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Bayesian D- and I-optimal designs for choice experiments involving mixtures and process variables

Mario Becerra
with Peter Goos

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Model-Oriented Data Analysis and Optimum Design
Southampton, England

Outline

1. Choice modeling and choice experiments
2. Mixture experiments
3. Combining choice models and mixture models
4. Optimality criteria for choice experiments
5. Examples

Choice modeling and choice experiments

Discrete choice experiments

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- Quantify consumer preferences

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- Quantify consumer preferences
- Preference data is collected
- Respondents are presented sets of alternatives (choice sets) and asked to choose
  - Example: choosing to buy product A, B or C
- Latent utility function → probability of making each decision

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Mixture experiments

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    - types of fish used to make a fish patty



Mixtures

- Many products and services can be described as mixtures of ingredients
- Examples:
  - ingredients of bread
  - ingredients used to make a cocktail
  - types of fish used to make a fish patty
  - primary colors to make new colors




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Mixtures

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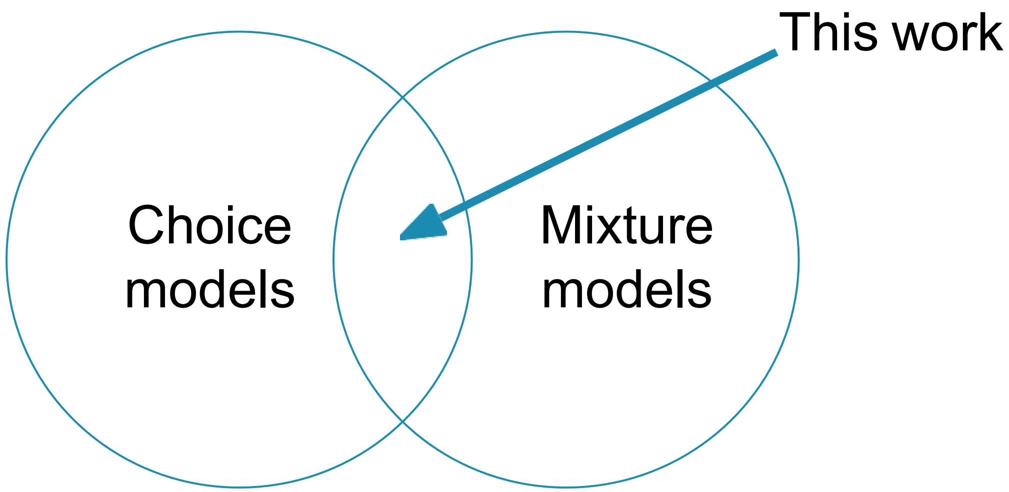
Mixtures

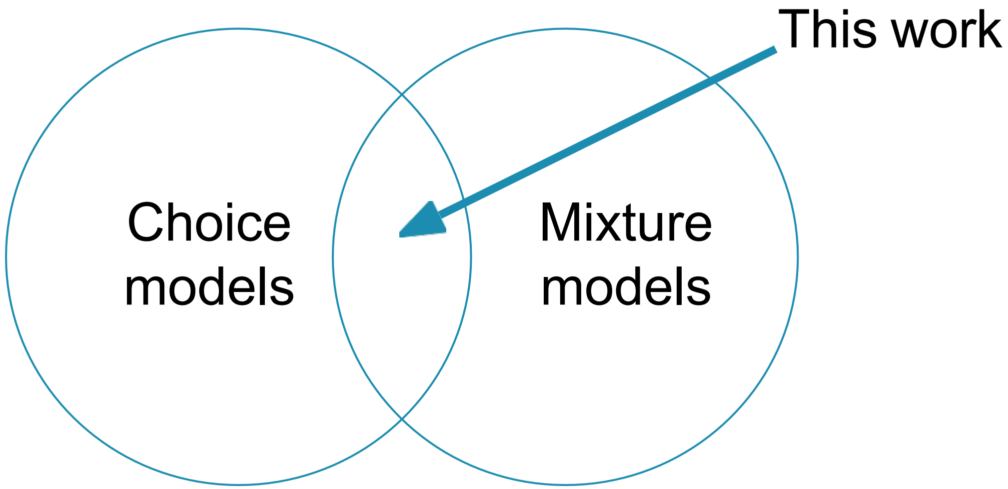
- In mixture experiments, products are expressed as combinations of **proportions** of ingredients
- The researchers' interest is generally in one or more characteristics of the mixture
- In this work, the characteristic of interest is the **preference** of respondents
- Choice experiments are ideal to collect data for quantifying and modeling preferences for mixtures

Combining choice models and mixture models

Choice experiments with mixtures



Choice experiments with mixtures



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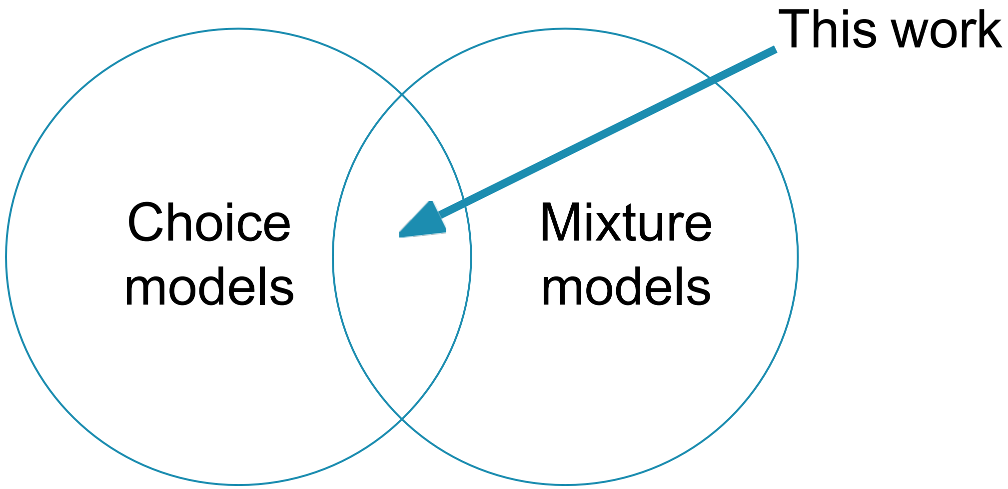

- First example by Courcoux and Séménou (1997), preferences for cocktails
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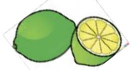
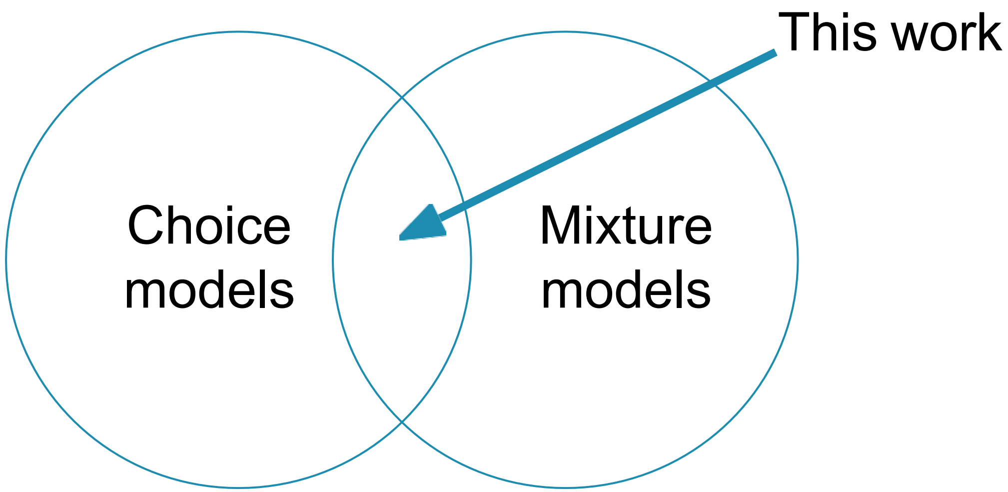
  - lemon juice 
  - blackcurrant syrup 

Choice experiments with mixtures



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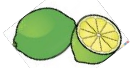
  - lemon juice 
  - blackcurrant syrup 
- 60 people, each making 8 pairwise comparisons

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Designing choice experiments with mixtures

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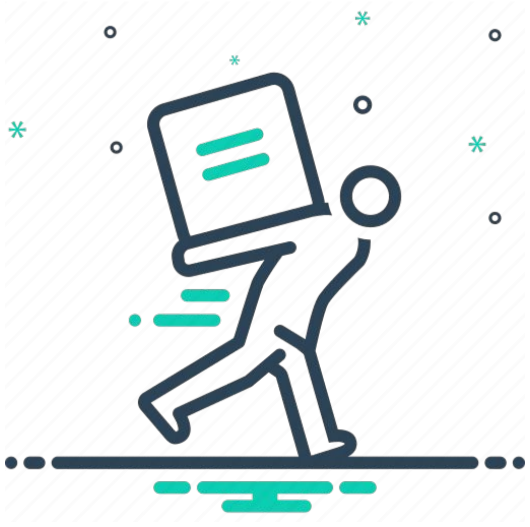

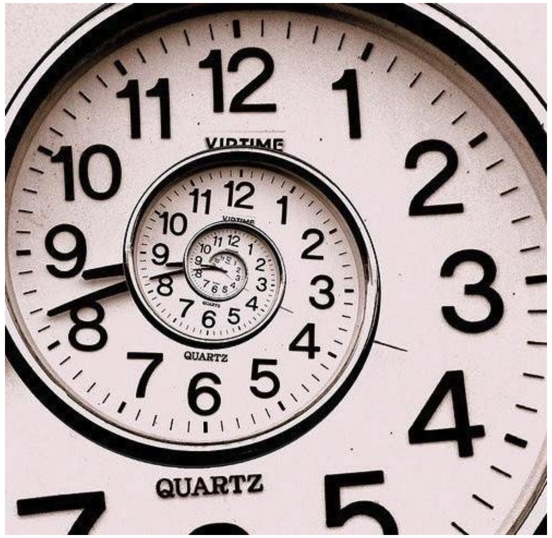

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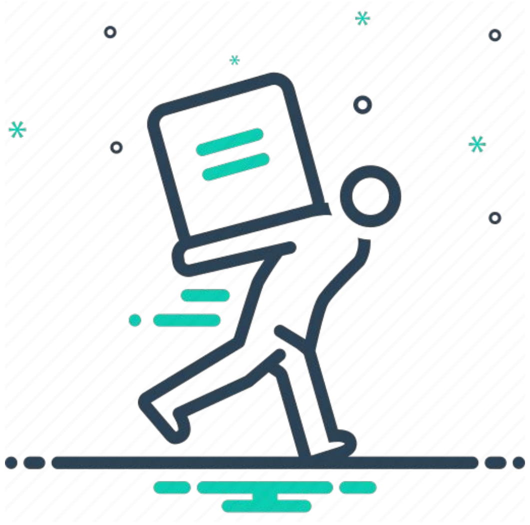
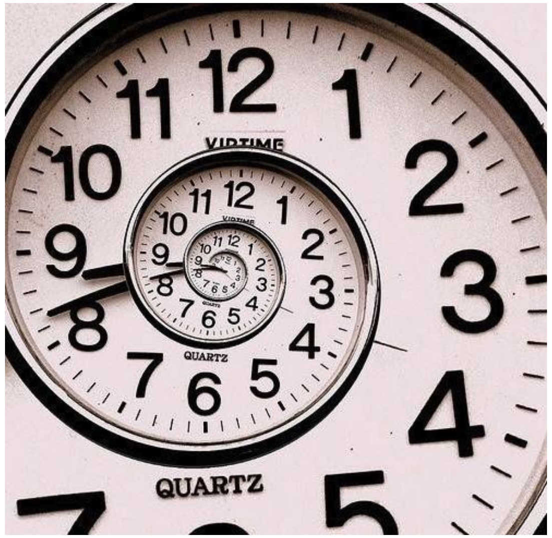
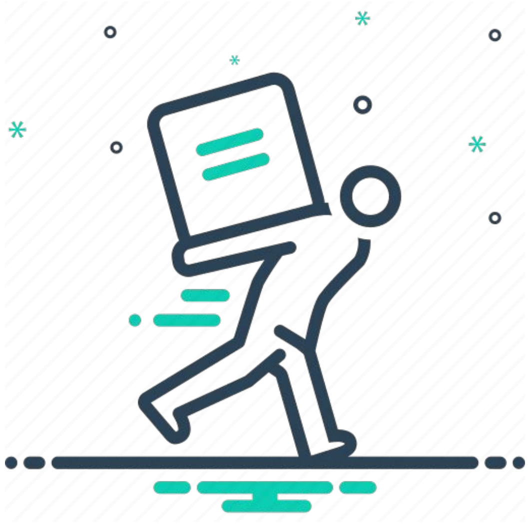
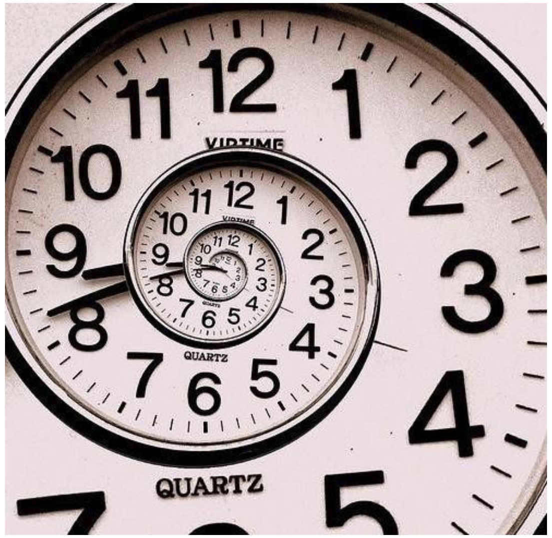




Designing choice experiments with mixtures

- Experiments are expensive, cumbersome and time-consuming
- Efficient experimental designs → reliable information
- Optimal design of experiments: the branch of statistics that deals with the construction of **efficient experimental designs**





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Optimality criteria for choice experiments

Optimal choice experiments with mixtures

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- **D-optimal** experimental designs → low-variance estimators
- We want to have a mixture that maximizes consumer preference
- Precise predictions are crucial
- **I-optimal** experimental designs → low-variance prediction

Models for data from mixture experiments

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- Each mixture is described as a combination of *q* ingredient proportions (0 to 1)
- Constraint: proportions sum up to one → perfect collinearity
- Special-cubic Scheffé model:

$$Y = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \beta_{ij} x_i x_j + \sum_{i=1}^{q-2} \sum_{j=i+1}^{q-1} \sum_{k=j+1}^{q} \beta_{ijk} x_i x_j x_k + \varepsilon$$

Including process variables

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$$Y = \sum_{k=1}^{q} \gamma_k^0 x_k + \sum_{k=1}^{q-1} \sum_{l=k+1}^{q} \gamma_{kl}^0 x_k x_l + \sum_{i=1}^{r} \sum_{k=1}^{q} \gamma_k^i x_k z_i + \sum_{i=1}^{r-1} \sum_{j=i+1}^{r} \alpha_{ij} z_i z_j + \sum_{i=1}^{r} \alpha_i z_i^2 + \varepsilon$$

Multinomial logit model for choice data

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Multinomial logit model for choice data

- A respondent faces *S* choice sets involving *J* alternatives each
- Respondent chooses the alternative that has the highest perceived utility
- The probability that a respondent chooses alternative $j \in \{1, ..., J\}$ in choice set s is

$$p_{js} = \frac{\exp\left[\boldsymbol{f}^T(\boldsymbol{x}_{js})\boldsymbol{\beta}\right]}{\sum_{t=1}^{J} \exp\left[\boldsymbol{f}^T(\boldsymbol{x}_{ts})\boldsymbol{\beta}\right]}$$

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Model for choice data concerning mixtures

- We assume vector $\boldsymbol{x}_{js}$ contains the q ingredient proportions and r process variables

Model for choice data concerning mixtures

- We assume vector $\boldsymbol{x}_{js}$ contains the *q* ingredient proportions and *r* process variables
- Perceived utility modeled as

$$u_{js} = \boldsymbol{f}(\boldsymbol{x}_{js})^T \boldsymbol{\beta}$$
$$= \sum_{i=1}^{q-1} \gamma_i^{0*} x_{ijs} + \sum_{i=1}^{q-1} \sum_{k=i+1}^{q} \gamma_{ik}^{0} x_{ijs} x_{kjs} + \sum_{i=1}^{r} \sum_{k=1}^{q} \gamma_k^{i} x_{kjs} z_{ijs} +$$
$$\sum_{i=1}^{r-1} \sum_{k=i+1}^{r} \alpha_{ik} z_{ijs} z_{kjs} + \sum_{i=1}^{r} \alpha_i z_{ijs}^2$$

D-optimal designs

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- D-optimality criterion

$$\mathcal{D} = \det\left(\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta})\right)$$

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$$\mathcal{D} = \det\left(\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta})\right) \longrightarrow \text{prior distribution } \pi(\boldsymbol{\beta})$$

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- Bayesian D-optimality criterion

$$\mathcal{D}_B = \int_{\mathbb{R}^m} \det\left(\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta})\right) \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}$$

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- Numerical approximation to Bayesian D-optimality criterion

$$\mathcal{D}_B \approx \frac{1}{R} \sum_{i=1}^{R} \det\left(\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta}^{(i)})\right)$$

I-optimal designs

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- I-optimality criterion

$$\mathcal{I} = \int_{\chi} \boldsymbol{f}^T(\boldsymbol{x}_{js})\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta})\boldsymbol{f}(\boldsymbol{x}_{js})d\boldsymbol{x}_{js}$$

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$$\mathcal{I} = \int_{\chi} \boldsymbol{f}^T(\boldsymbol{x}_{js})\boldsymbol{I}^{-1}(\boldsymbol{X},\boldsymbol{\beta})\boldsymbol{f}(\boldsymbol{x}_{js})d\boldsymbol{x}_{js}$$

$$= \text{tr}\left[\boldsymbol{I}^{-1}(\boldsymbol{X},\boldsymbol{\beta})\boldsymbol{W}_u\right]$$

$$\boldsymbol{W}_u = \int_{\chi} \boldsymbol{f}(\boldsymbol{x}_{js})\boldsymbol{f}^T(\boldsymbol{x}_{js})d\boldsymbol{x}_{js}$$

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- Numerical approximation to Bayesian I-optimality criterion

$$\mathcal{I}_B \approx \frac{1}{R}\sum_{i=1}^{R} \mathrm{tr}\left[\boldsymbol{I}^{-1}(\boldsymbol{X},\boldsymbol{\beta}^{(i)})\boldsymbol{W}_u\right]$$

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Example

Cocktail preferences

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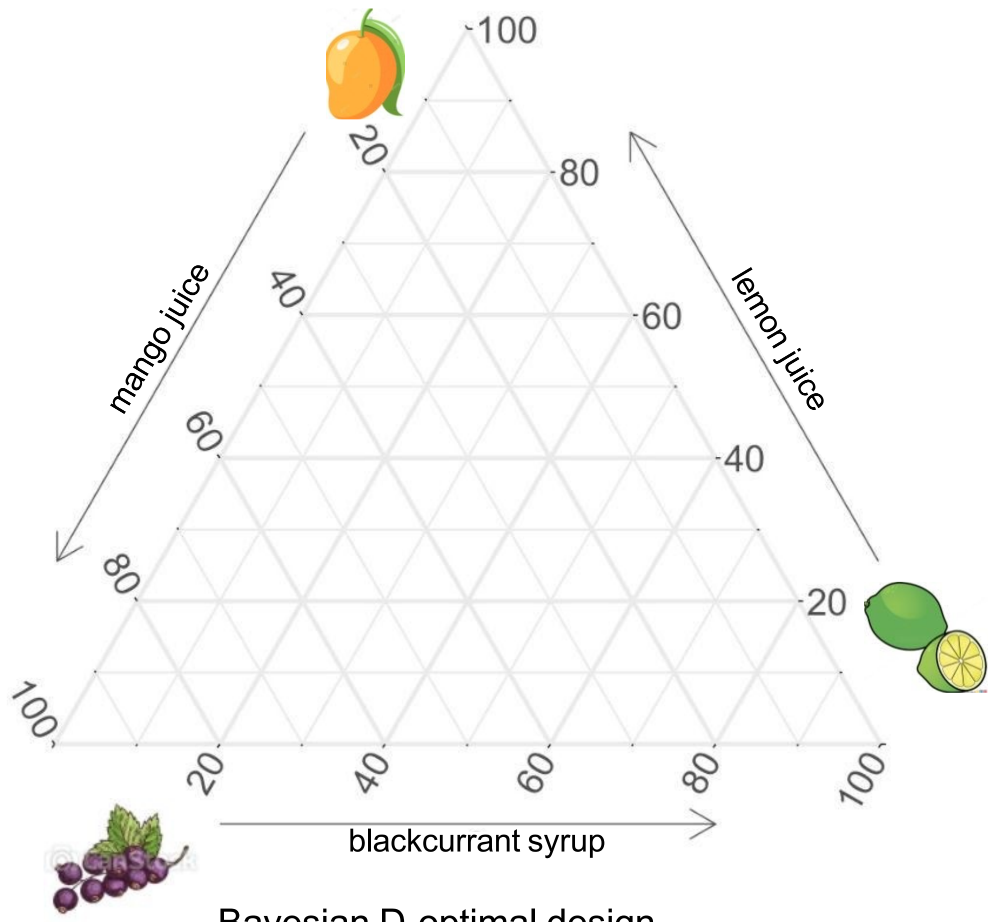
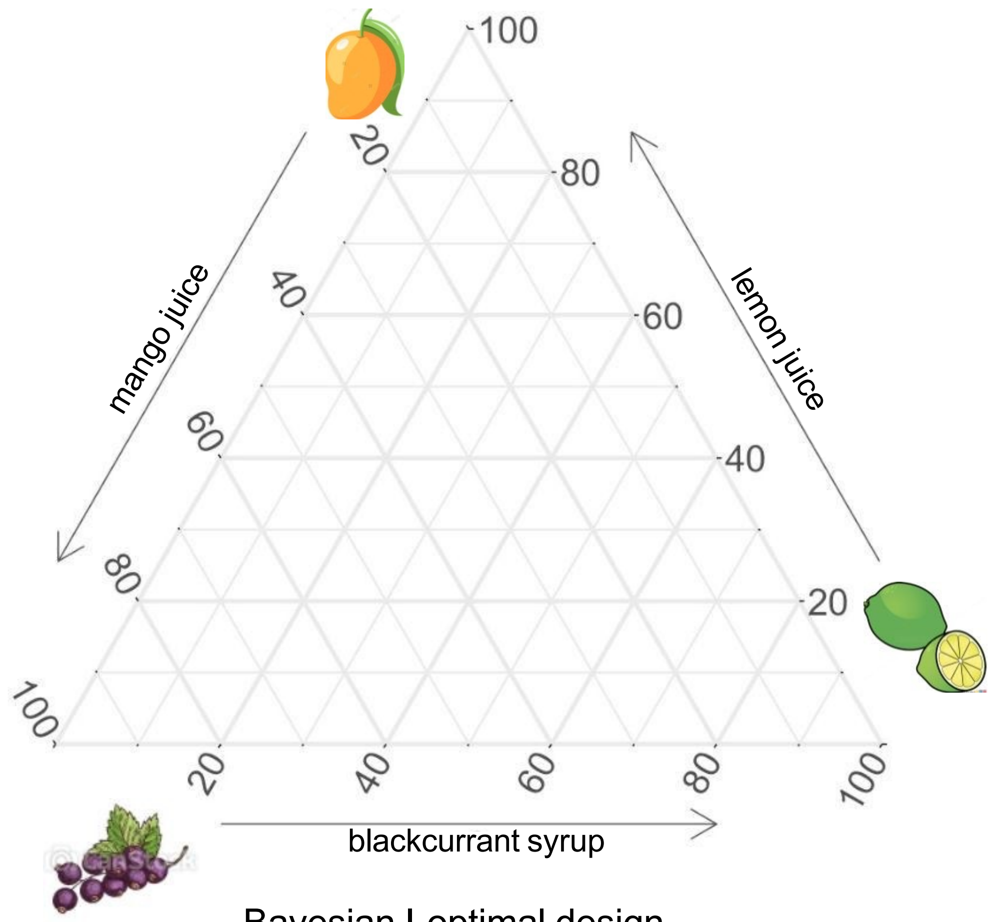
- Each respondent tasted 4 choice sets of size 2
- Simulated responses for temperature (process variable) → $\boldsymbol{\beta}$ parameter vector
- $\boldsymbol{\beta}$ used as prior distribution in a second-order Scheffé model and MNL model for **Bayesian D- and I-optimal** designs

Cocktail preferences



Bayesian D-optimal design



Bayesian I-optimal design

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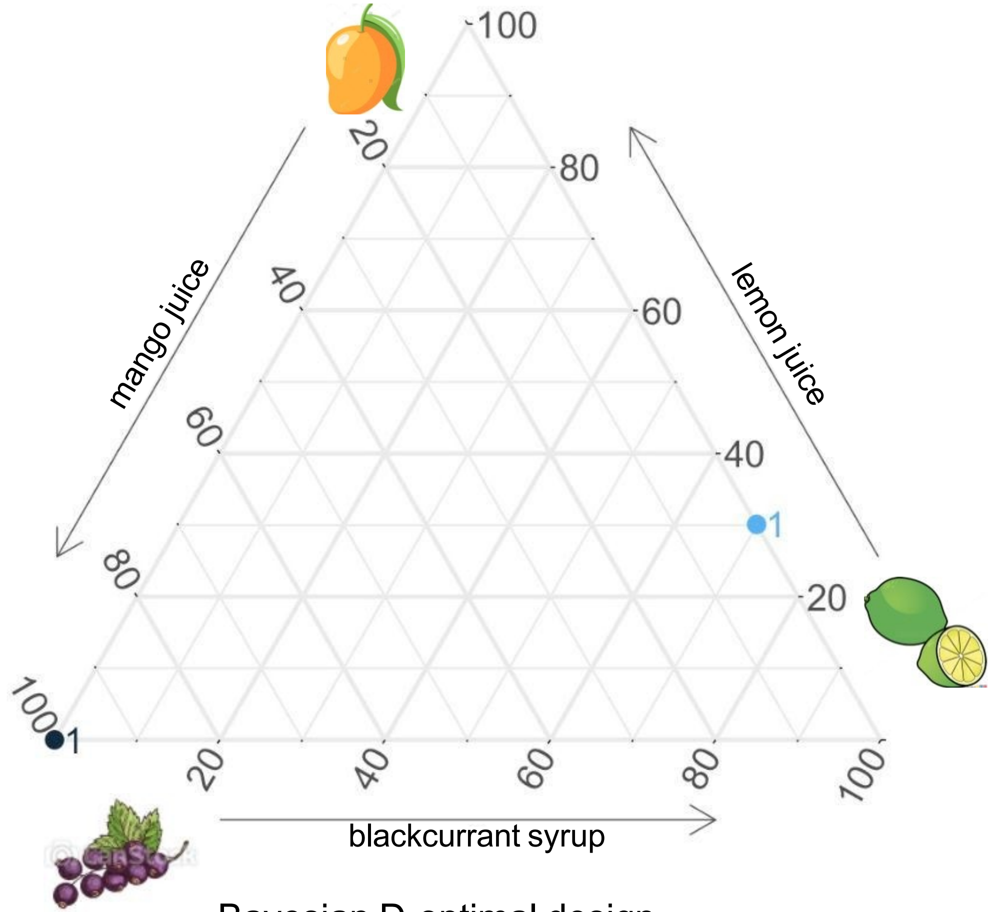

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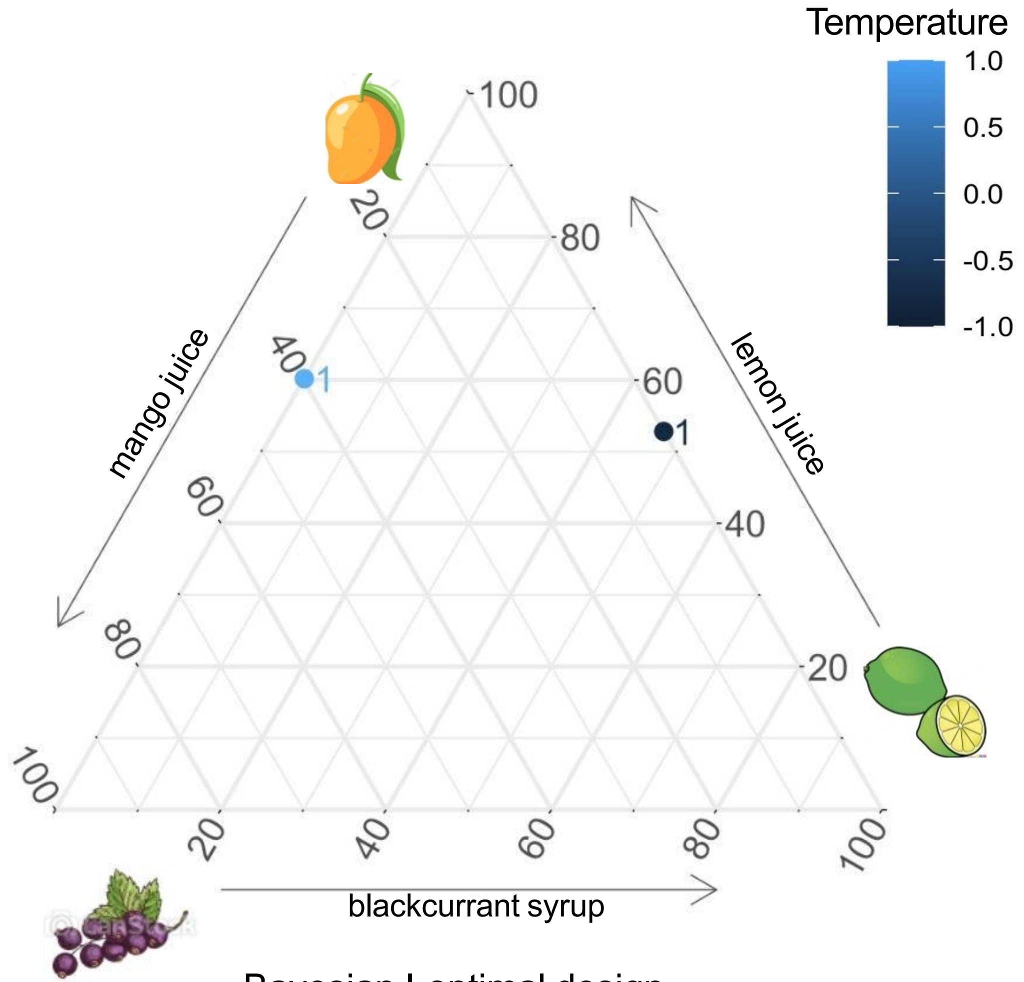

Bayesian I-optimal design

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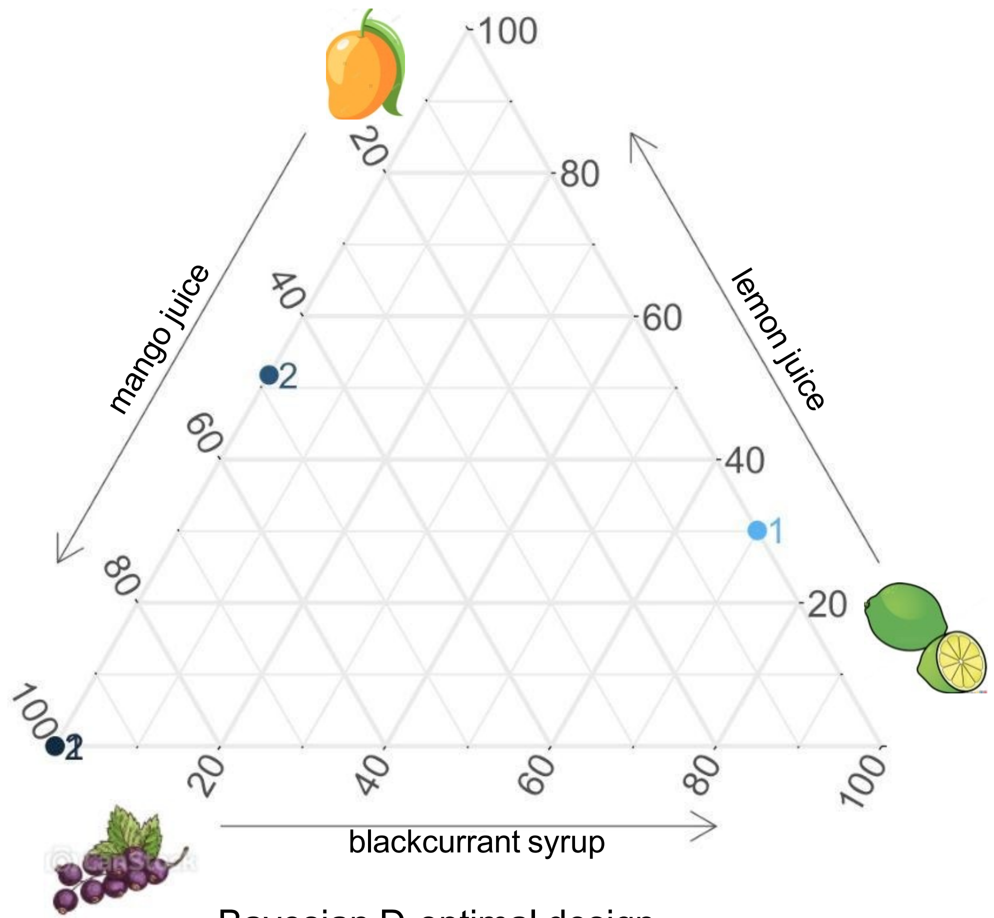

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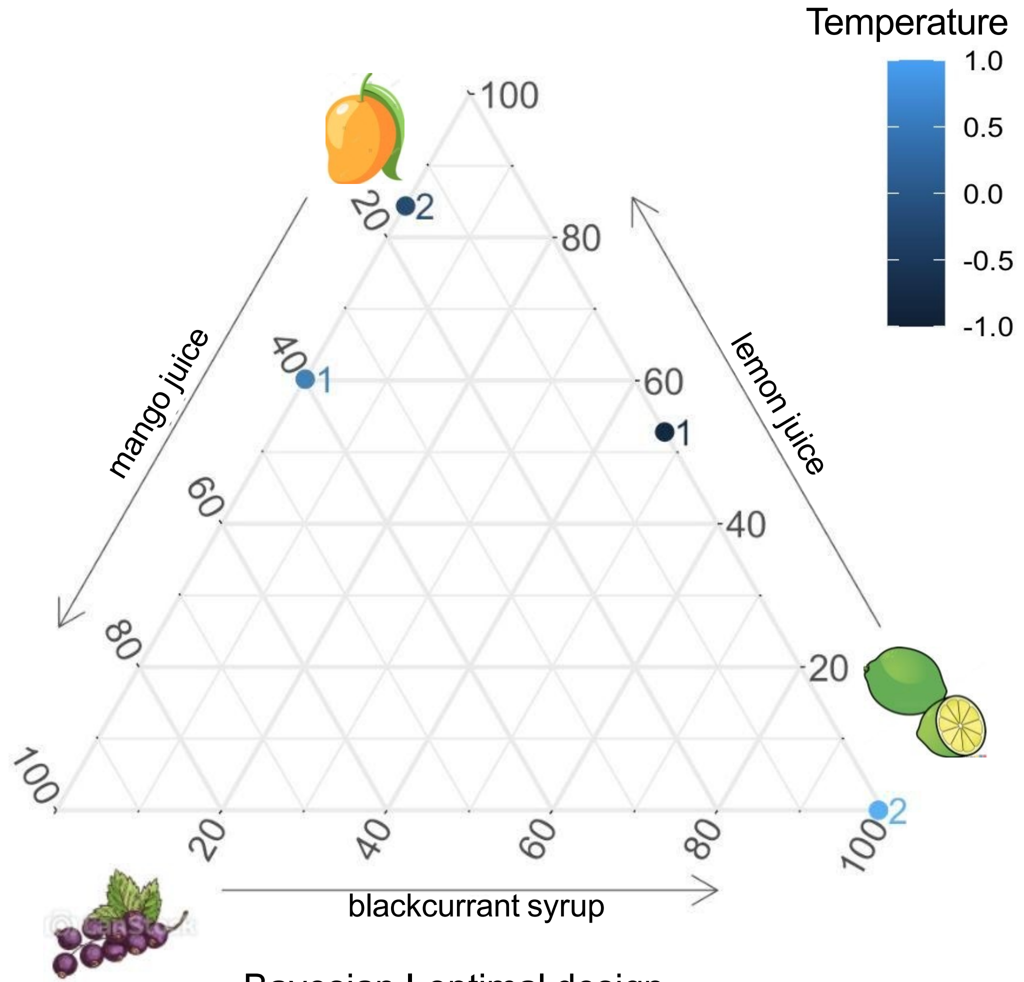

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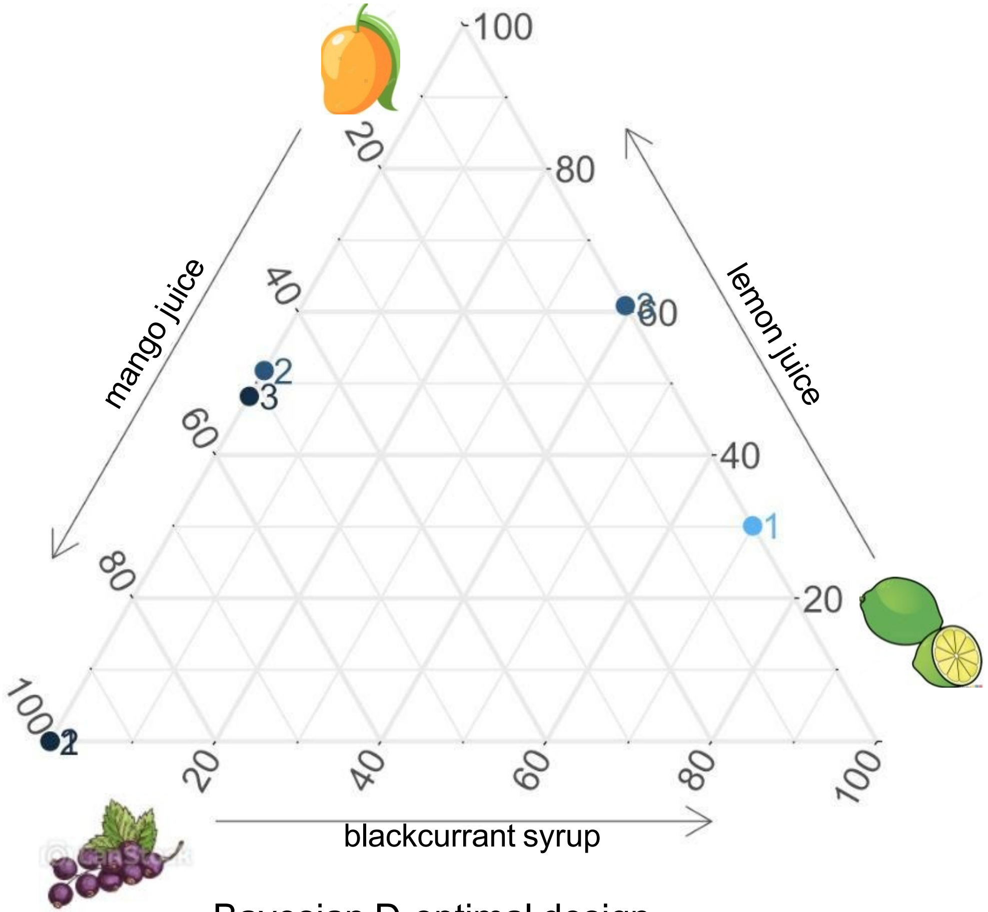

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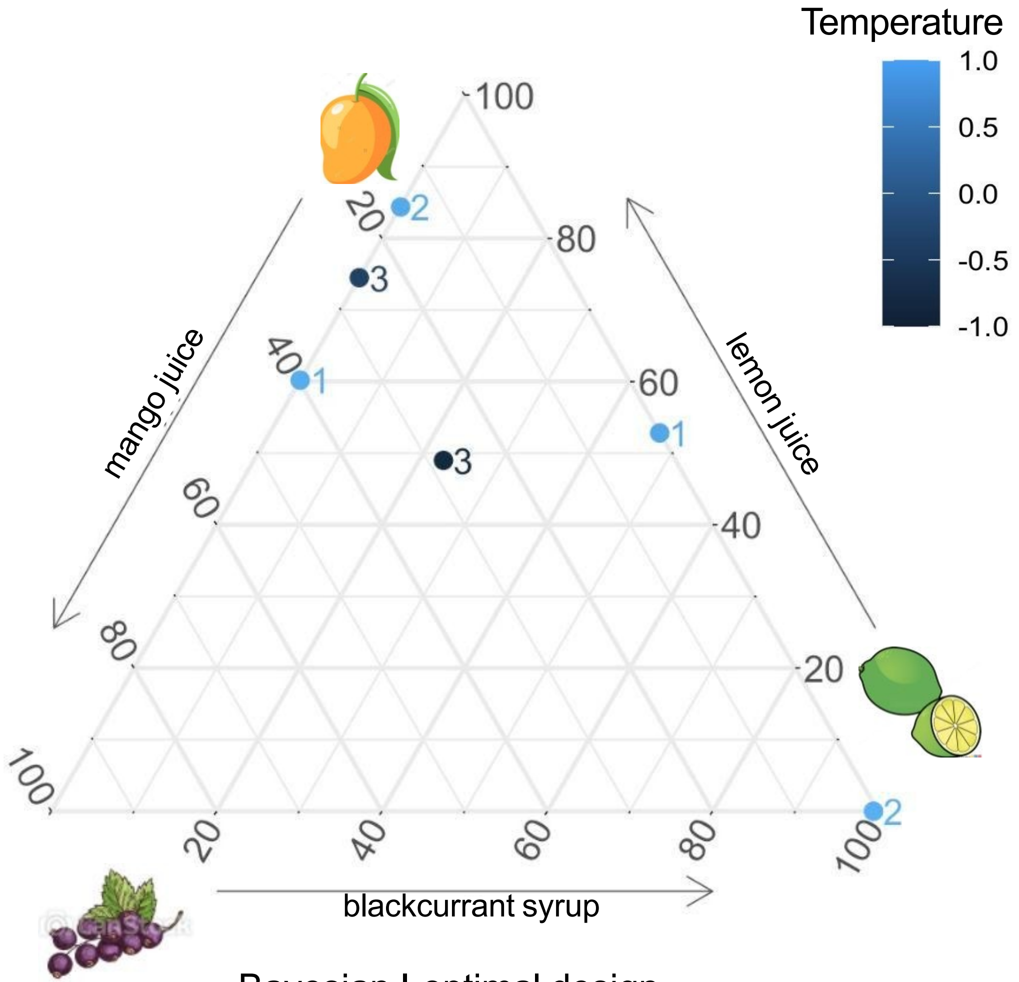

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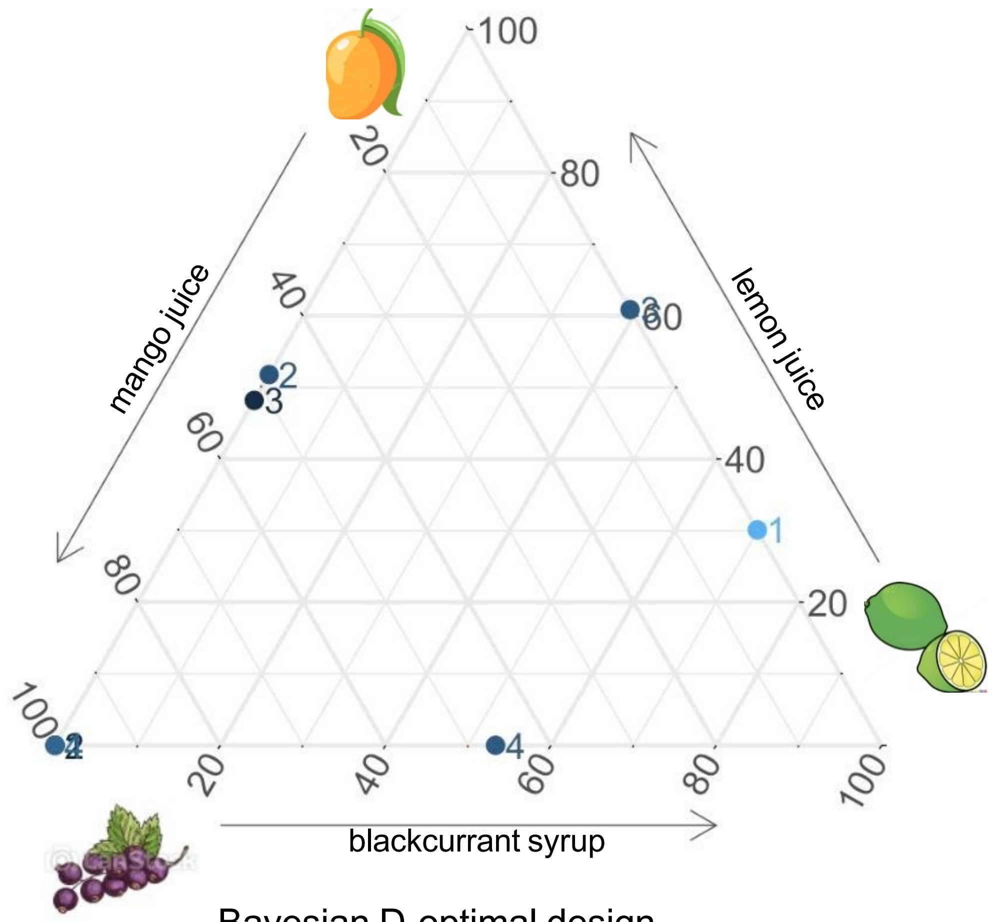

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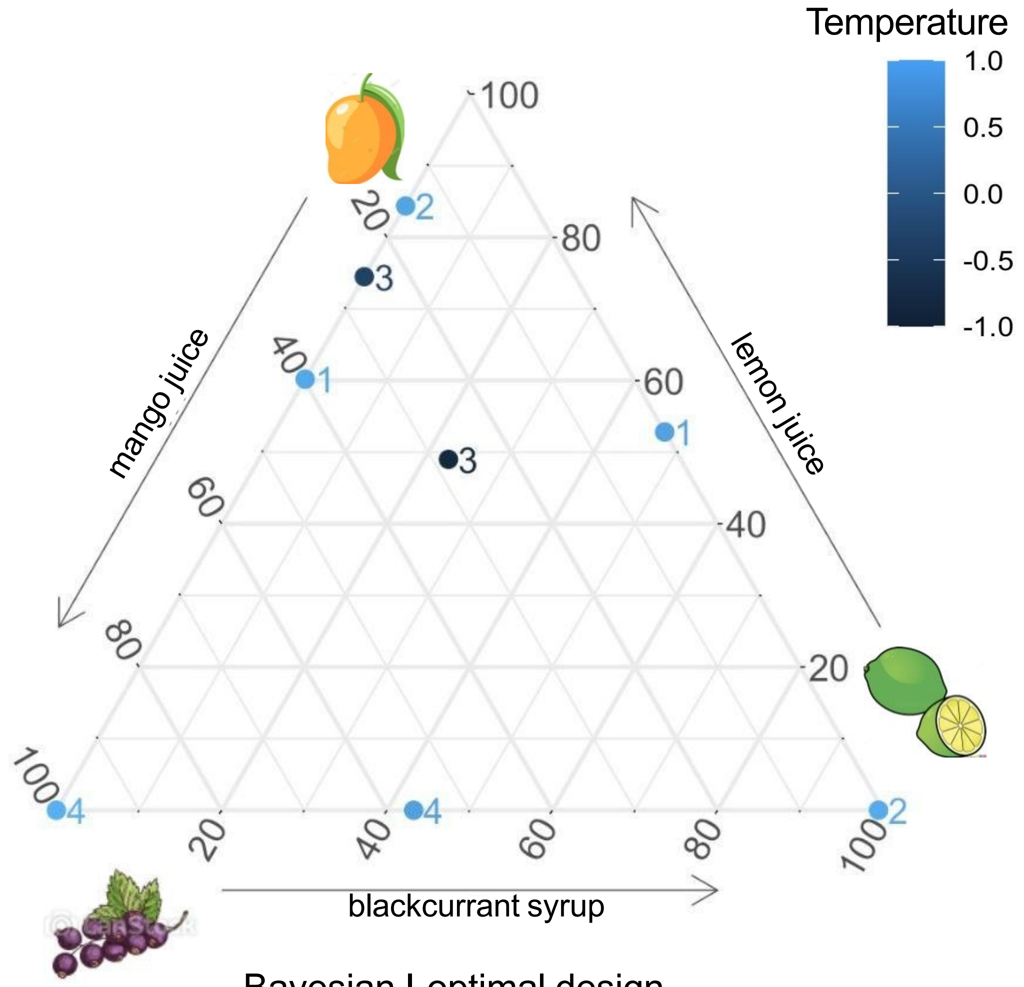

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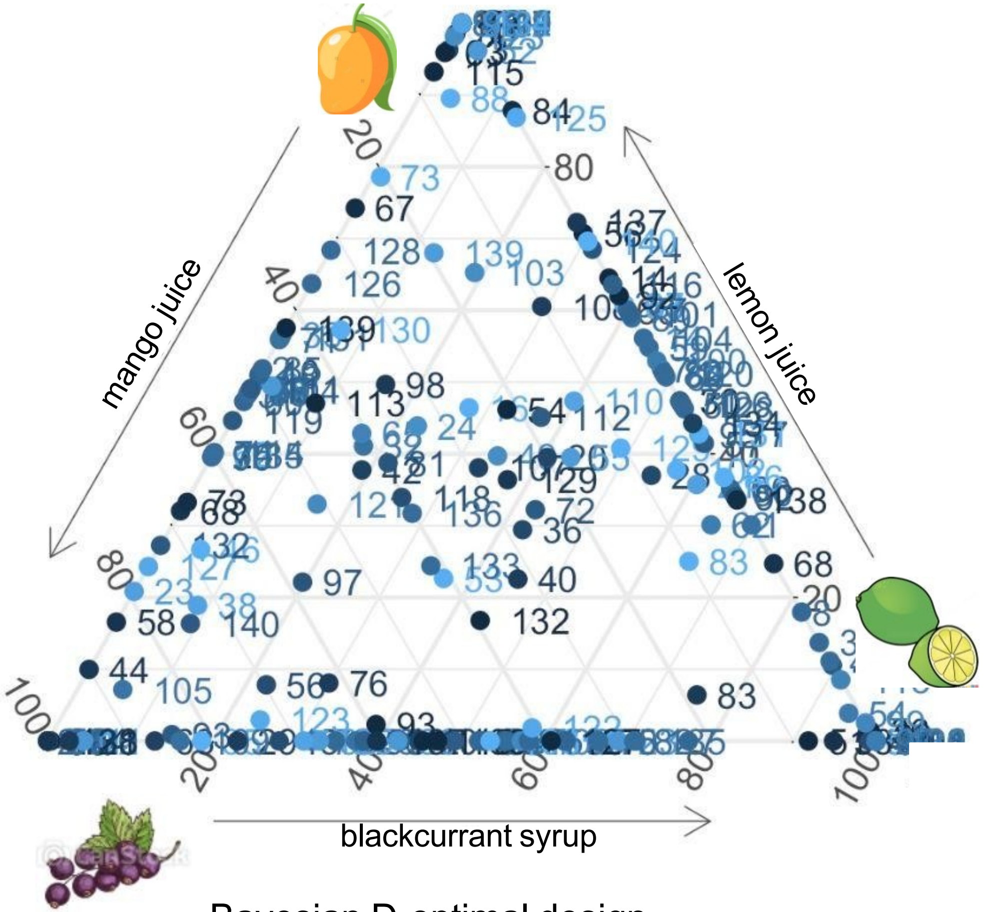

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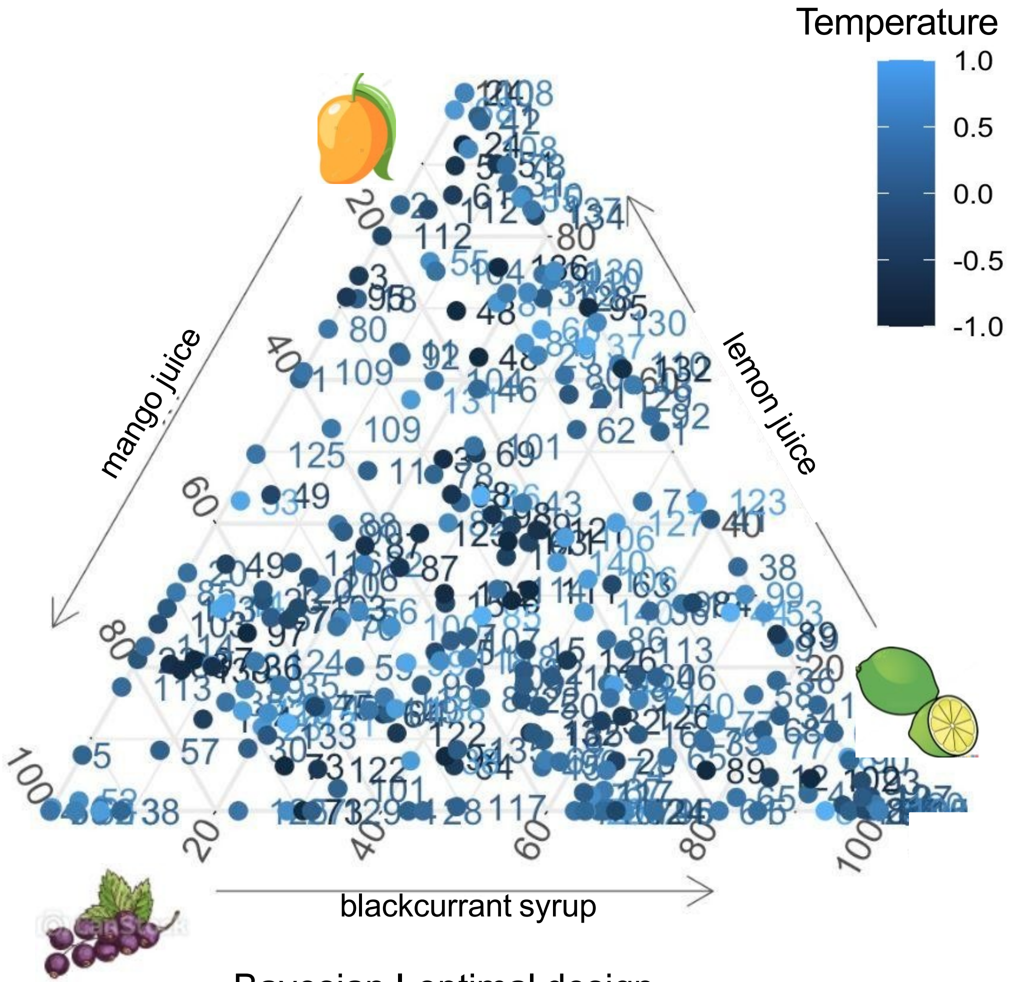

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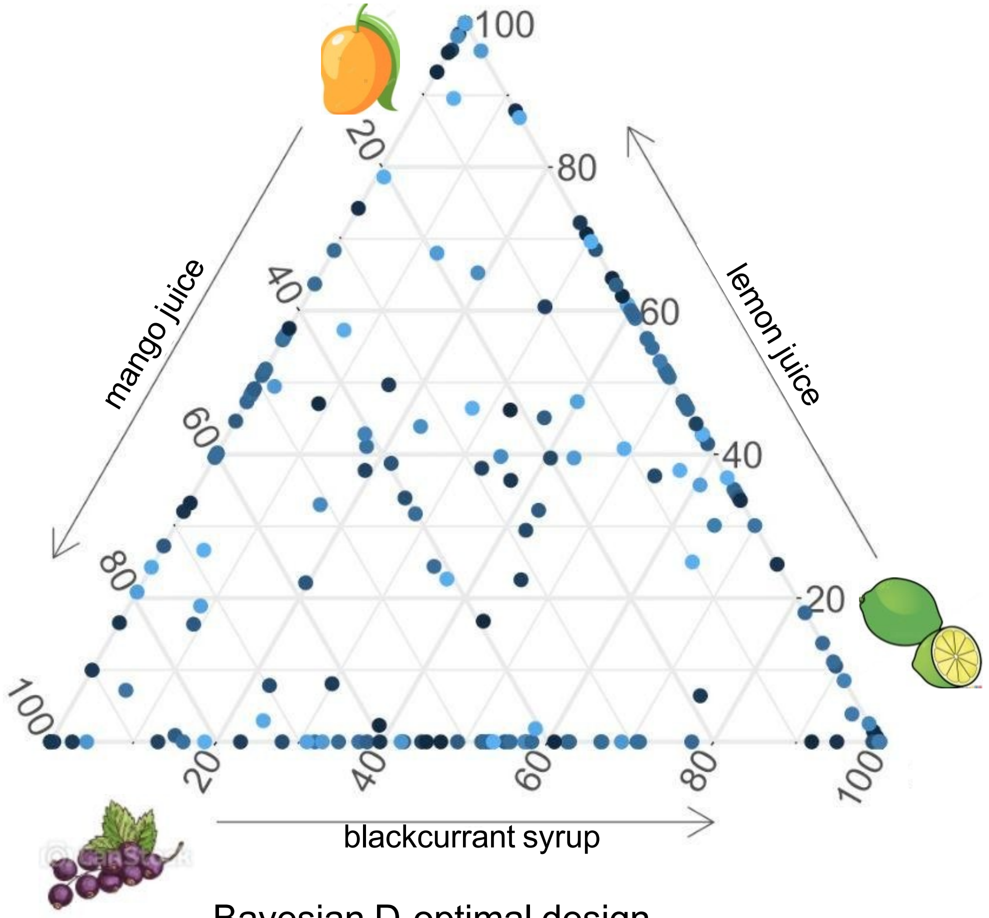

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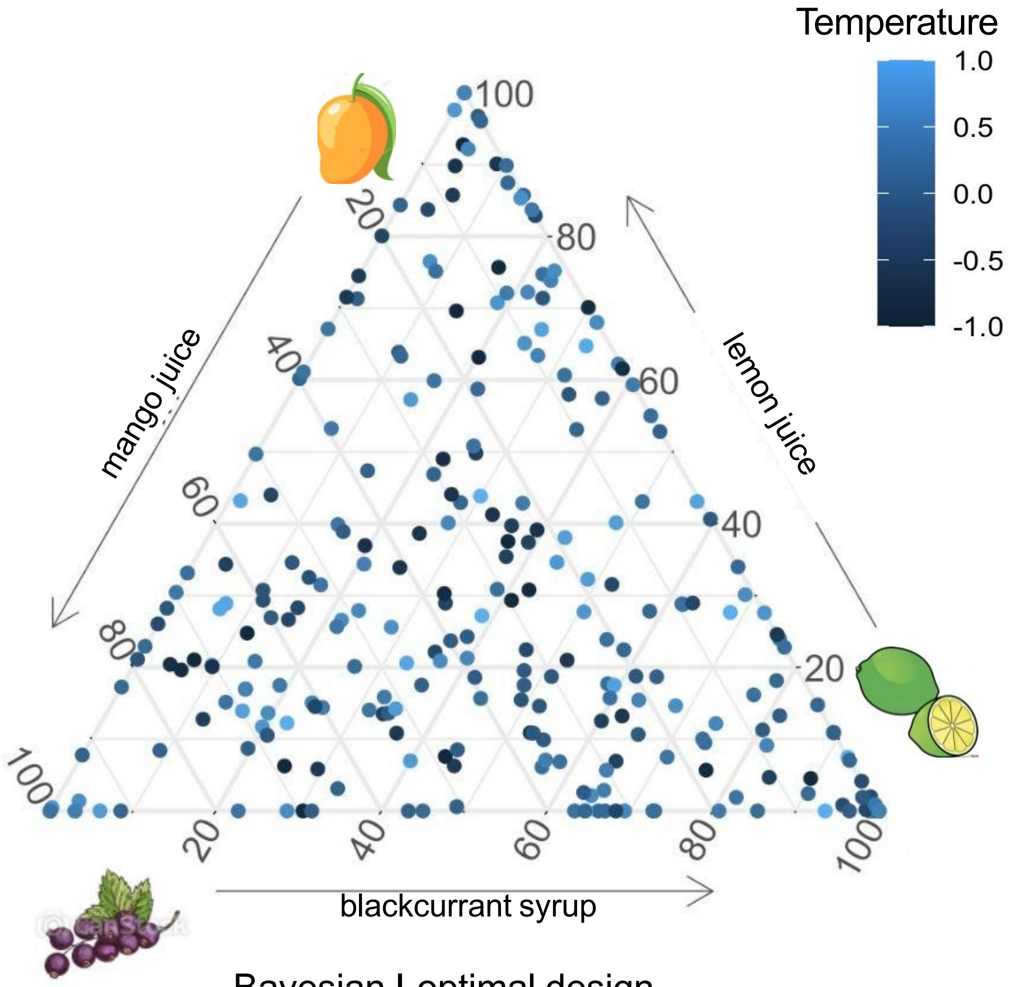

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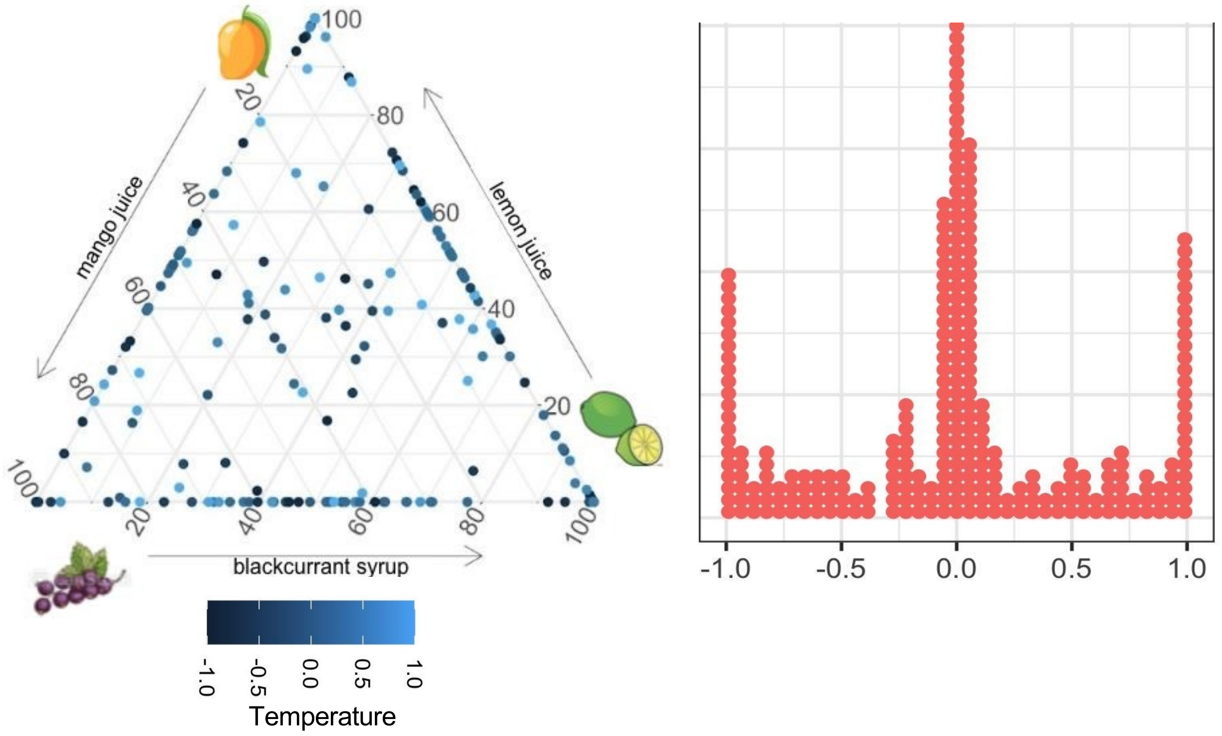

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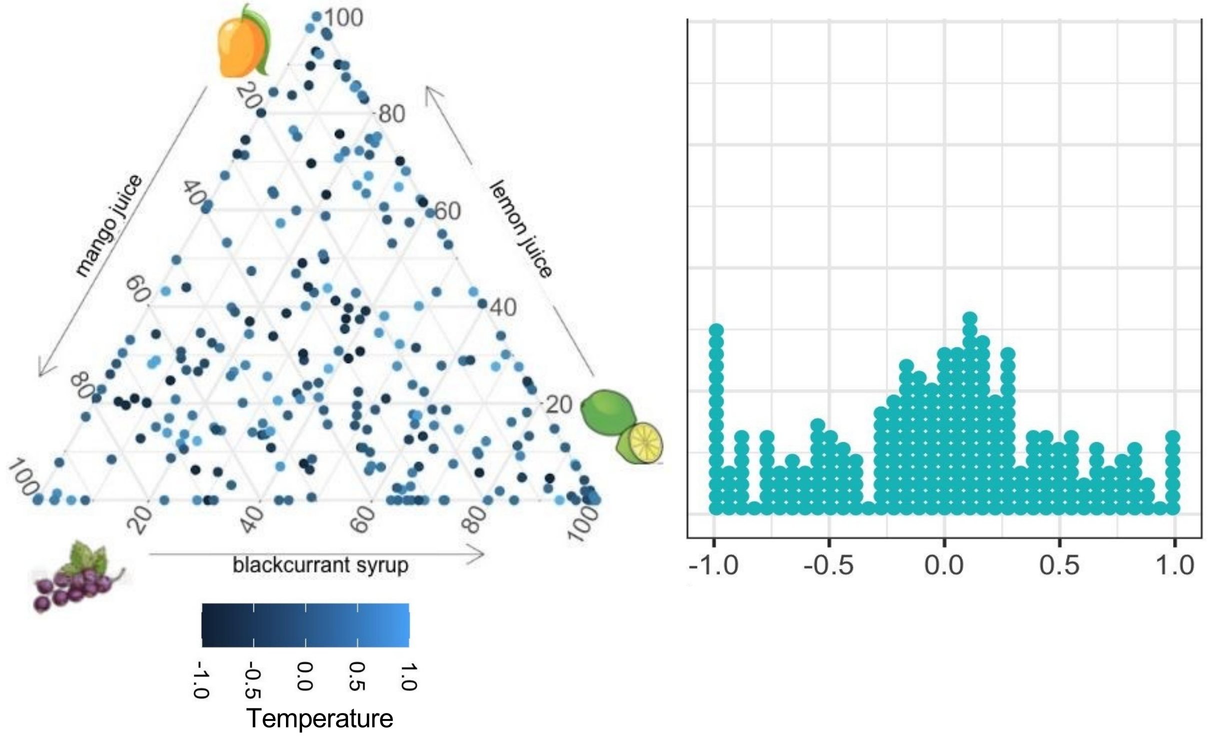

Bayesian I-optimal design

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Upper bound on the number of distinct mixtures

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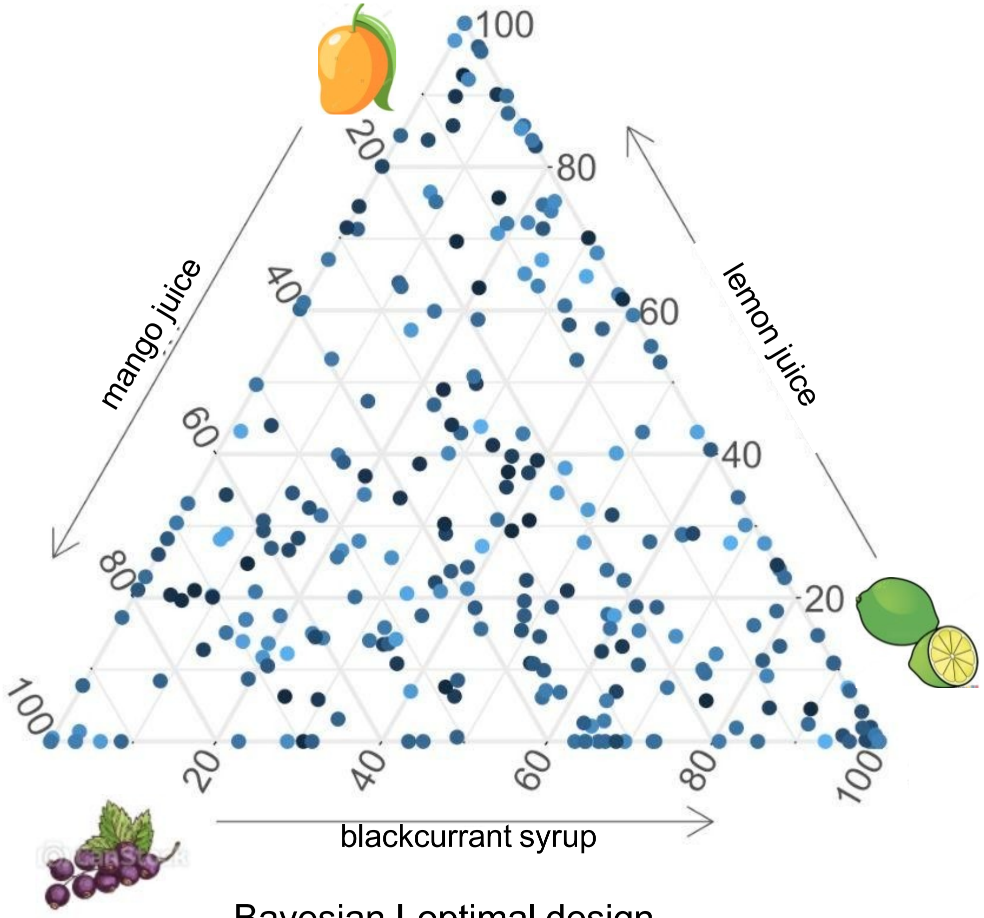

Bayesian I-optimal design

261 different mixtures

I-opt = 2.72

Cocktail preferences

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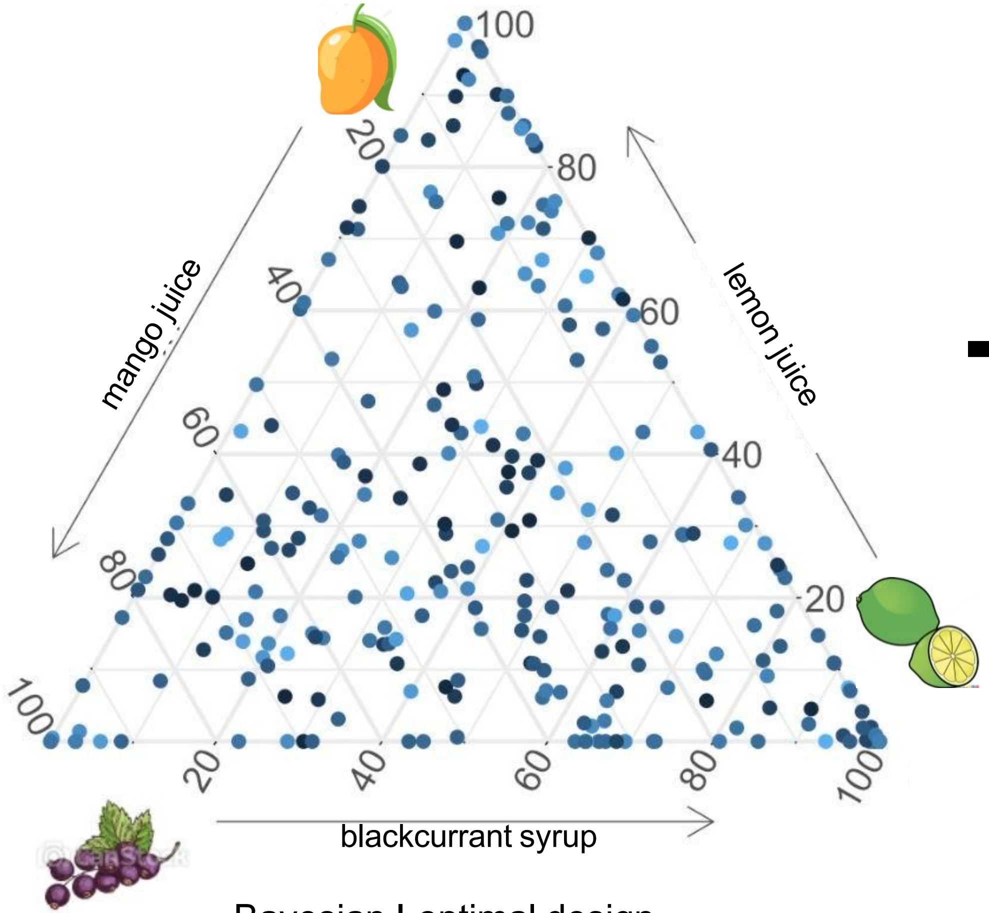

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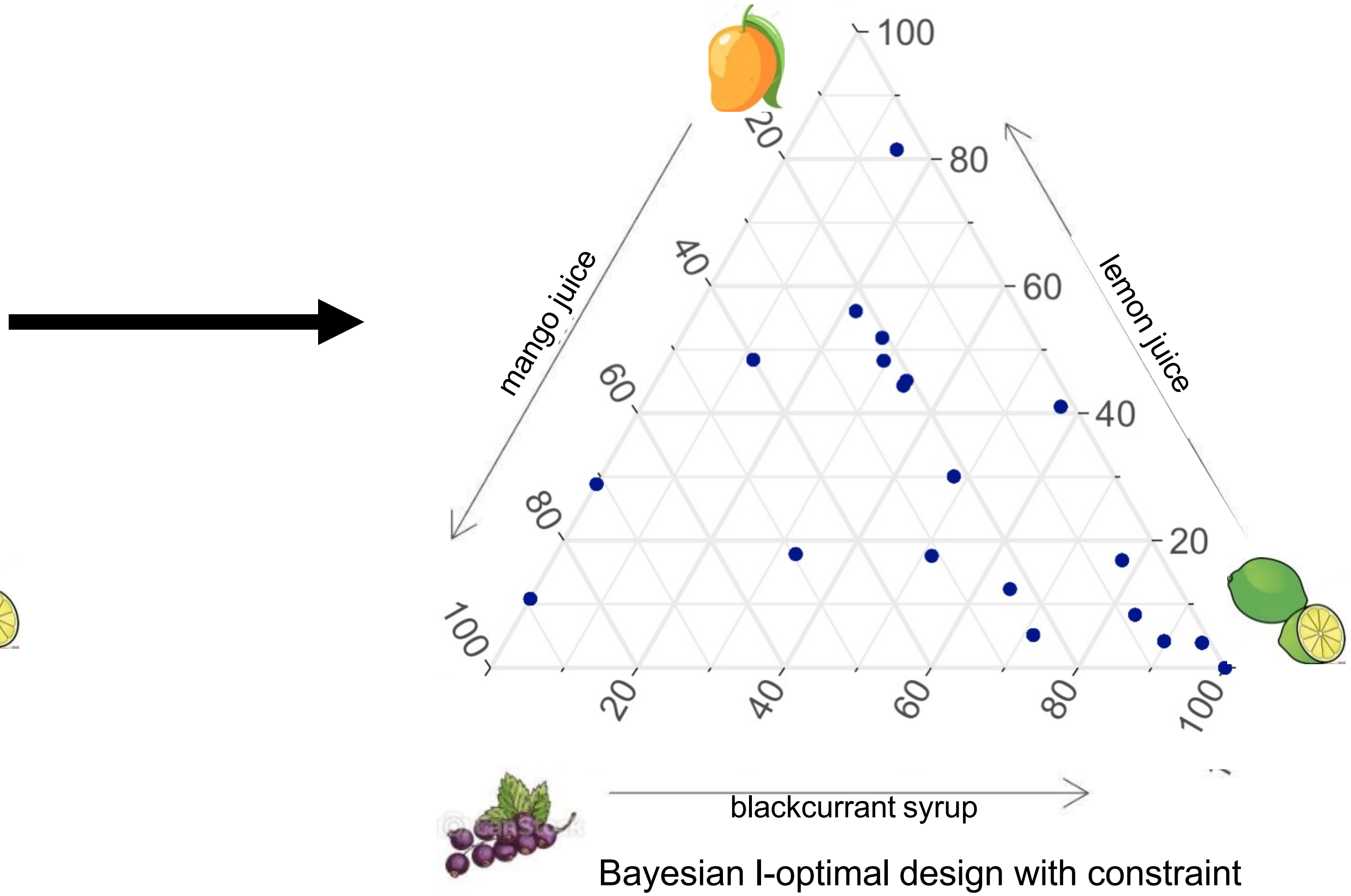

Bayesian I-optimal design with constraint

20 different mixtures

I-opt = 2.85

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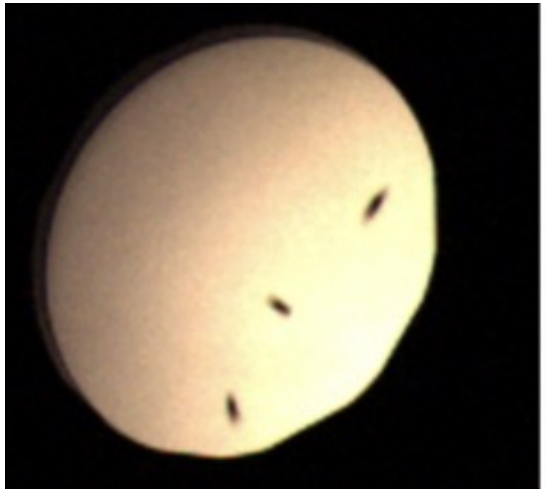
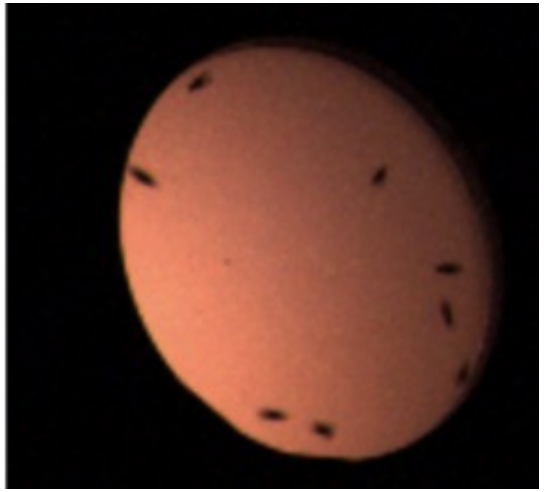
Fruit flies’ color preferences

Fruit flies' color preferences

Fruit flies' color preferences





More information

- *Bayesian I-optimal designs for choice experiments with mixtures* by Mario Becerra and Peter Goos. Chemometrics and Intelligent Laboratory Systems 217 (2021): 104395. DOI: 10.1016/j.chemolab.2021.104395

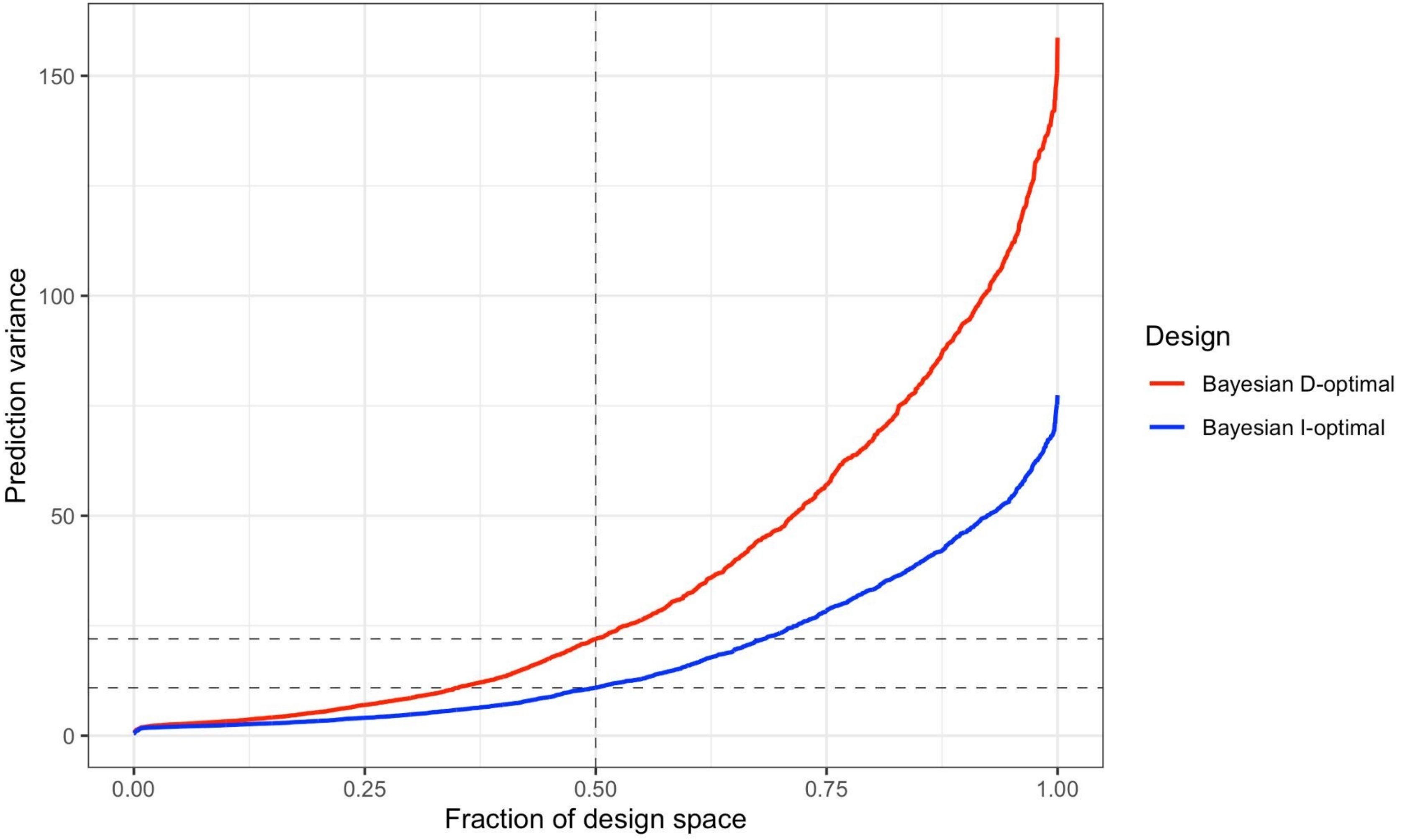
- *Bayesian D- and I-optimal designs for choice experiments involving mixtures and process variables* by Mario Becerra and Peter Goos. To appear in *Food Quality and Preference*. DOI: 10.1016/j.foodqual.2023.104928

- R package with our algorithms (https://github.com/mariobecerra/opdesmixr)

- Mario Becerra's website (with links to papers, R package, and code): mariobecerra.github.io/

Thank you

Cocktail preferences



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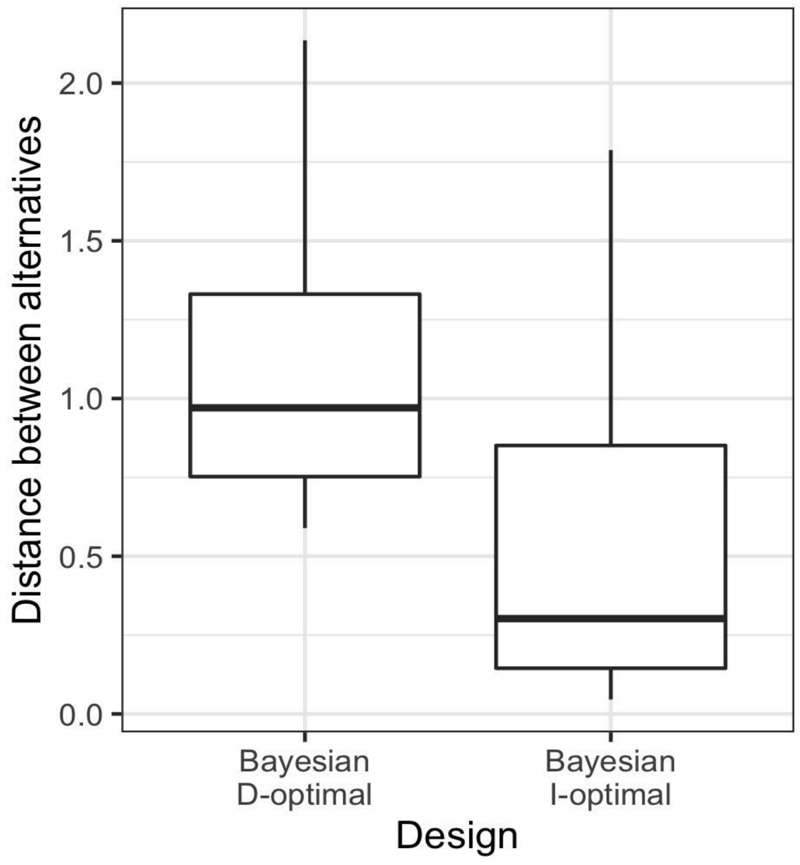
Extra: Cocktail preferences



Extra: Optimal design criteria

- D-optimal designs: low-variance estimators
- I-optimal designs: low-variance predictions
- Information matrix of multinomial logit model: $\boldsymbol{I}(\boldsymbol{X}, \boldsymbol{\beta}) = \sum_{s=1}^{S} \boldsymbol{X}_s^T (\boldsymbol{P}_s - \boldsymbol{p}_s \boldsymbol{p}_s^T) \boldsymbol{X}_s$
- With

$$\boldsymbol{P}_s = \text{diag}(\boldsymbol{p}_s)$$

$$\boldsymbol{p}_s = (p_{1s}, \ldots, p_{Js})^T$$

$$\boldsymbol{X}_s^T = [\boldsymbol{f}(\boldsymbol{x}_{js})]_{j \in \{1,\ldots,J\}}$$

$$\boldsymbol{X} = [\boldsymbol{X}_1, \ldots, \boldsymbol{X}_S]$$

$$p_{js} = \frac{\exp\left[\boldsymbol{f}^T(\boldsymbol{x}_{js})\boldsymbol{\beta}\right]}{\sum_{t=1}^{J} \exp\left[\boldsymbol{f}^T(\boldsymbol{x}_{ts})\boldsymbol{\beta}\right]}$$

Extra: Model for choice data concerning mixtures

- The attributes of the alternatives in a choice experiment are the ingredients of a mixture
- Vector $\boldsymbol{x}_{js}$ contains the *q* ingredient proportions and that $\boldsymbol{f}(\boldsymbol{x}_{js})$ represents the model expansion of these proportions
- Most natural thing to do:

$$U_{js} = \sum_{i=1}^{q} \beta_i x_{ijs} + \sum_{i=1}^{q-1} \sum_{k=i+1}^{q} \beta_{ik} x_{ijs} x_{kjs} + \sum_{i=1}^{q-2} \sum_{k=i+1}^{q-1} \sum_{l=k+1}^{q} \beta_{ikl} x_{ijs} x_{kjs} x_{ljs} + \varepsilon_{js}$$

- Rewrite x_{qjs} as $1 - x_{1js} - \ldots - x_{q-1,js}$

$$U_{js} = \boldsymbol{f}^T(\boldsymbol{x}_{js})\boldsymbol{\beta} = \sum_{i=1}^{q-1} \beta_i^* x_{ijs} + \sum_{i=1}^{q-1} \sum_{k=i+1}^{q} \beta_{ik} x_{ijs} x_{kjs} + \sum_{i=1}^{q-2} \sum_{k=i+1}^{q-1} \sum_{l=k+1}^{q} \beta_{ikl} x_{ijs} x_{kjs} x_{ljs} + \varepsilon_{js}$$

- With

$$\boldsymbol{f}(\boldsymbol{x}_{js}) = (x_{1js}, x_{2js}, \ldots, x_{q-1,js}, x_{1js}x_{2js}, \ldots, x_{q-1,js}x_{qjs}, x_{1js}x_{2js}x_{3js}, \ldots, x_{q-2,js}x_{q-1,js}x_{qjs})^T$$

$$\beta_i^* = \beta_i - \beta_q \text{ for } i \in \{1, \ldots, q-1\}$$

$$\boldsymbol{x}_{js} = (x_{1js}, x_{2js}, \ldots, x_{qjs})^T \qquad \boldsymbol{\beta} = (\beta_1^*, \beta_2^*, \ldots, \beta_{q-1}^*, \beta_{1,2}, \ldots, \beta_{q-1,q}, \beta_{123}, \ldots, \beta_{q-2,q-1,q})^T$$

KU LEUVEN