Research

Reconciling mixture designs and factorial designs in order to identify best recipes in a holistic way

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Agrostat 2016

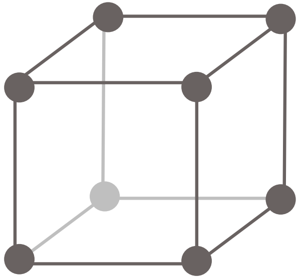
Process
- Soaking (short-long)
- Cooking (mild-strong)
- Drying (mild-strong)

Ingredients
- Sucrose (0-10%)
- Glucose (0-10%)
- Fructose (0-10%)

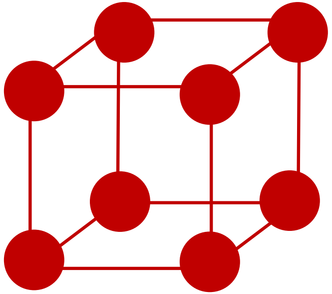
P x I

P & I

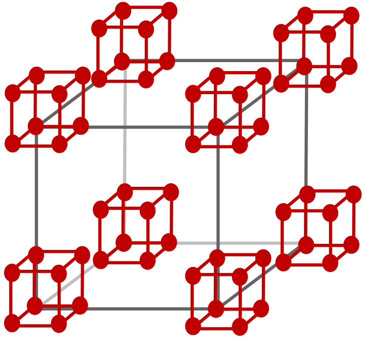
Full



2^3 = 8 experiments



2^3 = 8 experiments



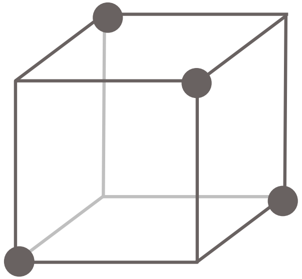
$2^3 \times 2^3 = 2^6$ = 64 experiments

Strength=2

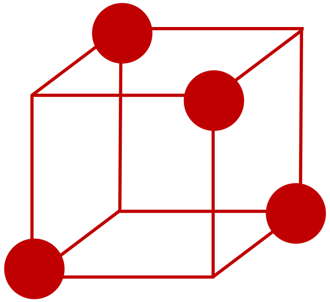
	A	B	C	AB	AC	ABC
E01	0	0	0	0	0	0
E02	0	0	1	0	1	1
E03	0	1	0	1	0	1
E04	0	1	1	1	1	0
E05	1	0	0	1	1	1
E06	1	0	1	1	0	0
E07	1	1	0	0	1	0
E08	1	1	1	0	0	1

Strength=3 Strength=3

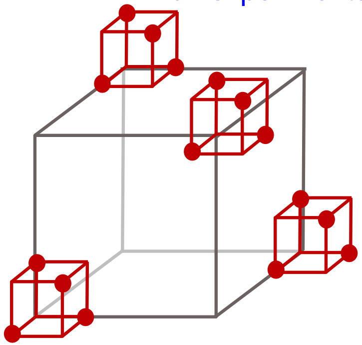
Fraction



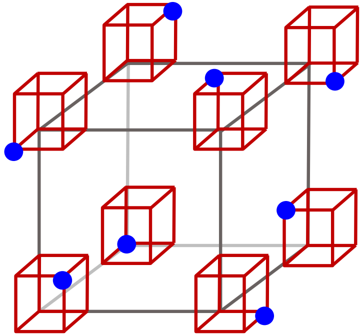
2^{3-1} = 4 experiments



2^{3-1} = 4 experiments



$2^{3-1} \times 2^{3-1} = 2^{6-2}$ = 16 experiments
(Barton, 1999)



2^{6-3} = 8 experiments
(Hedayat, Sloane, Stufken, 1999)

Nestlé Research

Process

- Soaking (short-long)
- Cooking (mild-strong)
- Drying (mild-strong)

Mixture

- Sucrose (0-10%)
- Glucose (0-10%)
- Fructose (0-10%)

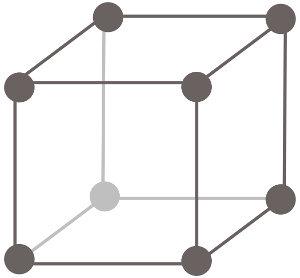
Sum = 10%

P x M

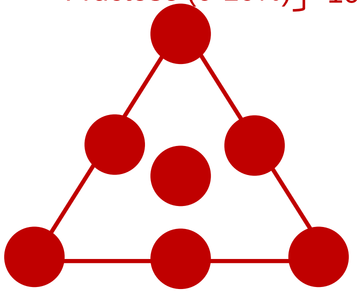
P & M

	A	B	C	AB'	AC'	ABC'
E01	0	0	0	3.3	3.3	3.3
E02	0	0	1	0	5	5
E03	0	1	0	5	0	5
E04	0	1	1	5	5	0
E05	1	0	0	3.3	3.3	3.3
E06	1	0	1	10	0	0
E07	1	1	0	0	10	0
E08	1	1	1	0	0	10

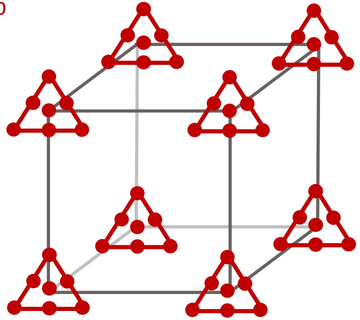
Full



2^3 = 8 experiments

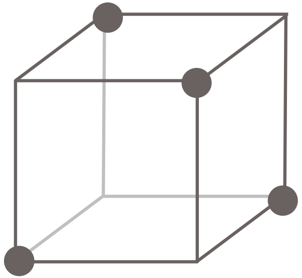


Simplex-Lattice {3,2,+2} = 8

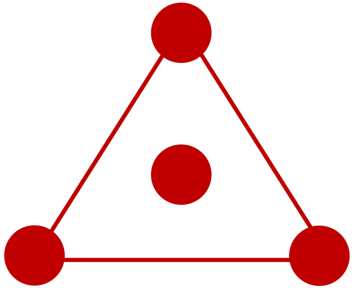


2^3 x SL {3,2,+2} = 64

Fraction

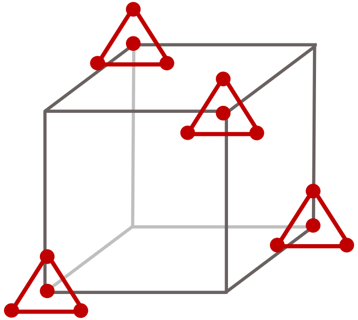


2^{3-1} = 4 experiments

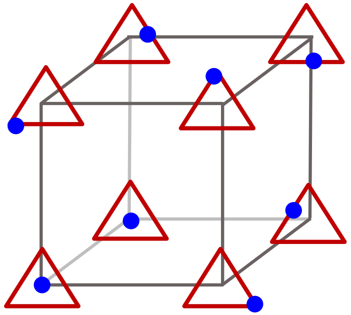


SL {3,1,+1} = 4

(Cornell, 2002)



2^{3-1} x SL {3,1,+1} = 16



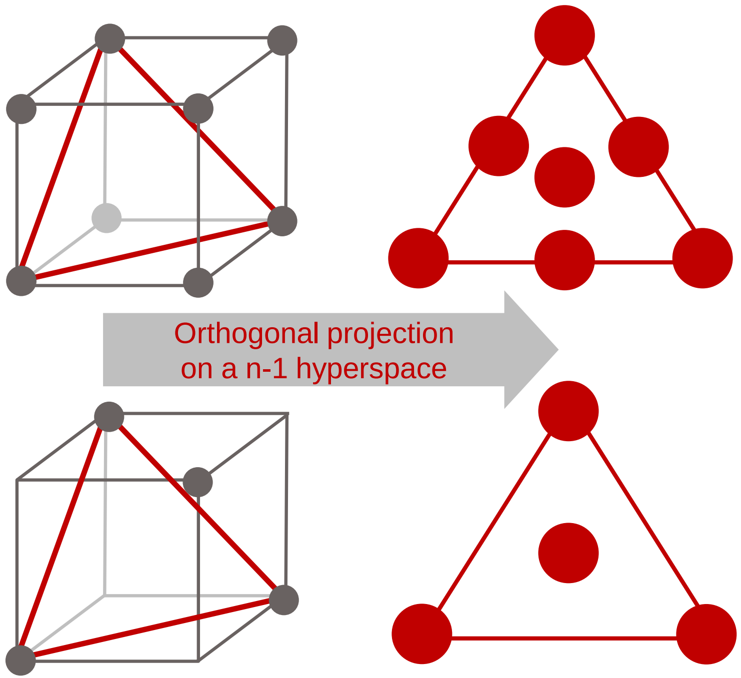
2^{6-3} = 8 experiments

Nestlé Research

Method for transforming an orthogonal array into a mixture

Full

Fraction



(Box, Hau, 2001)

	D_{Init}			$D_{Intermediate}$					D_{Final}		
	AB	AC	ABC	AB	AC	ABC	Sum	Vs. {SUM=10}	AB'	AC'	ABC'
E01	0	0	0	0	0	0	0	-10	3.3	3.3	3.3
E02	0	1	1	0	10	10	20	10	0	5	5
E03	1	0	1	10	0	10	20	10	5	0	5
E04	1	1	0	10	10	0	20	10	5	5	0
E05	1	1	1	10	10	10	30	20	3.3	3.3	3.3
E06	1	0	0	10	0	0	10	0	10	0	0
E07	0	1	0	0	10	0	10	0	0	10	0
E08	0	0	1	0	0	10	10	0	0	0	10

0	0	0	0
1	10	10	10

- Start with the initial orthogonal array D_{Init}. For each of the *n* experiments and each of the *q* ingredients, replace the low level by the lower bound a_i and the high level by the upper bound b_i, leading to an intermediate design $D_{Intermediate}$ with elements p_{ti} (t=1...n, i=1...q).
- In $D_{Intermediate}$, none or almost none of the mixtures sum to the constant *c*.
- Transform $D_{Intermediate}$ into D_{Final} by adjusting the mixtures according to their excess or lack vs. total amount *c*:
  - In case of a mixtures summing to less than *c*, let the lack of total amount be *w-*. Focus on the low level setting components p_{ti} of this mixture. One has to increase by *w-* the sum of the selected levels. In order to accomplish it, allocate a portion of *w-* to each of these levels proportionally to the range of variation of their respective components.
  - In case of a mixture t in excess of amount *w+*, the principle remains the same. In this situation, one has simply to select the high levels p_{ti} of the mixture. And then decrease the selected high levels proportionally to the range of variation of their respective components.

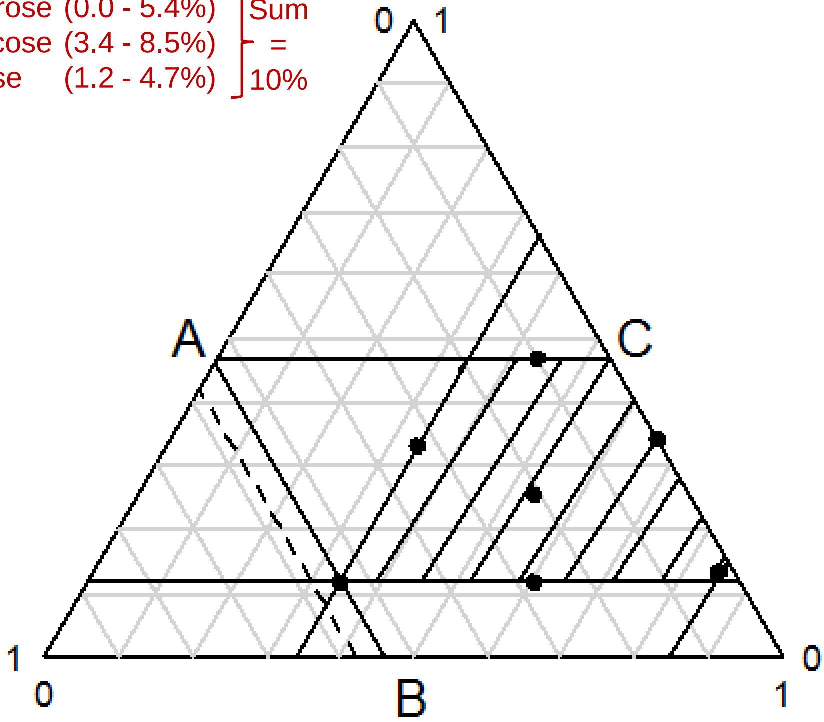
Nestlé Research

Method for transforming an orthogonal array into a constrained mixture

Mixture

- A=Sucrose (0.0 - 5.4%)
- B=Glucose (3.4 - 8.5%)
- Fructose (1.2 - 4.7%)

Sum = 10%



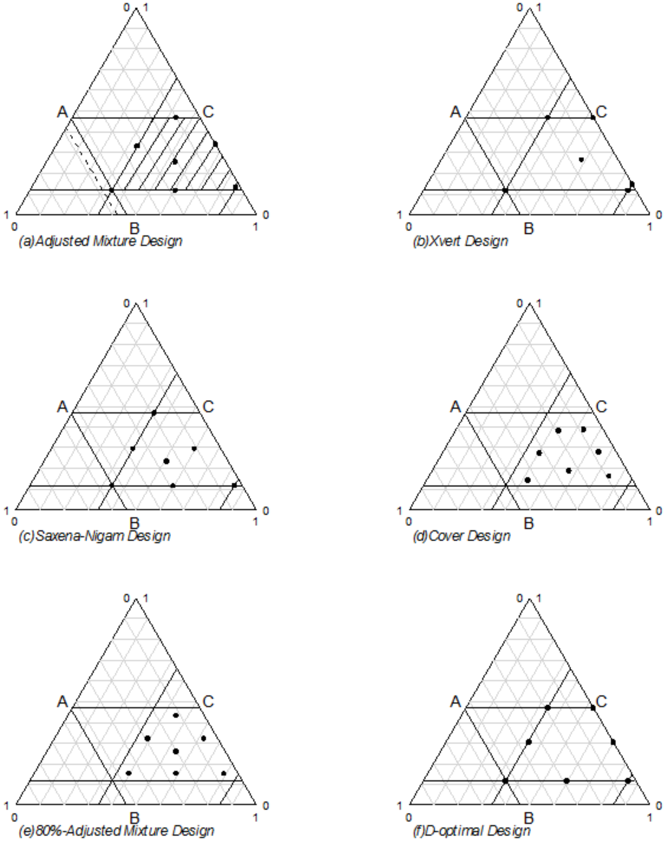
	D_{Init}			$D_{Intermediate}$					D_{Final}		
	AB	AC	ABC	AB	AC	ABC	Sum	Vs. {SUM=10}	AB'	AC'	ABC'
E01	0	0	0	0.0	3.4	1.2	4.6	-5.4	2.1	5.4	2.5
E02	0	1	1	0.0	8.5	4.7	13.2	3.2	0.0	6.6	3.4
E03	1	0	1	5.4	3.4	4.7	13.5	3.5	3.3	3.4	3.3
E04	1	1	0	5.4	8.5	1.2	15.1	5.1	2.8	6.0	1.2
E05	1	1	1	5.4	8.5	4.7	18.6	8.6	2.1	5.4	2.5
E06	1	0	0	5.4	3.4	1.2	10	0	5.4	3.4	1.2
E07	0	1	0	0.0	8.5	1.2	9.7	-0.3	0.2	8.5	1.3
E08	0	0	1	0.0	3.4	4.7	8.1	-1.9	1.0	4.3	4.7

0	0	3.4	1.2
1	5.4	8.5	4.7

The method works for

- Any type of constraints
- Multiple mixtures
- Nested mixtures

This method is a consensus between established methods



	D-efficiency (2nd order)	Coverage Index
(a) Adjusted Mixture	0.513	0.579
(b) Extreme Vertices	0.070	0.300
(c) Saxena-Nigam	0.215	0.588
(d) Space-Filling	0.001	1.000
(e) Adjusted Mixture (80%)	0.008	0.944
(f) D-optimal (2nd order)	1.000	0.435

The proposed design reaches best consensus between

- D-efficiency (Atkinson, 1992)
- Coverage (Johnson, 1990)

In this case, it is the only technique yielding values higher than 0.5 for both indexes.

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This method allows handling complex problems very easily

Phase 1 (2^{7-4} → 8 experiments)

- Main effects of 4 orthogonal factors (partial replacement of wheat by up to 3 alternative grains + humectant type)
- First order model of 3 mixture factors (Mixture of 3 sugars summing to 10%)

Phase 2 (2^{9-5} → 16 experiments)

- R=V for 4 process factors (humectant, soaking, cooking, drying)
- First order model of 5 mixture factors (Mixture of 5 alternative grains summing to 15%)

	D_{Init} A	B	C	AB	AC	BC	ABC	$D_{Intermediate}$ A	B	C	vs. c	D_{Final} A Sugar A	B Sugar B	C Sugar C	AB Grain 1	AC Grain 2	BC Grain 3	ABC humect.
C1	0	0	0	0	0	0	0	0.0	3.4	1.2	-5.4	2.1	5.4	2.5	0	0	0	W
C2	1	0	0	1	1	0	1	5.4	3.4	1.2	0.0	5.4	3.4	1.2	2	2	0	W+
C3	0	1	0	1	0	1	1	0.0	8.5	1.2	-0.3	0.2	8.5	1.3	2	0	2	W+
C4	1	1	0	0	1	1	0	5.4	8.5	1.2	5.1	2.8	6.0	1.2	0	2	2	W
C5	0	0	1	0	1	1	1	0.0	3.4	4.7	-1.9	1.0	4.3	4.7	0	2	2	W+
C6	1	0	1	1	0	1	0	5.4	3.4	4.7	3.5	3.3	3.4	3.3	2	0	2	W
C7	0	1	1	1	1	0	0	0.0	8.5	4.7	3.2	0.0	6.6	3.4	2	2	0	W
C8	1	1	1	0	0	0	1	5.4	8.5	4.7	8.6	2.1	5.4	2.5	0	0	0	W+

(Illmann, 2009)

	A Humect.	B Soaking duration	C Cooking condition	D Drying condition	ABC Grain1	ABD Grain2	ACD Grain3	BCD Grain4	ABCD Grain5	∑Grains
P01	W	short	mild	mild	2.0	2.0	3.0	0.0	8.0	15.0
P02	W	short	mild	strong	2.0	5.8	6.3	0.9	0.0	15.0
P03	W	short	strong	mild	4.0	2.0	7.7	1.3	0.0	15.0
P04	W	short	strong	strong	3.3	5.4	3.0	0.0	3.4	15.0
P05	W	long	mild	mild	3.8	6.9	3.0	1.2	0.0	15.0
P06	W	long	mild	strong	3.3	2.0	6.1	0.0	3.6	15.0
P07	W	long	strong	mild	2.0	4.8	5.4	0.0	2.8	15.0
P08	W	long	strong	strong	2.7	3.8	4.6	2.0	1.8	15.0
P09	W+	short	mild	mild	3.3	5.6	6.1	0.0	0.0	15.0
P10	W+	short	mild	strong	3.8	2.0	3.0	1.2	4.9	15.0
P11	W+	short	strong	mild	2.0	5.6	3.0	0.9	3.6	15.0
P12	W+	short	strong	strong	2.1	2.4	10.0	0.1	0.4	15.0
P13	W+	long	mild	mild	2.0	2.0	6.3	0.9	3.8	15.0
P14	W+	long	mild	strong	2.0	10.0	3.0	0.0	0.0	15.0
P15	W+	long	strong	mild	5.0	3.6	4.4	0.4	1.6	15.0
P16	W+	long	strong	strong	2.9	4.3	5.0	0.6	2.3	15.0

(Addelman, 1962)

Phase 1 (2^{7-4} → 8 experiments)

- Initial product ~ 80% Wheat + 20% sucrose
- Perceived sweetness is a key liking driver
- Idea : generate biscuit flavor (congruent with perceived sweetness) through Maillard to reduce sugars

→ Identify best combination

Processing (AA from grains + Sugars + Humectant)

Phase 2 (2^{9-5} → 16 experiments)

- On top of grains necessary for AA, include grains with additional nutritional benefits
- Fine-tune process conditions

→ New product

~ 75% Wheat + 15% grains + 10% sugars

→ Nutritionally balanced & more liked

Nestlé Research

Reconciling mixture designs and factorial designs in order to identify best recipes in a holistic way

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