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

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

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

**$2^3 = 8$ experiments**

**$2^3 x 2^3 = 2^6 = 64$ experiments**

**$2^{3-1} = 4$ experiments**

**$2^{3-1} x 2^{3-1} = 2^{6-2} = 16$ experiments**

**$2^{6-3} = 8$ experiments**

(Hedayat, Sloane, Stufken, 1999)
**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**
- $2^3 = 8$ experiments
- $2^3 \times SL\{3,2,+2\} = 64$
- $2^3 - 1 = 4$ experiments
- $2^3 - 1 \times SL\{3,1,+1\} = 16$
- $2^6 - 3 = 8$ experiments

**Full**
- $2^3 = 8$ experiments

**Fraction**
- $2^3 - 1 = 4$ experiments

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**P & M**

<table>
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<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>AB'</th>
<th>AC'</th>
<th>ABC'</th>
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(Cornell, 2002)
Method for transforming an orthogonal array into a mixture

- Start with the initial orthogonal array $D_{\text{Init}}$. 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 $D_{\text{Intermediate}}$ with elements $p_{ti}$ ($t = 1...n, i = 1...q$).
- In $D_{\text{Intermediate}}$, none or almost none of the mixtures sum to the constant $c$.
- Transform $D_{\text{Intermediate}}$ into $D_{\text{Final}}$ 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 this mixture. And then decrease the selected high levels proportionally to the range of variation of their respective components.

(Box, Hau, 2001)
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%)

\[ \text{Sum} = 10\% \]

The method works for
- Any type of constraints
- Multiple mixtures
- Nested mixtures

The table shows the transformation process with initial, intermediate, and final mixtures.

The diagram visually represents the transformation process.
This method is a consensus between established methods

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.

<table>
<thead>
<tr>
<th>D-efficiency (2nd order)</th>
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<td>(a) Adjusted Mixture</td>
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<td>(b) Extreme Vertices</td>
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<td>(c) Saxena-Nigam</td>
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<td>(d) Space-Filling</td>
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This method allows handling complex problems very easily

Phase 1 (27-4 → 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 (29-5 → 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%)
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