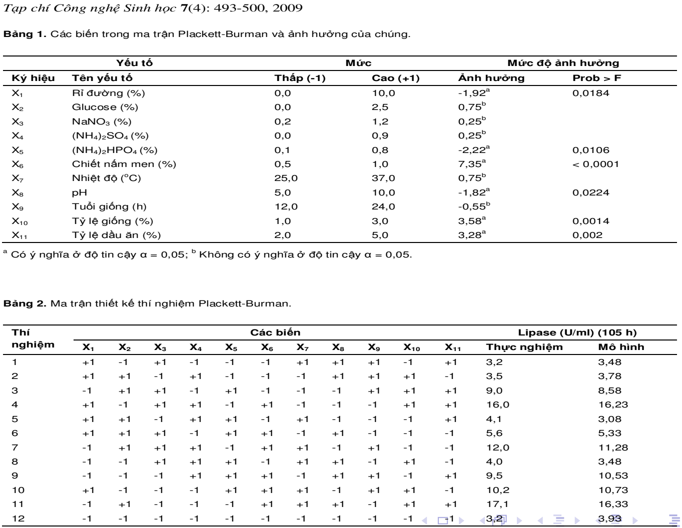
Screening designs are designs conducted at the primary stage of the experiment to screen out significant factors from a large number of factors for further studies. In some situations, the number of runs minus 1 is not greater than the number of factor, then the screening designs is referred as saturated or supersaturated designs. Popular screening designs are

- 2-level screening designs such as fractional factorial designs.
- Saturated designs:
    - 2-level saturated designs (Placket-Burman designs).
    - 3-level saturated designs (Nguyen & Pham(2017)).
- DSD-based screening designs:
    - 3-level DSDs (Jones and Nachtsheim, 2011; Xiao et al., 2012; Nguyen and Stylianou, 2013).
    - Mix-level Screening designs (Jones & Nachtsheim (2013), Yang et al. (2014), Nguyen & Pham (2016)).

Screening design

- Supersaturated designs (SSDs):
  - 2-level SSDs (Booth & Cox (1962), Lin (1993), Wu (1993), Nguyen (1996) and other authors (See Gilmour, 2005, Georgiou, 2014)).
  - 3-level Supersaturated Designs (Nguyen & Pham (2017)).
  - The mixed-level SSDs (Yamaha & Lin (1999), Yamaha et al. (1999), Fang et al. (2000) and other authors (See Georgiou, 2014)).

Placket-Burman design: Lipase experiment



Tạp chí Công nghệ Sinh học **7**(4): 493-500, 2009

Bảng 1. Các biến trong ma trận Plackett-Burman và ảnh hưởng của chúng.

Yếu tố		Mức		Mức độ ảnh hưởng	
Ký hiệu	**Tên yếu tố**	**Thấp (-1)**	**Cao (+1)**	**Ảnh hưởng**	**Prob > F**
X_1	Rỉ đường (%)	0,0	10,0	-1,92[a]	0,0184
X_2	Glucose (%)	0,0	2,5	0,75[b]	
X_3	$NaNO_3$ (%)	0,2	1,2	0,25[b]	
X_4	$(NH_4)_2SO_4$ (%)	0,0	0,9	0,25[b]	
X_5	$(NH_4)_2HPO_4$ (%)	0,1	0,8	-2,22[a]	0,0106
X_6	Chiết nấm men (%)	0,5	1,0	7,35[a]	< 0,0001
X_7	Nhiệt độ (°C)	25,0	37,0	0,75[b]	
X_8	pH	5,0	10,0	-1,82[a]	0,0224
X_9	Tuổi giống (h)	12,0	24,0	-0,55[b]	
X_{10}	Tỷ lệ giống (%)	1,0	3,0	3,58[a]	0,0014
X_{11}	Tỷ lệ dầu ăn (%)	2,0	5,0	3,28[a]	0,002

[a] Có ý nghĩa ở độ tin cậy α = 0,05; [b] Không có ý nghĩa ở độ tin cậy α = 0,05.

Bảng 2. Ma trận thiết kế thí nghiệm Plackett-Burman.

Thí nghiệm	Các biến											Lipase (U/ml) (105 h)	
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}	X_{11}	Thực nghiệm	Mô hình
1	+1	-1	+1	-1	-1	-1	+1	+1	+1	-1	+1	3,2	3,48
2	+1	+1	-1	+1	-1	-1	-1	+1	+1	+1	-1	3,5	3,78
3	-1	+1	+1	-1	+1	-1	-1	-1	+1	+1	+1	9,0	8,58
4	+1	-1	+1	+1	-1	+1	-1	-1	-1	+1	+1	16,0	16,23
5	+1	+1	-1	+1	+1	-1	+1	-1	-1	-1	+1	4,1	3,08
6	+1	+1	+1	-1	+1	+1	-1	+1	-1	-1	-1	5,6	5,33
7	-1	+1	+1	+1	-1	+1	+1	-1	+1	-1	-1	12,0	11,28
8	-1	-1	+1	+1	+1	-1	+1	+1	-1	+1	-1	4,0	3,48
9	-1	-1	-1	+1	+1	+1	-1	+1	+1	-1	+1	9,5	10,53
10	+1	-1	-1	-1	+1	+1	+1	-1	+1	+1	-1	10,2	10,73
11	-1	+1	-1	-1	-1	+1	+1	+1	-1	+1	+1	17,1	16,33
12	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	3,2	3,93

DSD-based screening designs: 3-level screening designs

Definitive Screening Designs (DSDs) for 3-level factors are used to found the important effects in the model

$$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \varepsilon = X\beta + \varepsilon \tag{1}$$

where β_i are main effects and β_{ii} are pure-quadratic effects.

- Jones & Nachtsheim (2011) introduced an general structure for DSDs as:

  $$\begin{pmatrix} \mathbf{C} \\ \mathbf{0} \\ -\mathbf{C} \end{pmatrix}, \tag{2}$$

  where $\mathbf{C}_{m\times m}$ is a $(0, \pm 1)$-matrix with zero diagonal.
- Stylianou (2011) and Xiao et al. (2012) point out that if m is even and we can use a *conference* matrix order m for $\mathbf{C}$ then the DSD is global optimum.
- Nguyen & Stylianou (2013) provide cyclic generators for the construction of $\mathbf{C}$ in (3) for both even and odd m.

DSD for 6 factors

0	1	1	1	1	1
1	0	-1	1	1	-1
1	-1	0	-1	1	1
1	1	-1	0	-1	1
1	1	1	-1	0	-1
1	-1	1	1	-1	0

0	0	0	0	0	0

0	-1	-1	-1	-1	-1
-1	0	1	-1	-1	1
-1	1	0	1	-1	-1
-1	-1	1	0	1	-1
-1	-1	-1	1	0	1
-1	1	-1	-1	1	0

DSD-based screening designs: Mix-level screening designs (MLSD)

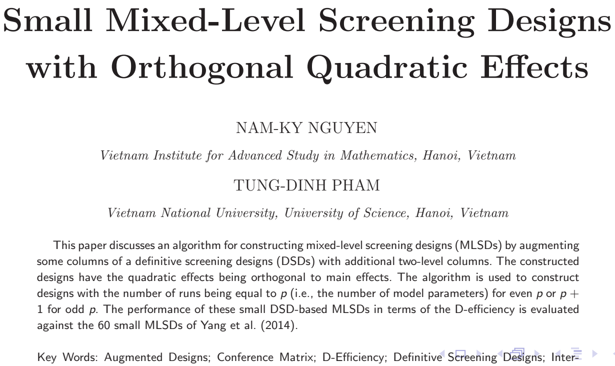
The following linear model for an MLSD with m_3 3-level factors and m_2 2-level factors or categorical factors in n runs:

$$y = \beta_0 + \sum_{i=1}^{m_3} \beta_{ii} x_i^2 + \sum_{i=1}^{m_3+m_2} \beta_i x_i + \varepsilon = X\beta + \varepsilon.$$

- Jones & Nachtsheim (2013) introduced DSD-augmented designs (ADSDs) and ORTH-augmented designs (OADs). They can be obtained by converting some columns of a DSD to 2-level ones. Note that the main effects of ADSDs are orthogonal to the quadratic effects. In this talk, we will denote the MLSDs whose the above property of ADSDs as MLSD*'s.
- Yang et al. (2014) introduced a new class of minimal-run MLSDs constructed from conference matrices and maximal determinant matrices (cf. `http://indiana.edu/~maxdet/`). YLL's MLSDs are small and are not MLSD*'s.

DSD-based screening designs: Mix-level screening designs (MLSD)

- Nguyen & Pham (2016) introduced the AUGMENT algorithm for constructing the small MLSDs* and improved an amount of YLL's designs.



Small Mixed-Level Screening Designs with Orthogonal Quadratic Effects

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This paper discusses an algorithm for constructing mixed-level screening designs (MLSDs) by augmenting some columns of a definitive screening designs (DSDs) with additional two-level columns. The constructed designs have the quadratic effects being orthogonal to main effects. The algorithm is used to construct designs with the number of runs being equal to p (i.e., the number of model parameters) for even p or $p+1$ for odd p. The performance of these small DSD-based MLSDs in terms of the D-efficiency is evaluated against the 60 small MLSDs of Yang et al. (2014).

Key Words: Augmented Designs; Conference Matrix; D-Efficiency; Definitive Screening Designs; Inter-

DSD-based screening designs: small MLSDs*

Idea: Augmenting 2-level factors to some columns of a DSD.

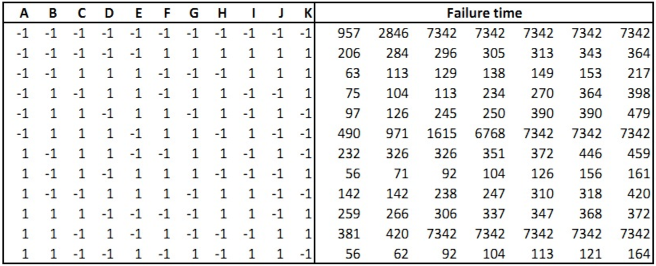
(1)	(2)	(3)	(4)
`++0+---`	`++0++--`	`++0+---`	`++0+--+`
`0-+-+++`	`0-+----`	`0-+----`	`0-+----`
`-++0---`	`-++0-++`	`-++0+++`	`-++0+++`
`+++-+++`	`+++--+-`	`+++--+-`	`+++--+-`
`+-++---`	`+-+++-+`	`+-+++-+`	`+-+++-+`
`-0+++++`	`-0++--+`	`-0++--+`	`-0++---`
`0000---`	`0000-++`	`0000-++`	`0000-++`
`--0-+++`	`--0-++-`	`--0-++-`	`--0-++-`
`0+-+---`	`0+-++++`	`0+-++++`	`0+-++++`
`+--0+++`	`+--0---`	`+--0---`	`+--0---`
`---+---`	`---+-+-`	`---+-+-`	`---+-+-`
`-+--+++`	`-+--+-+`	`-+--+-+`	`-+--+-+`
`+0-----`	`+0--+++`	`+0--+++`	`+0--+++`
`0000+++`	`0000+--`	`0000+--`	`0000+--`

Figure 1: Steps of AUGMENT to produce a DSD-based MLSD* for four 3-level factors and three 2-level factors in 14 runs.

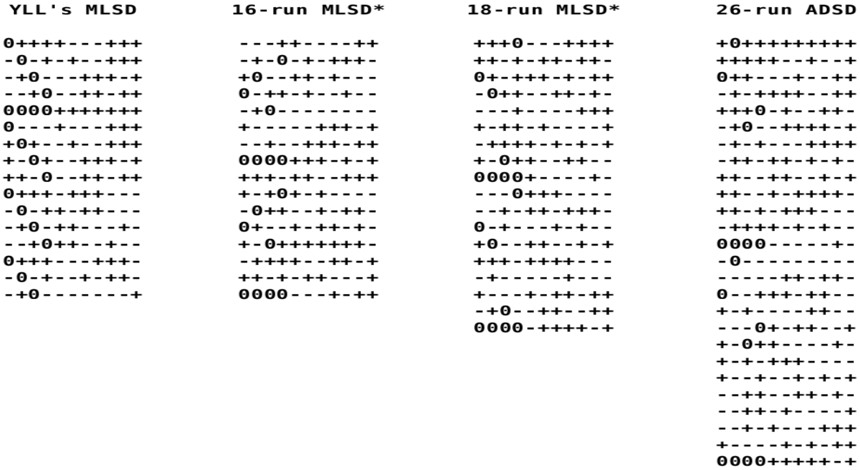
Thermostats experiment

Bullington et al. (1993) reported the use of a 12-run Plackett-Burman design in an experiment to improve the reliability of industrial thermostats. Ten thermostats were manufactured at each of the 12 factor settings and tested up to 7342 (x 1000) cycles. The failure time data are recorded in table and used for fitting the lognormal linear regression model.

Table 1: Lifetime data of Themorstats Experiment



A	B	C	D	E	F	G	H	I	J	K	Failure time						
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	957	2846	7342	7342	7342	7342	7342
-1	-1	-1	-1	-1	1	1	1	1	1	1	206	284	296	305	313	343	364
-1	-1	1	1	1	-1	-1	-1	1	1	1	63	113	129	138	149	153	217
-1	1	-1	1	1	-1	1	1	-1	-1	1	75	104	113	234	270	364	398
-1	1	1	-1	1	1	-1	1	-1	1	-1	97	126	245	250	390	390	479
-1	1	1	1	-1	1	1	-1	1	-1	-1	490	971	1615	6768	7342	7342	7342
1	-1	1	1	-1	-1	1	1	-1	1	-1	232	326	326	351	372	446	459
1	-1	1	-1	1	1	1	-1	-1	-1	1	56	71	92	104	126	156	161
1	-1	-1	1	1	1	-1	1	1	-1	-1	142	142	238	247	310	318	420
1	1	1	-1	-1	-1	-1	1	1	-1	1	259	266	306	337	347	368	372
1	1	-1	1	-1	1	-1	-1	-1	1	1	381	420	7342	7342	7342	7342	7342
1	1	-1	-1	1	-1	1	-1	1	1	-1	56	62	92	104	113	121	164



YLL's MLSD	16-run MLSD*	18-run MLSD*	26-run ADSD
0++++---+++	---++----++	+++0---++++	+0+++++++++
-0-+-+--+++	-+-0-+-+++-	++-+-++-++-	+++++--+--+
-+0---+++-+	+0--++-+---	0+-+++-+-++	0++---+--++
--+0--++-++	0-++-+--+--	-0++--++-+-	-+-++++--++
0000+++++++	-+0--------	---+----+++	+++0-+--++-
0---+---+++	+-----+++-+	+-++-+----+	-+0--++++-+
+0+--+--+++	--+--+++-++	-++++-+-+-+	-+-+---++++
+-0+--+++-+	0000+++-+-+	+-0++--++--	-++-++-+-+-
++-0--++-++	+++-++--+++	0000+----+-	++--++--+-+
0+++-+++---	+-+0+-+----	---0+++----	++--+-++++-
-0-++-++---	-0++--+-++-	--+-++-+++-	++-+-+++---
-+0-++---+-	0+--+-++-+-	0-+---+-+--	-++++-+-+--
--+0++--+--	+-0+++++++-	+0--++--+-+	0000-----+-
0+++---+++-	-++++--++-+	+++-++++---	-0---------
-0-+--+-++-	++-+-++---+	-+-----+---	-----++-++-
-+0-------+	0000---+-++	+---+-++-++	0--+++-++--
		-+0--++--++	+-+----++--
		0000-++++-+	---0+-++--+
			+-0++----+-
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			+--+--+-+-+
			--++--++-+-
			--++-+----+
			--+-+---+++
			+----+-+-++
			0000+++++-+

Figure 2: Four candidate MLSDs for the thermostats experiment described in Bullington et al. (1993).

Thermostats experiment : Summary of four MLSDs

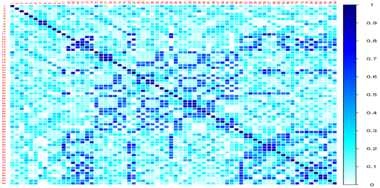
Table 2. Comparison of five candidate MLSDs for the thermostats exper
described in Bullington et al. (1993).

MLSDs	(d_1, d_2)	$r_{\max}$	$r'_{\max}$	v_Q	v_{M3}
YLL's MLSD	(77.9, 67.3)	0.75	0.76 (1)‡	0.803	0.167†
16-run MLSD*	(94.1, 88.6)	0.33	0.60 (3)	0.417†	0.139
18-run MLSD*	(99.1, 89.9)	0.36	0.29 (48)	0.414†	0.080
26-run ADSD	(105.7, 86.9)	0.41	0.00†(495)	0.408†	0.048
36-run OA	(100.0, 100.0)	0.00†	0.54 (3)	0.125†	0.042†

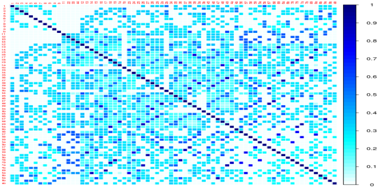
†Maximum value is the same as minimum value.

‡Frequencies.

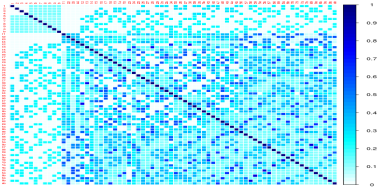
Thermostats experiment: Correlation Cell Plot For Four MLSDs



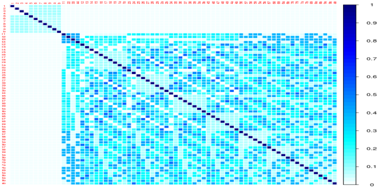
(a-YLL16)



(b-MLSD*16)



(c-MLSD*18)

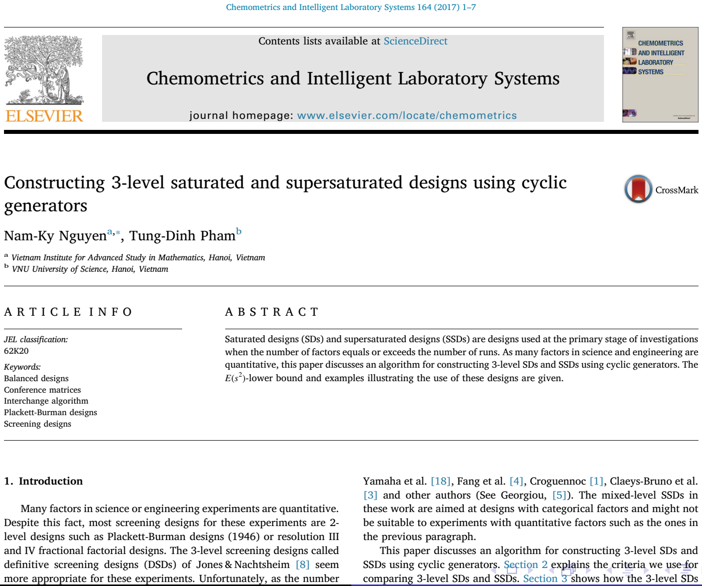


(d-ADSD26)

Pharmaceutical experiment

Phan (2006) described an experiment on robustness of a pharmaceutical experiment with 35 factors: (1) change of pyridine $\pm 5\%$, (2) addition temperature $\pm 3^0 C$, (3) reaction temperature $\pm 3\%$, (4) reaction time 90-15 min, (5) addition H_2O 120-140 min, (6) charge acetone $\pm 5\%$, etc. (35) drying $45 \pm 5^0 C$. Assume that the factors of both experiment are quantitative, Nguyen & Pham (2017) suggest an Es^2-optimal 3-level Saturated design for this experiment.

Saturated and Supersaturated designs



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Constructing 3-level saturated and supersaturated designs using cyclic generators

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ABSTRACT

Saturated designs (SDs) and supersaturated designs (SSDs) are designs used at the primary stage of investigations when the number of factors equals or exceeds the number of runs. As many factors in science and engineering are quantitative, this paper discusses an algorithm for constructing 3-level SDs and SSDs using cyclic generators. The $E(s^2)$-lower bound and examples illustrating the use of these designs are given.

1. Introduction

Many factors in science or engineering experiments are quantitative. Despite this fact, most screening designs for these experiments are 2-level designs such as Plackett-Burman designs (1946) or resolution III and IV fractional factorial designs. The 3-level screening designs called definitive screening designs (DSDs) of Jones & Nachtsheim [8] seem more appropriate for these experiments. Unfortunately, as the number

Yamaha et al. [18], Fang et al. [4], Croguennoc [1], Claeys-Bruno et al. [3] and other authors (See Georgiou, [5]). The mixed-level SSDs in these work are aimed at designs with categorical factors and might not be suitable to experiments with quantitative factors such as the ones in the previous paragraph.

This paper discusses an algorithm for constructing 3-level SDs and SSDs using cyclic generators. Section 2 explains the criteria we use for comparing 3-level SDs and SSDs. Section 3 shows how the 3-level SDs

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