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

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with Peter Goos

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Outline

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

Choice modeling and choice experiments

Discrete choice experiments

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- Quantify consumer preferences

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- Preference data is collected

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- 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

Mixture experiments

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- Examples:
  - wheat varieties in bread
  - ingredients used to make a cocktail
  - types of fish used to make a fish patty



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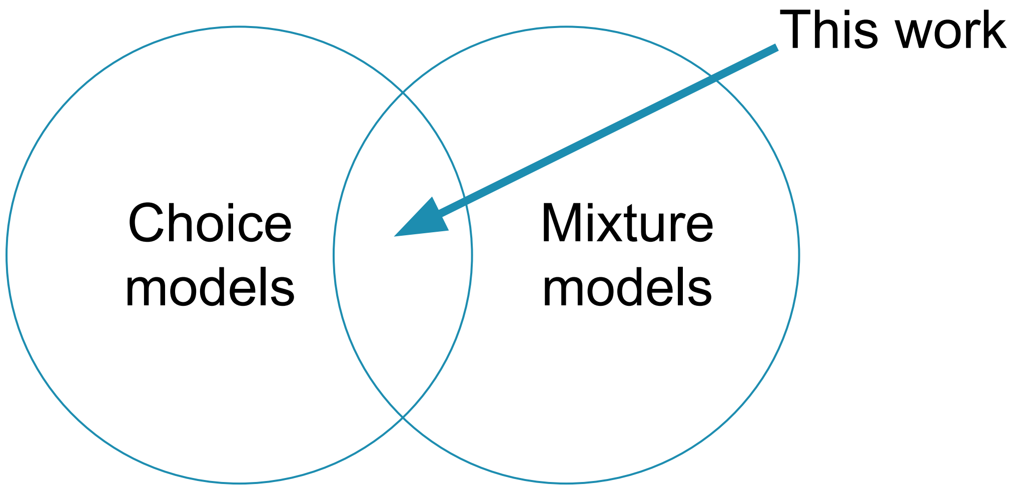
Mixtures

- 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



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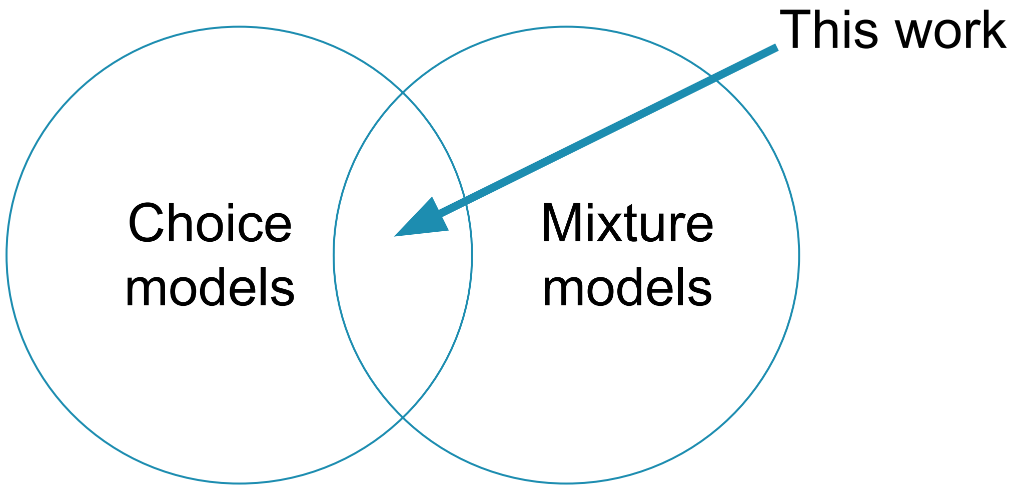

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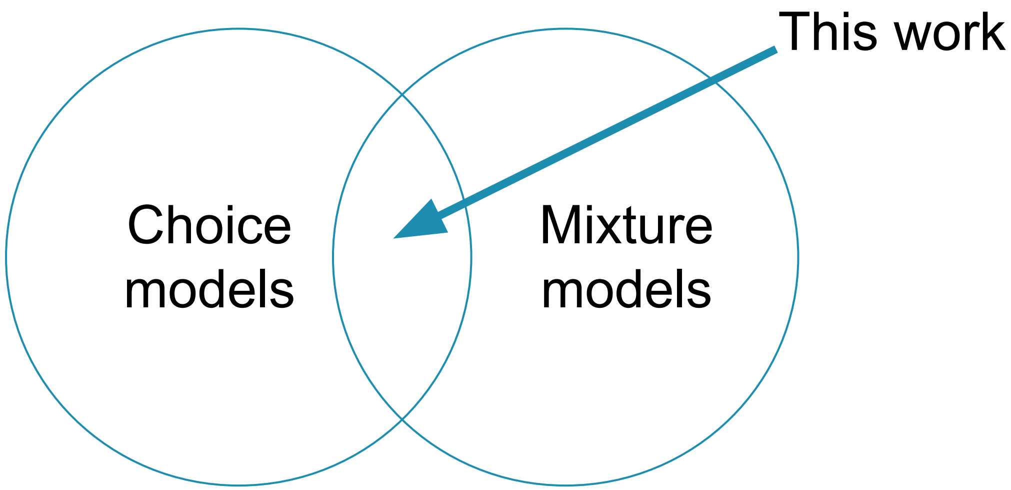

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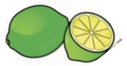
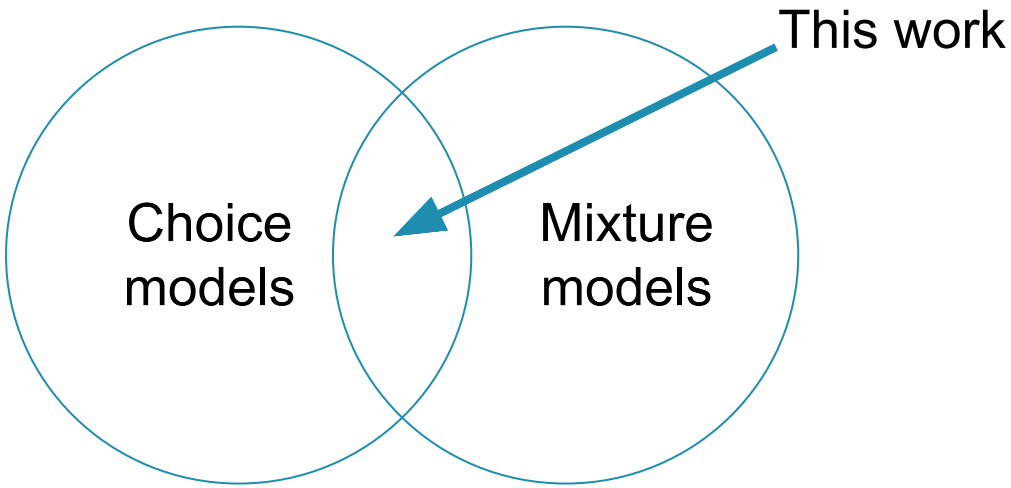
  - lemon juice 
  - blackcurrant syrup 

Choice experiments with mixtures



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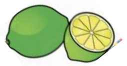
  - lemon juice 
  - blackcurrant syrup 
- 60 people, each making 8 pairwise comparisons

Designing choice experiments with mixtures

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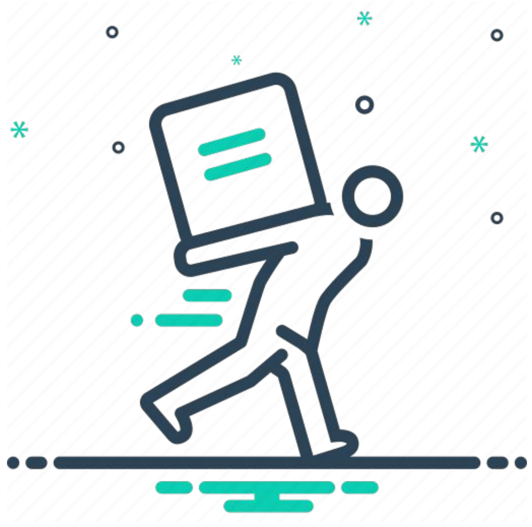
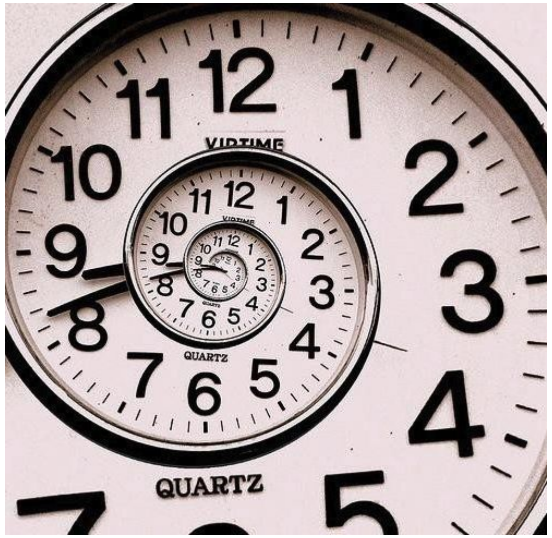

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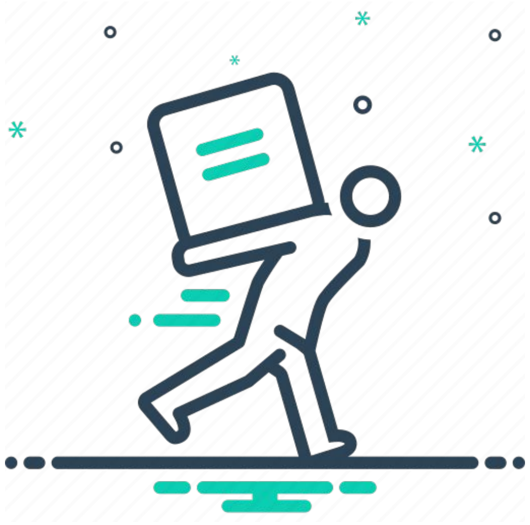
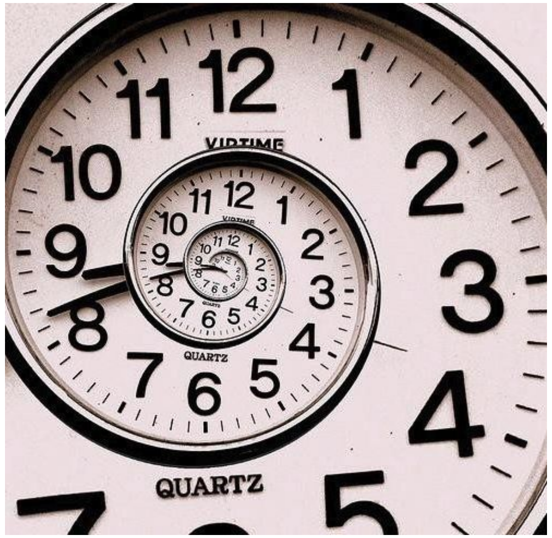
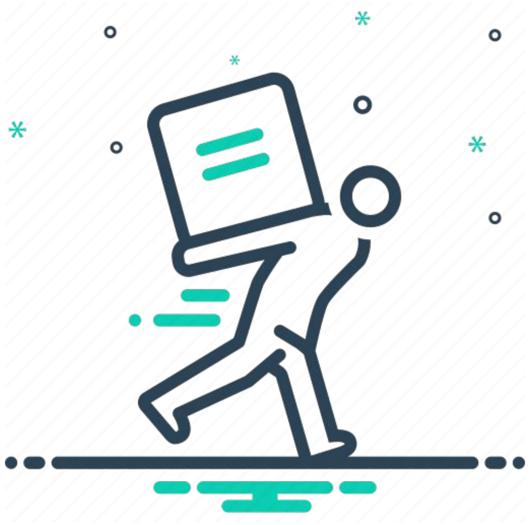
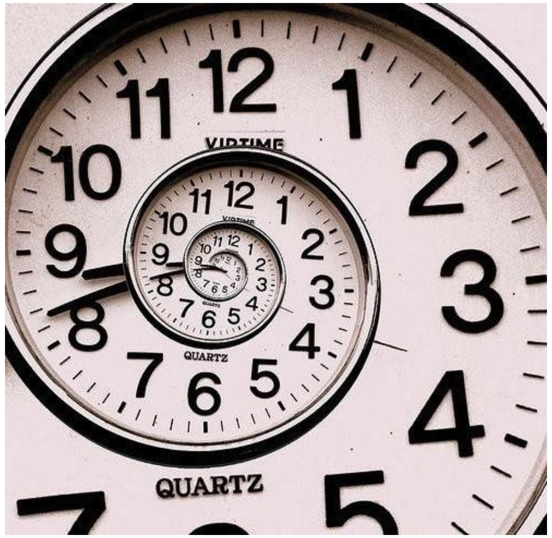




Designing choice experiments with mixtures

- 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**





Optimality criteria for choice experiments

Optimal choice experiments with mixtures

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- We want to have a mixture that maximizes consumer preference
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- **I-optimal** experimental designs → low-variance prediction

Models for data from mixture experiments

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- 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* ∈ *{1, ..., J}* in choice set *s* is

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

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

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

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

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

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

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

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

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

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Results

Cocktail preferences

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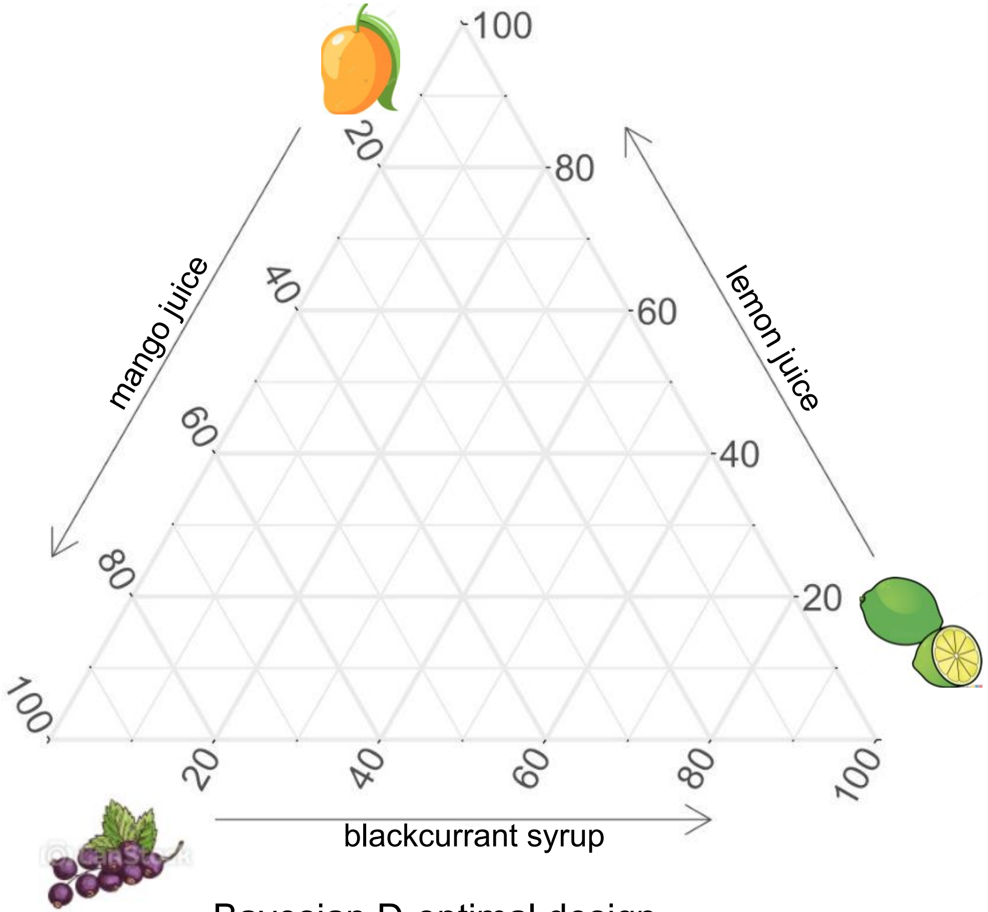
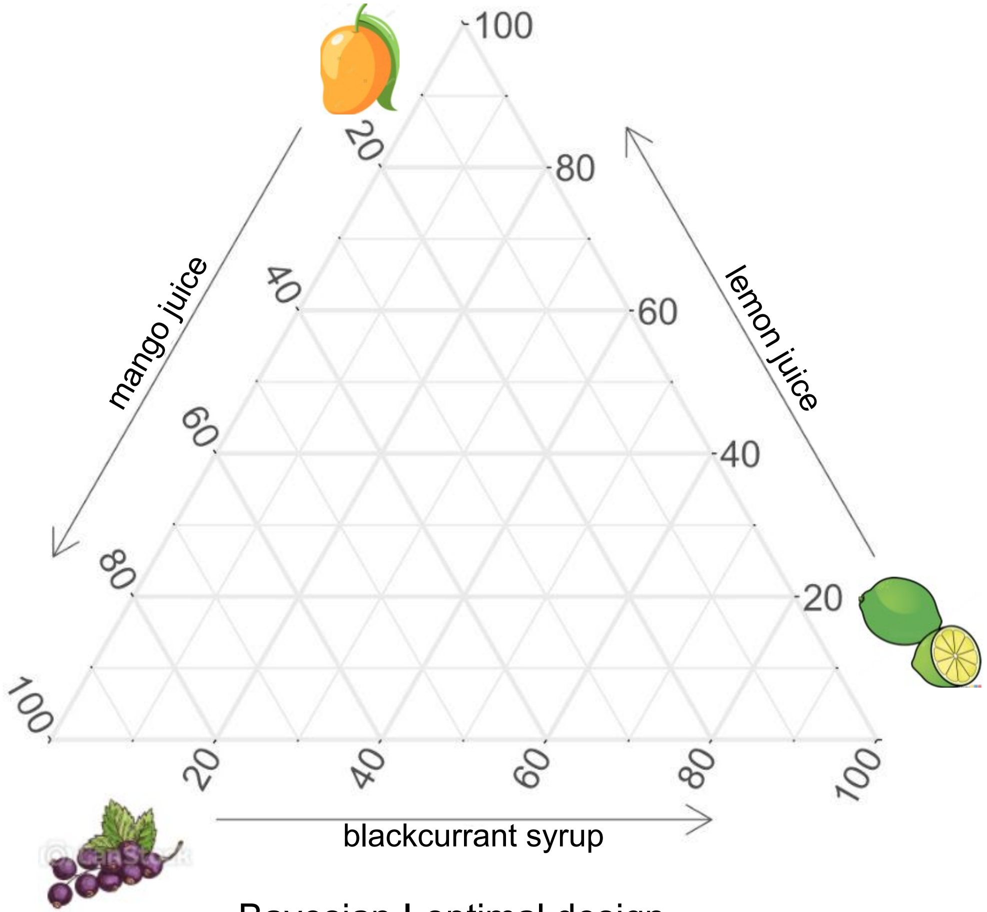
- Prior distribution for parameter vector $\boldsymbol{\beta}$ in a second-order Scheffé model and MNL model for **Bayesian D- and I-optimal** designs

Cocktail preferences



Bayesian D-optimal design



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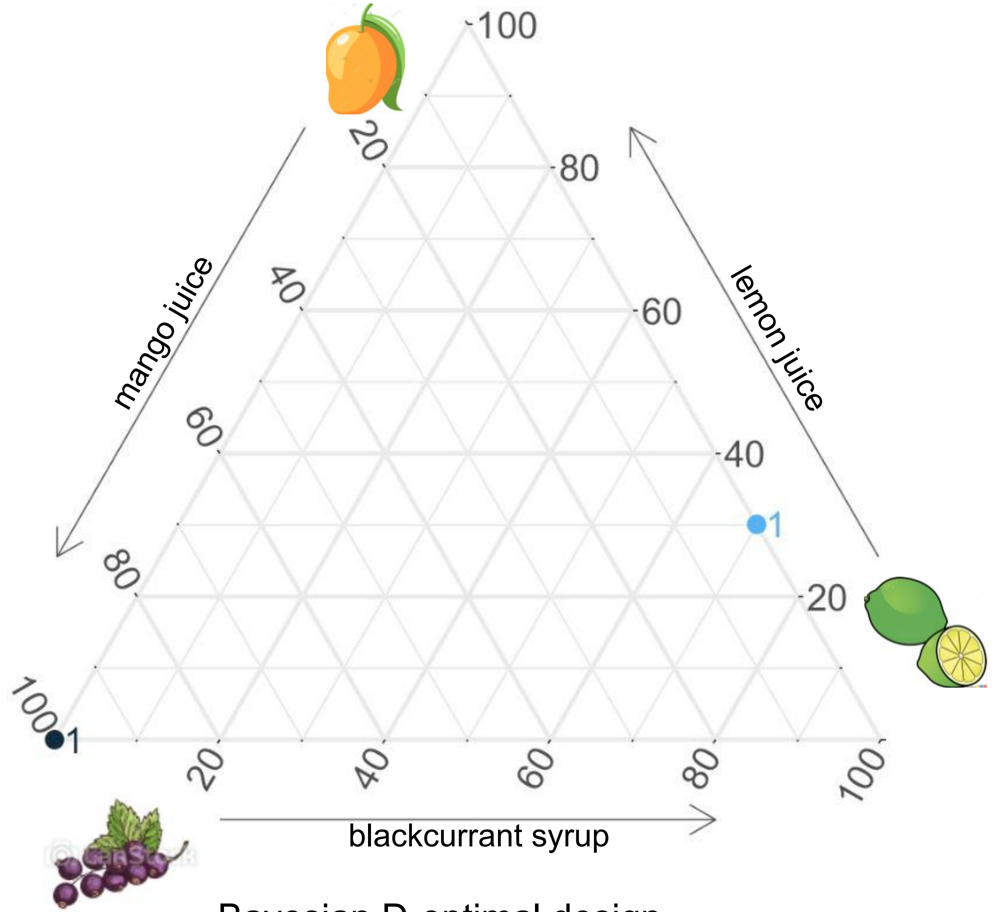

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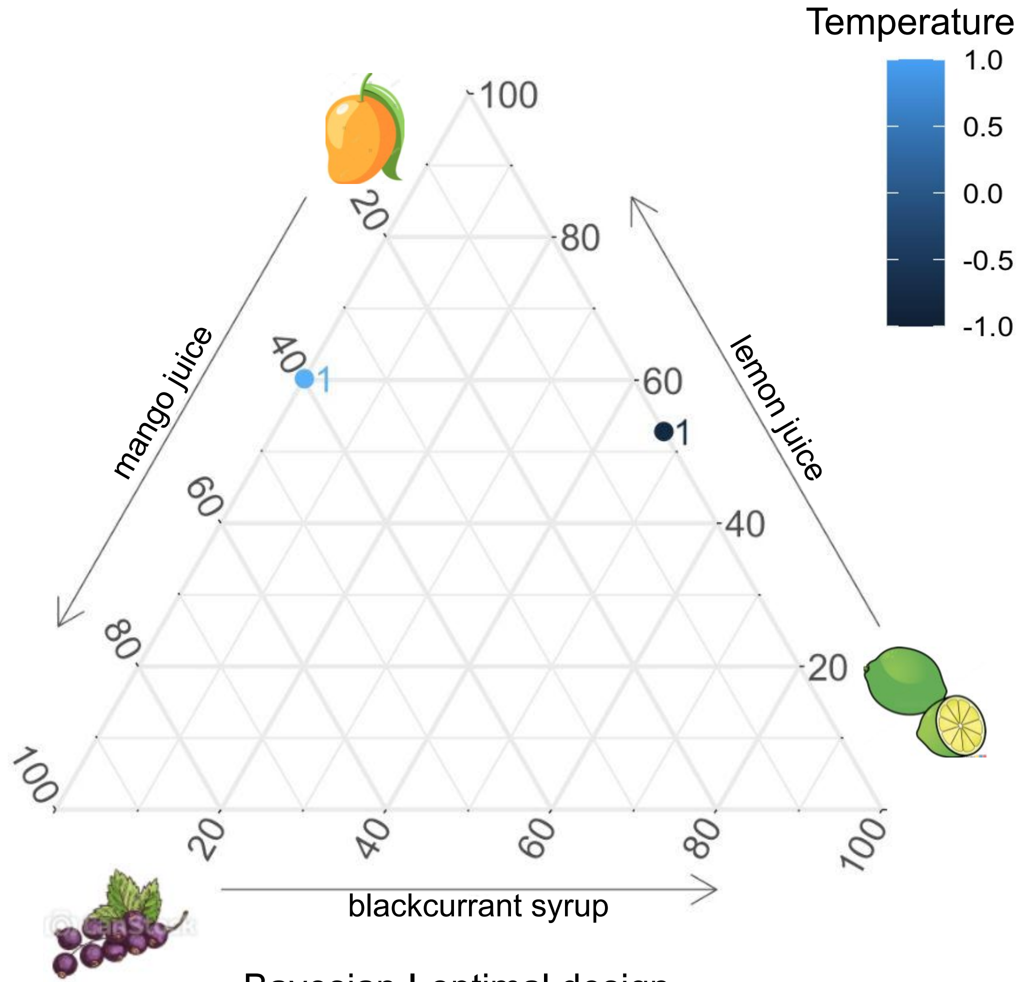

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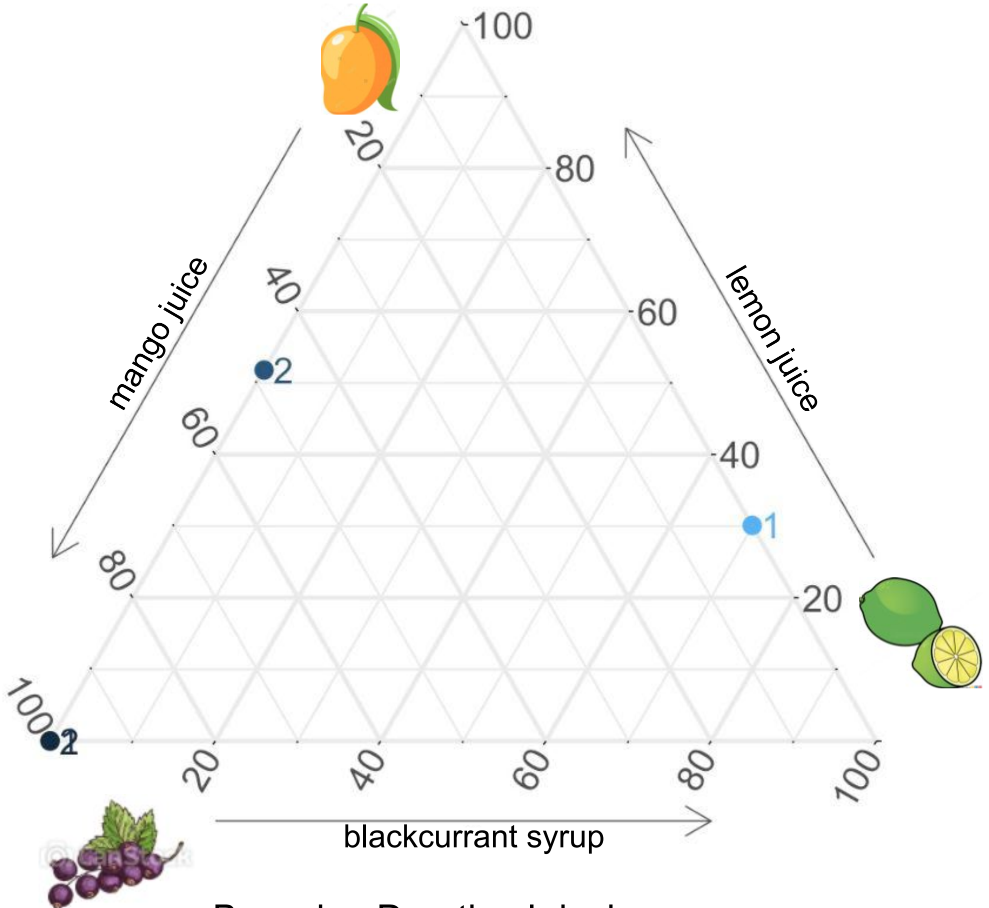

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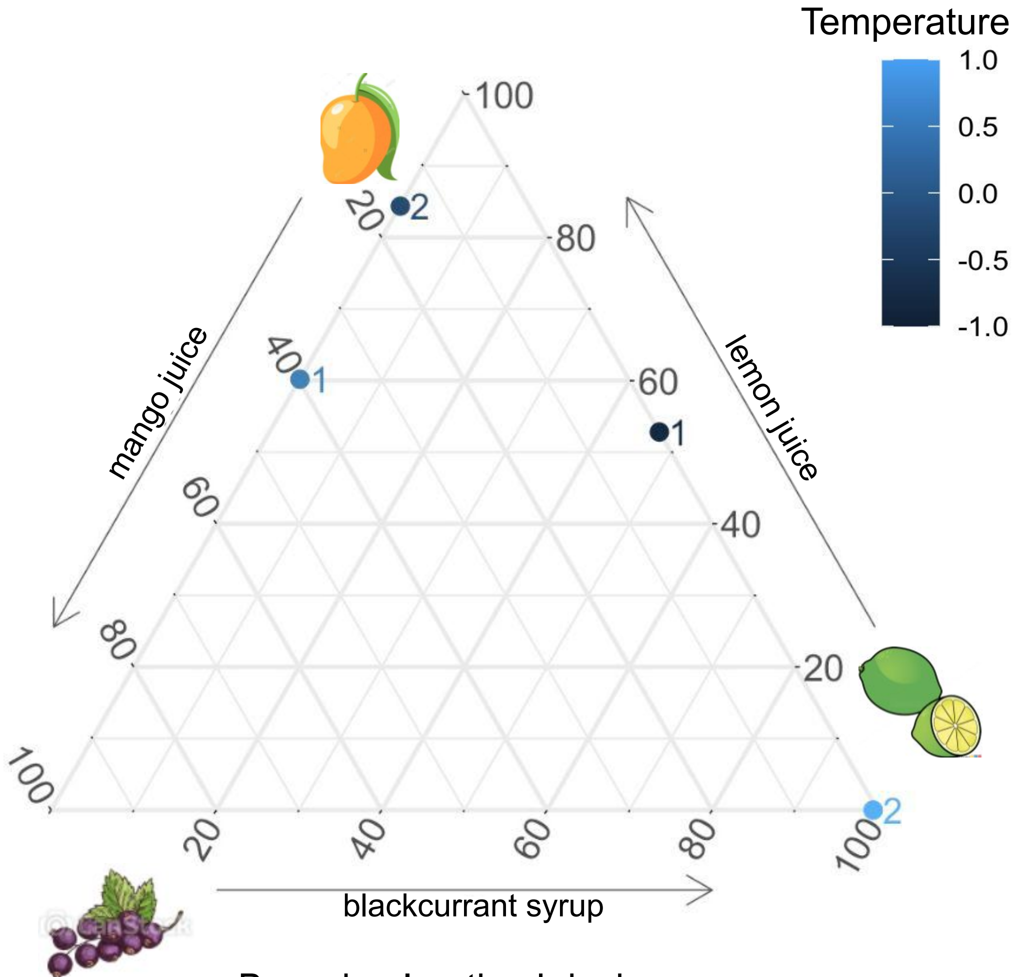

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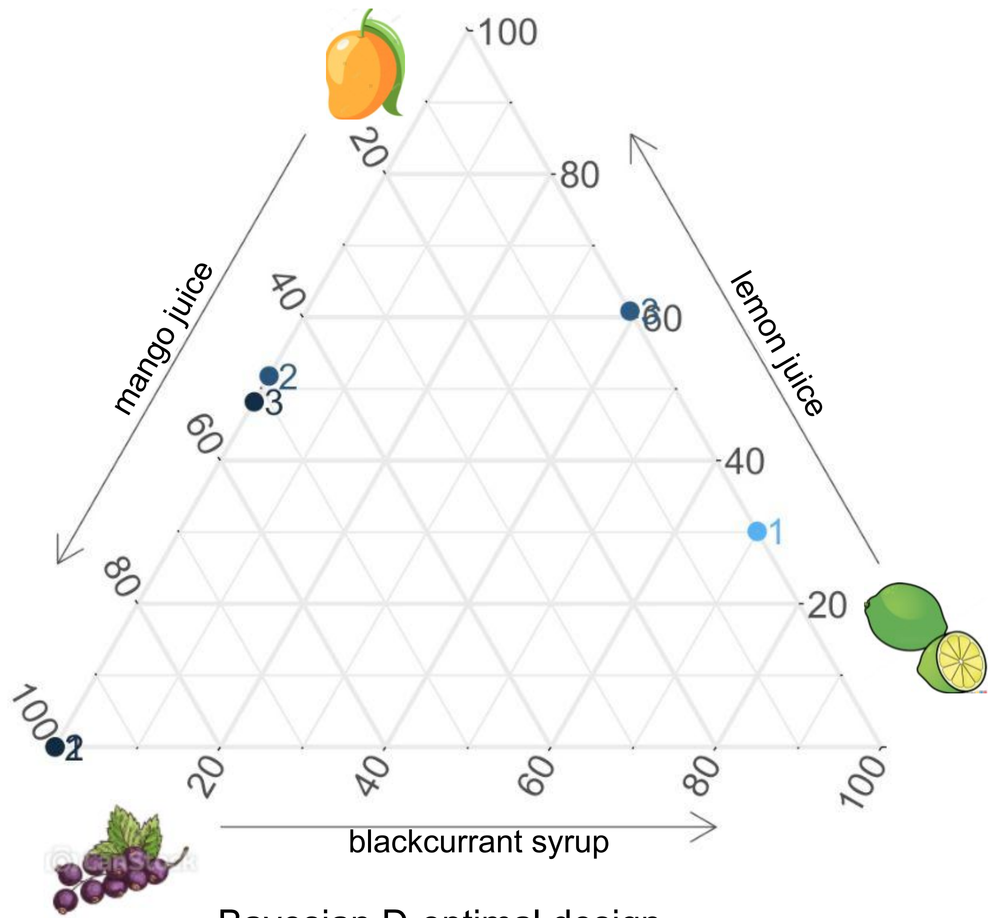

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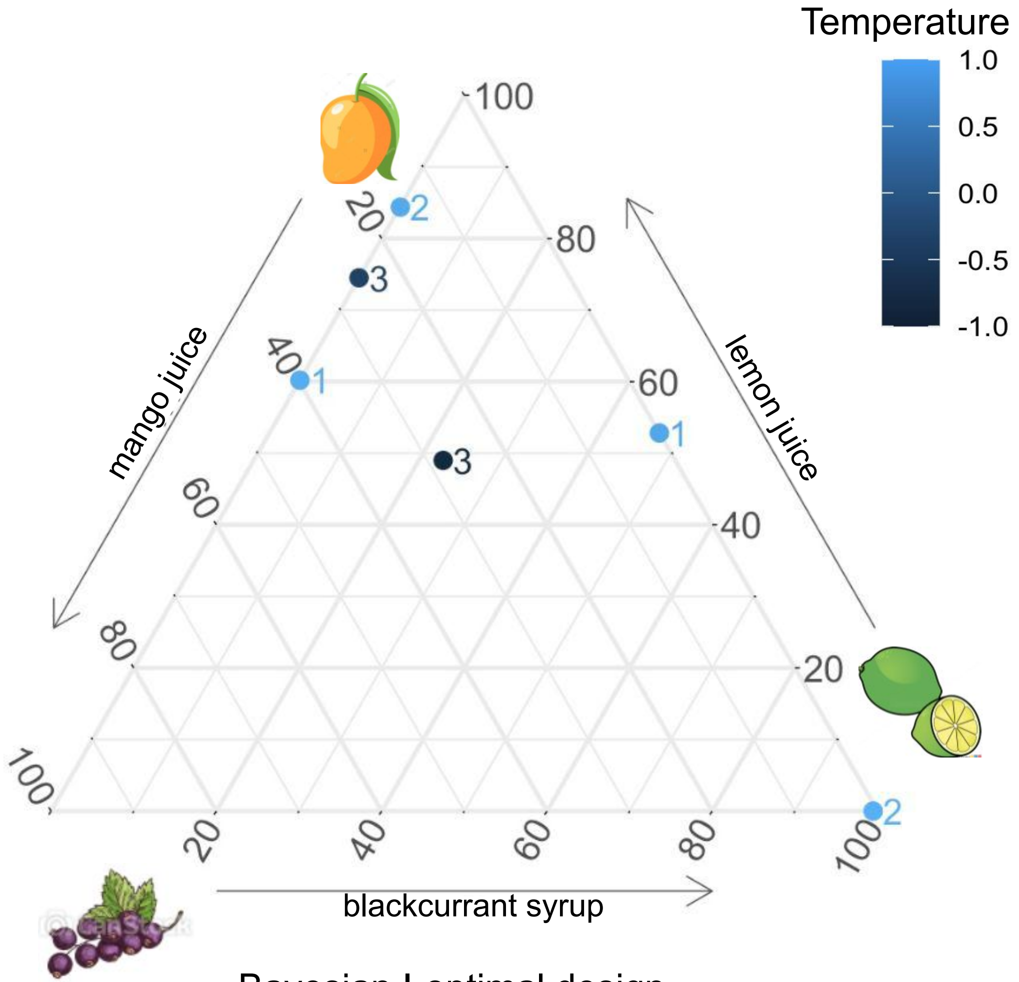

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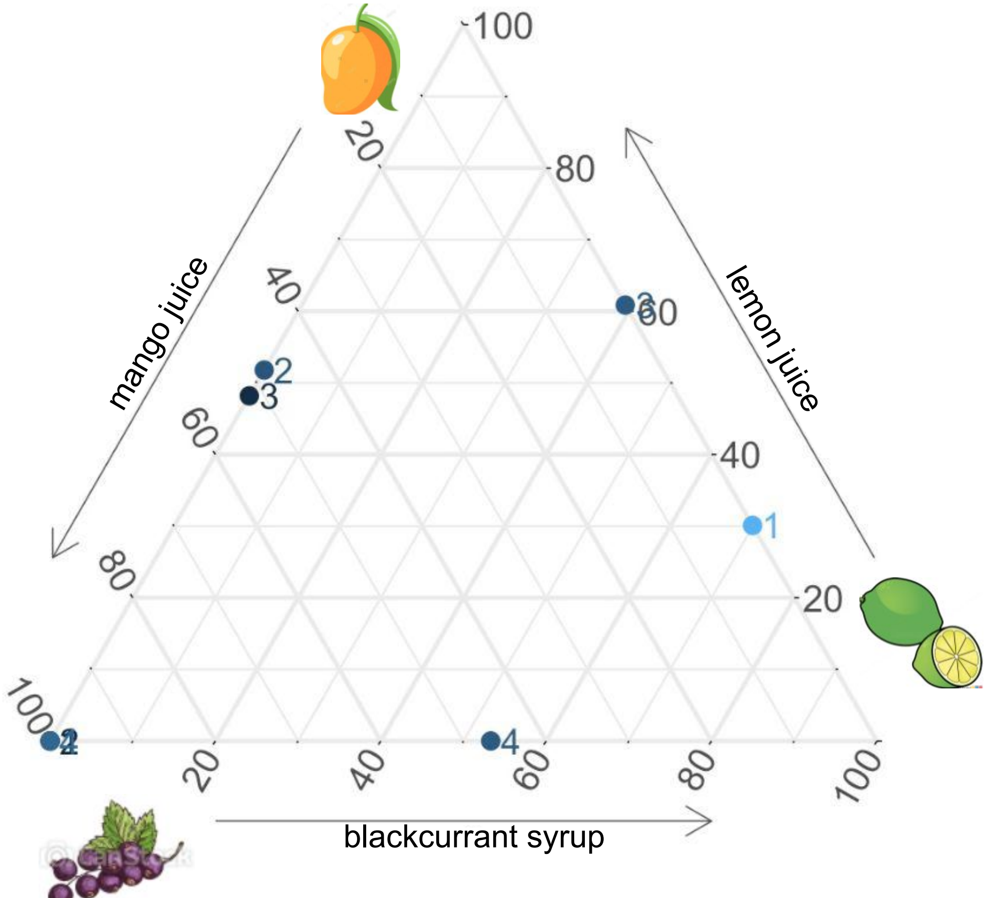

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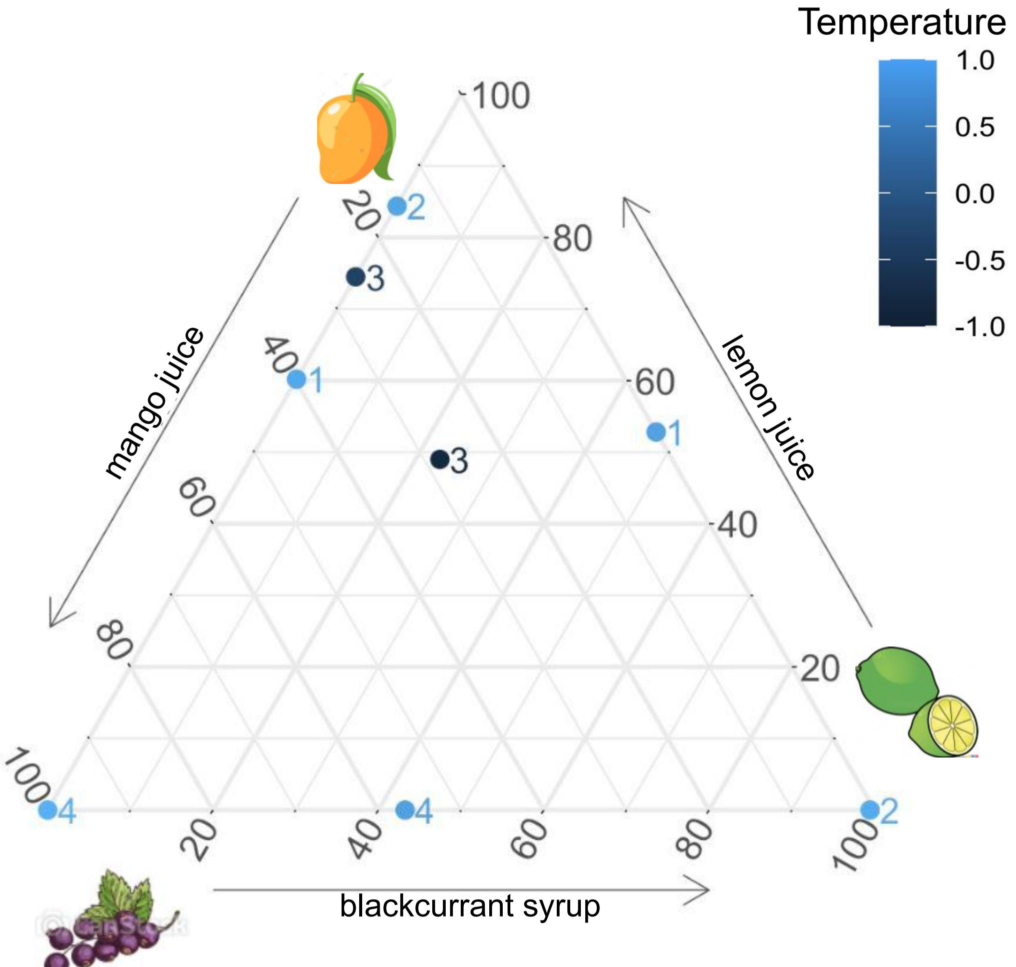

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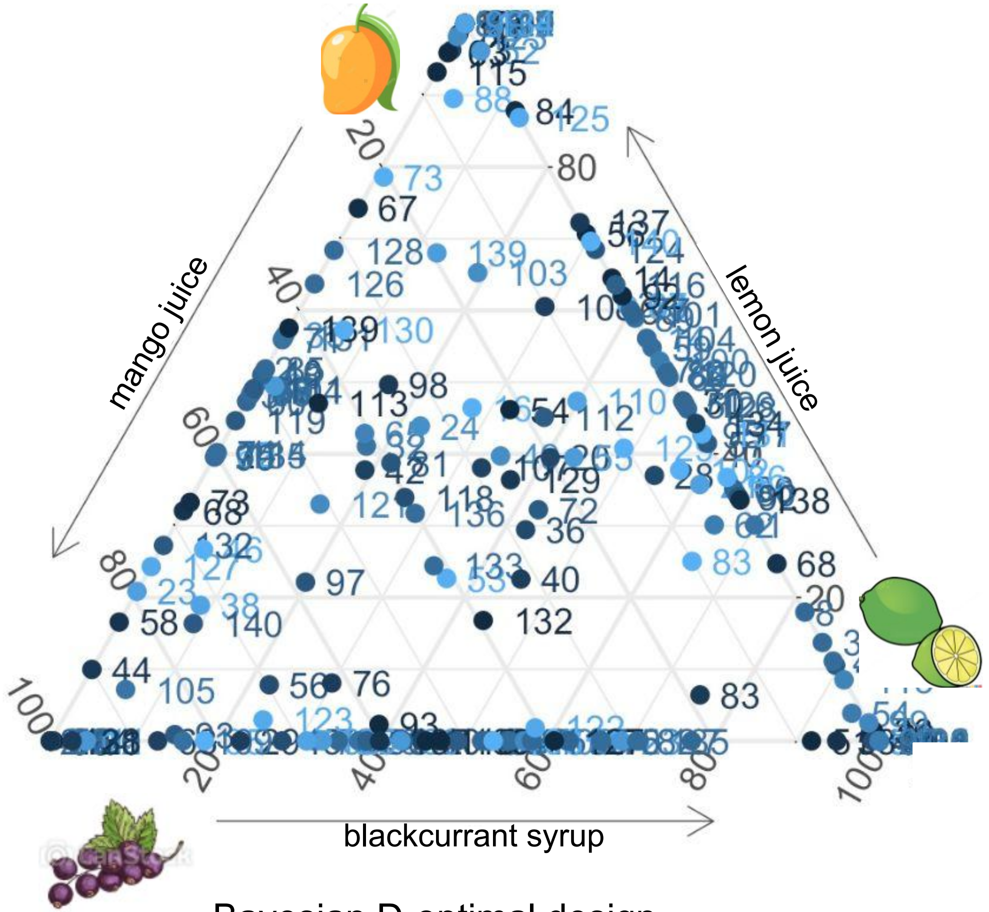

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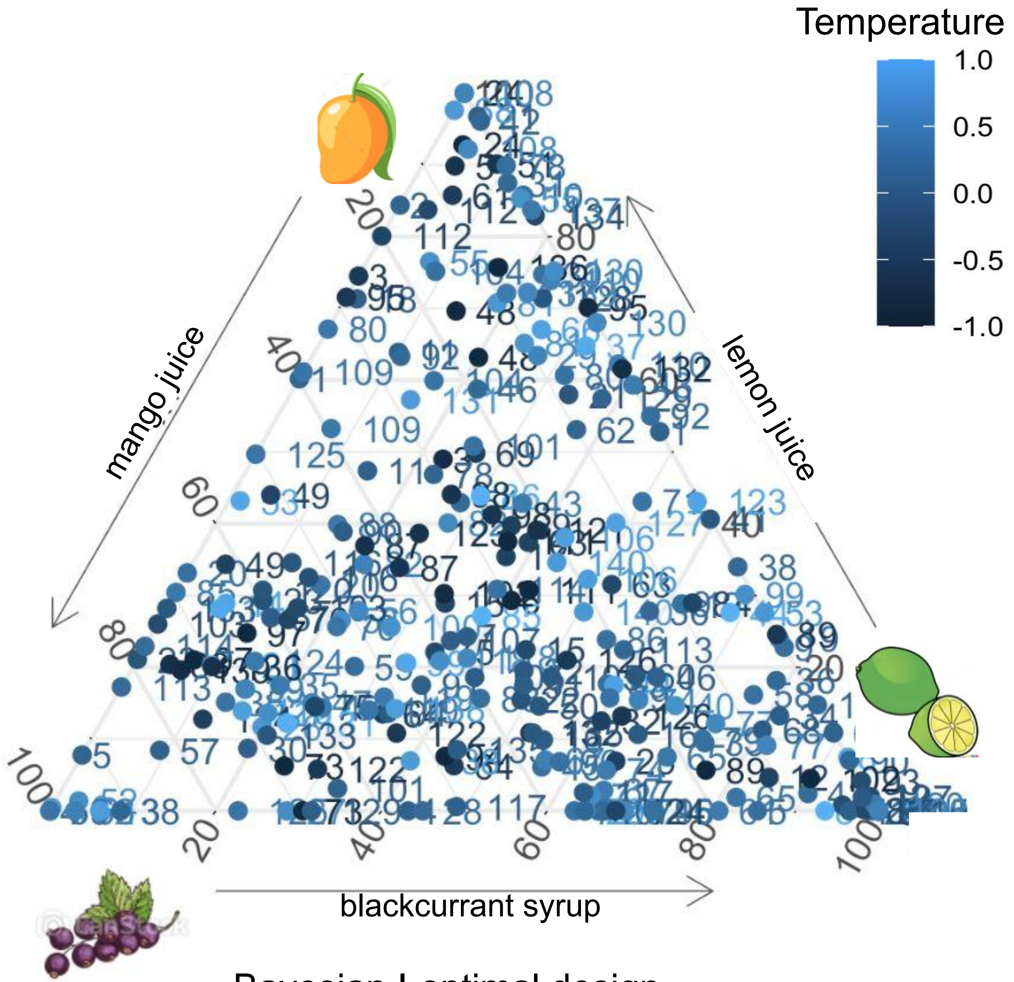

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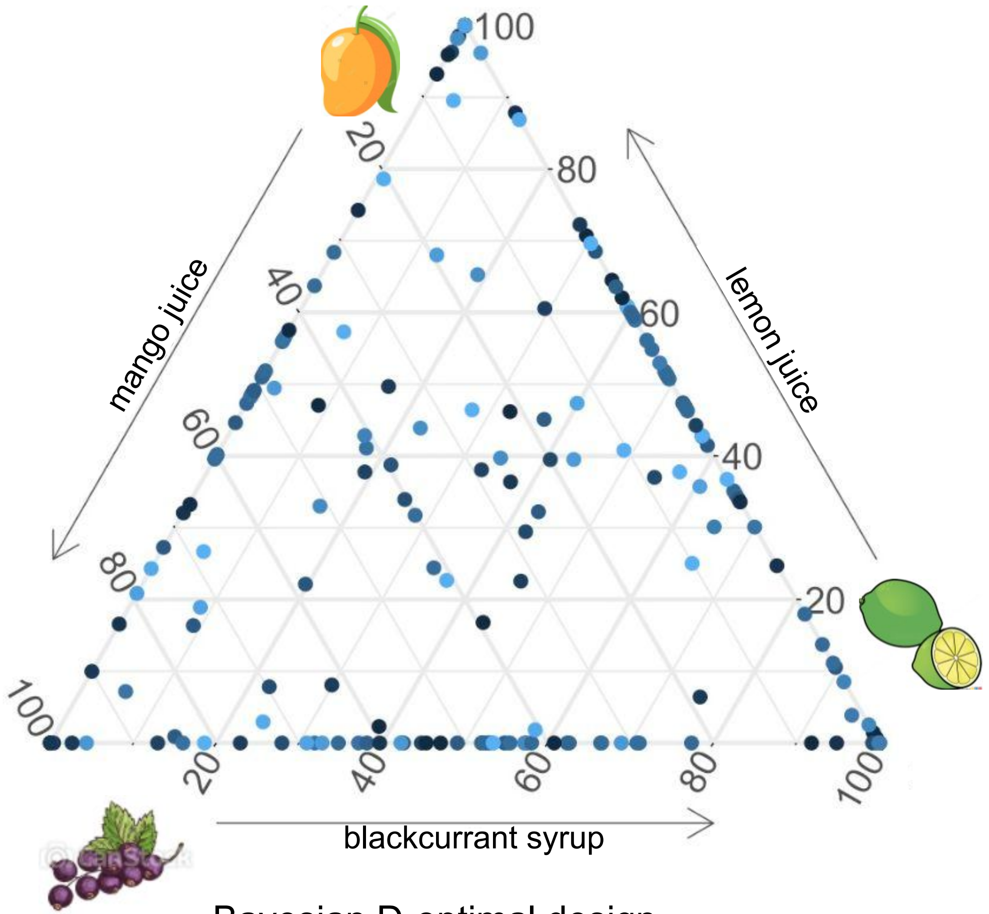

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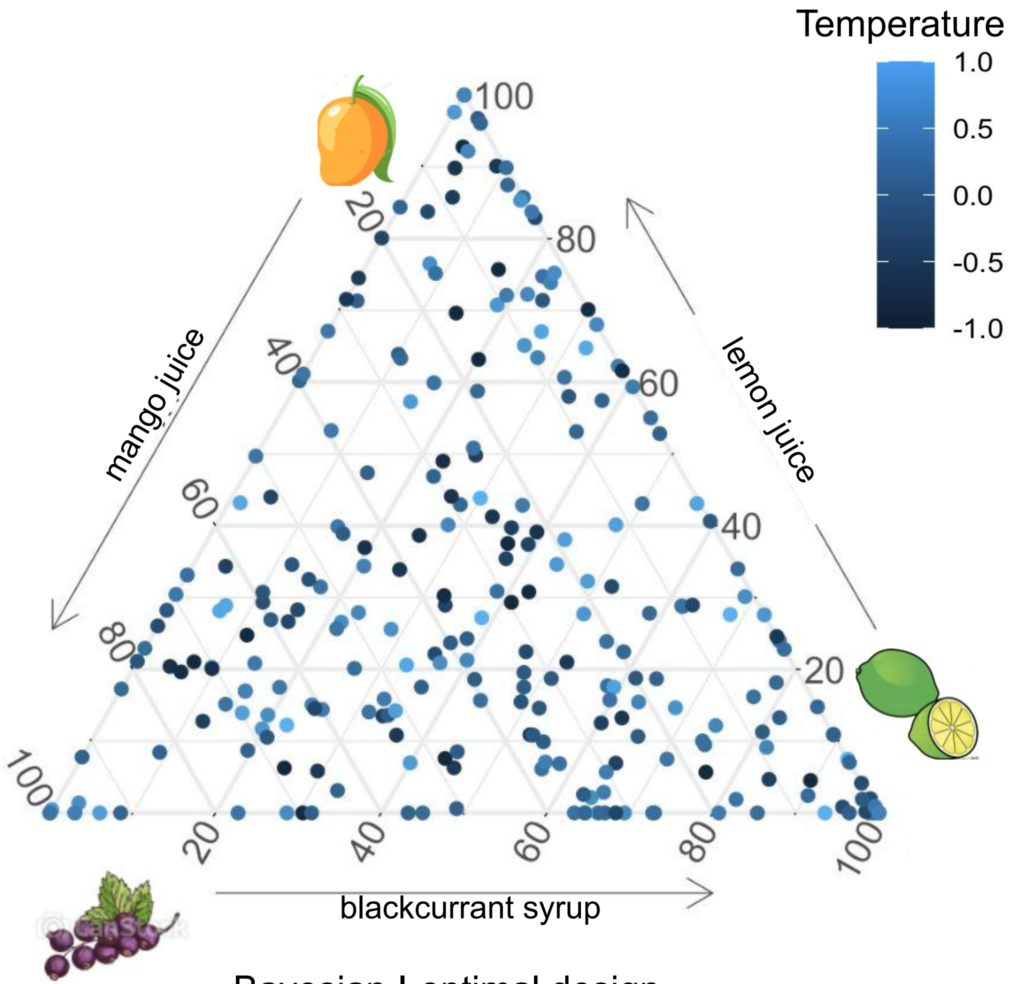

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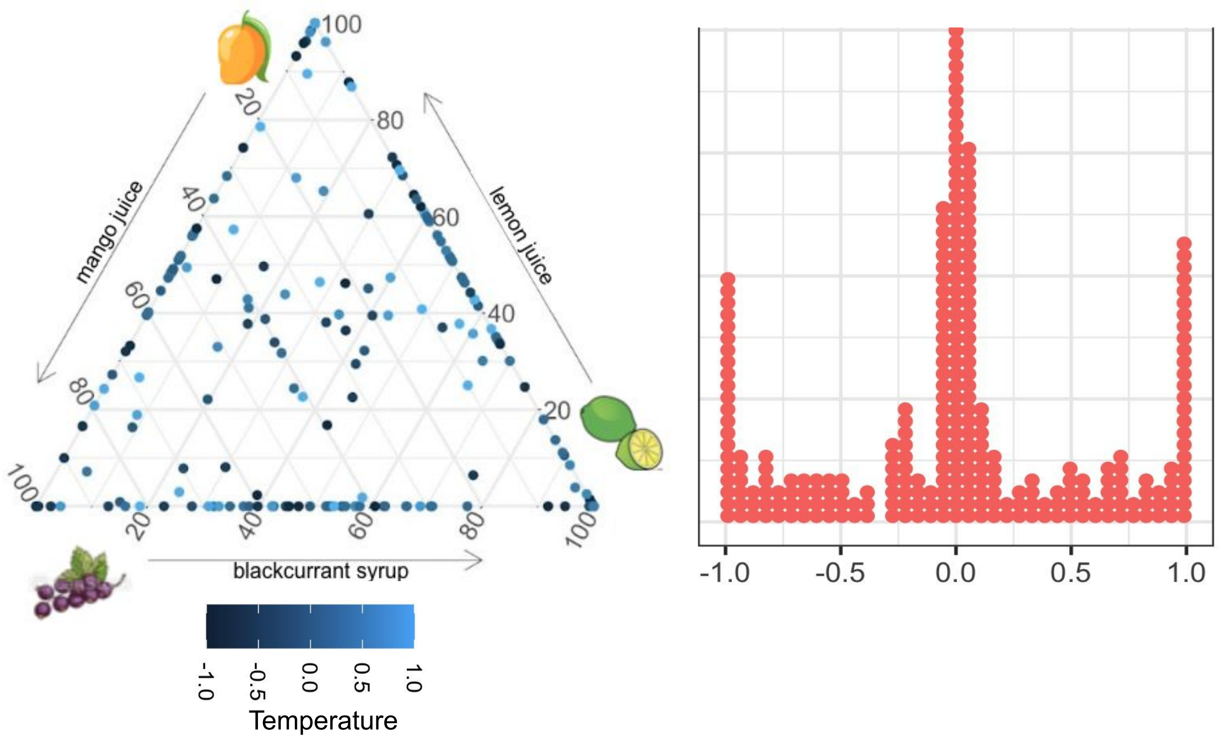

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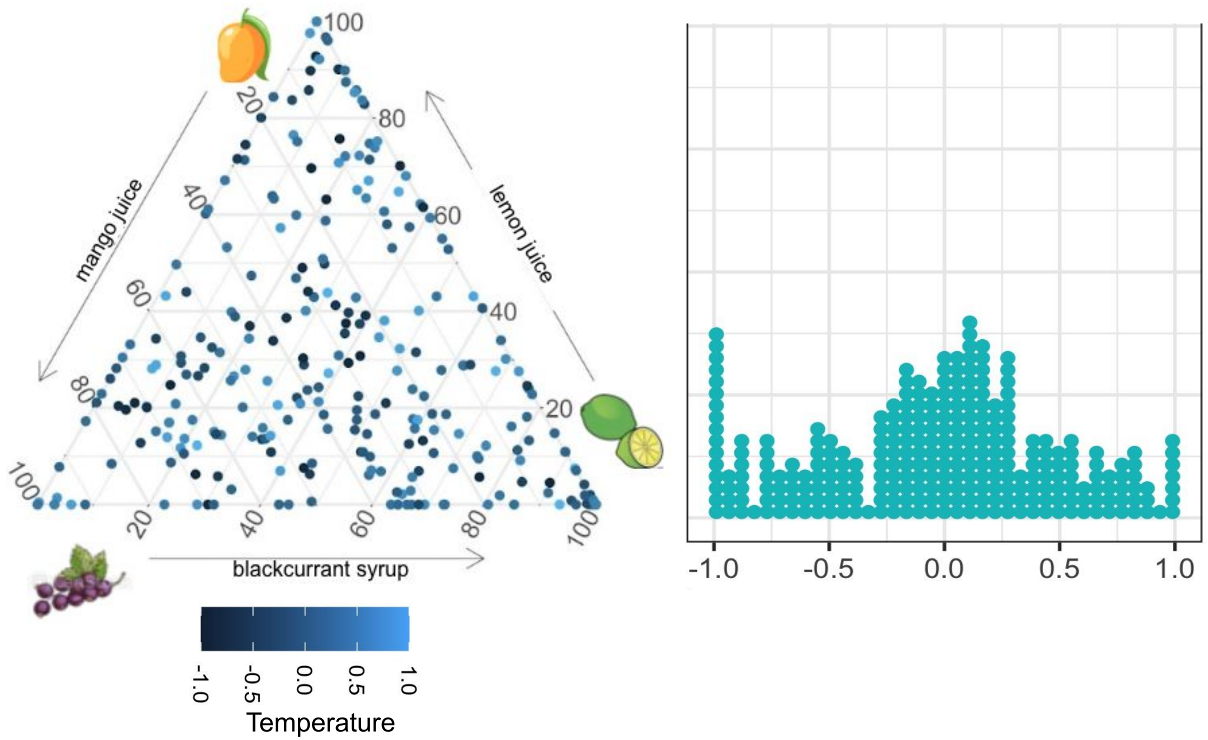

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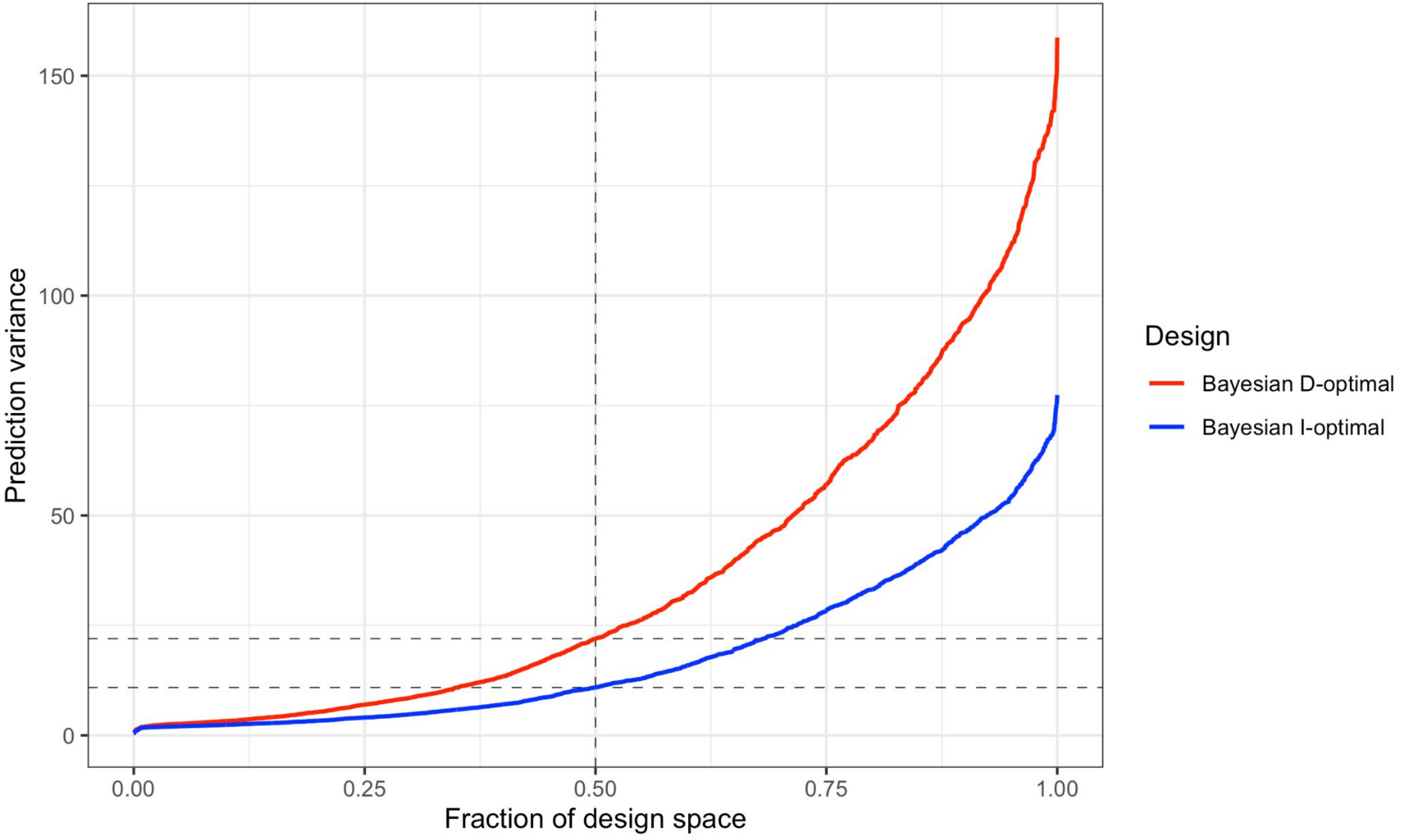

Fish patty experiment

Fish patty experiment

- Experiment from the 1980s by Cornell

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- Interest in firmness of patties

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    - oven cooking temperature (375 or 425 degrees Fahrenheit)

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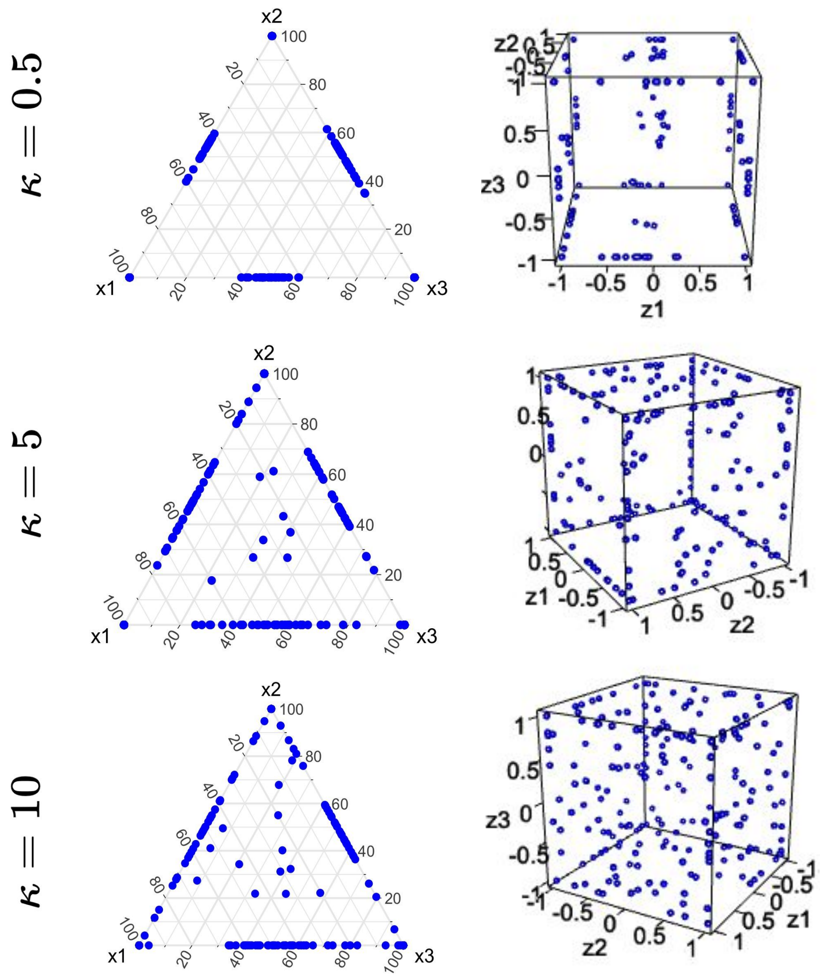
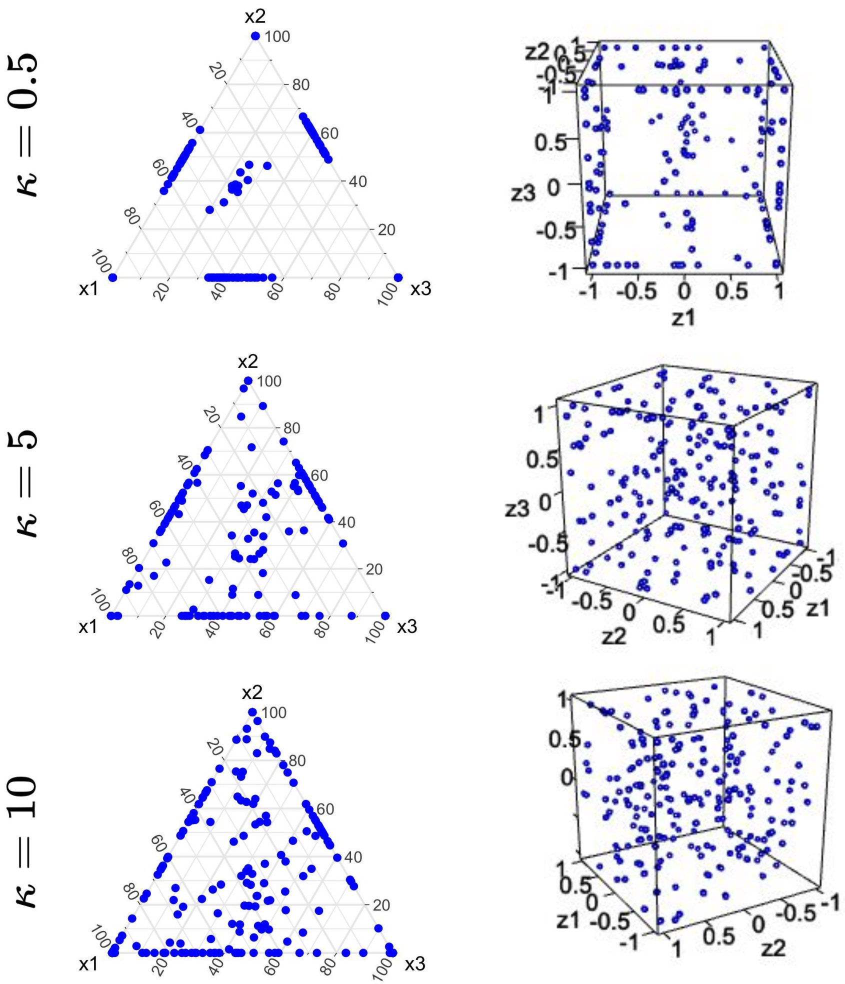
- Assuming firmness is proportional to utility
- Point estimates with 3 levels of uncertainty controlled by κ parameter

Fish patty experiment

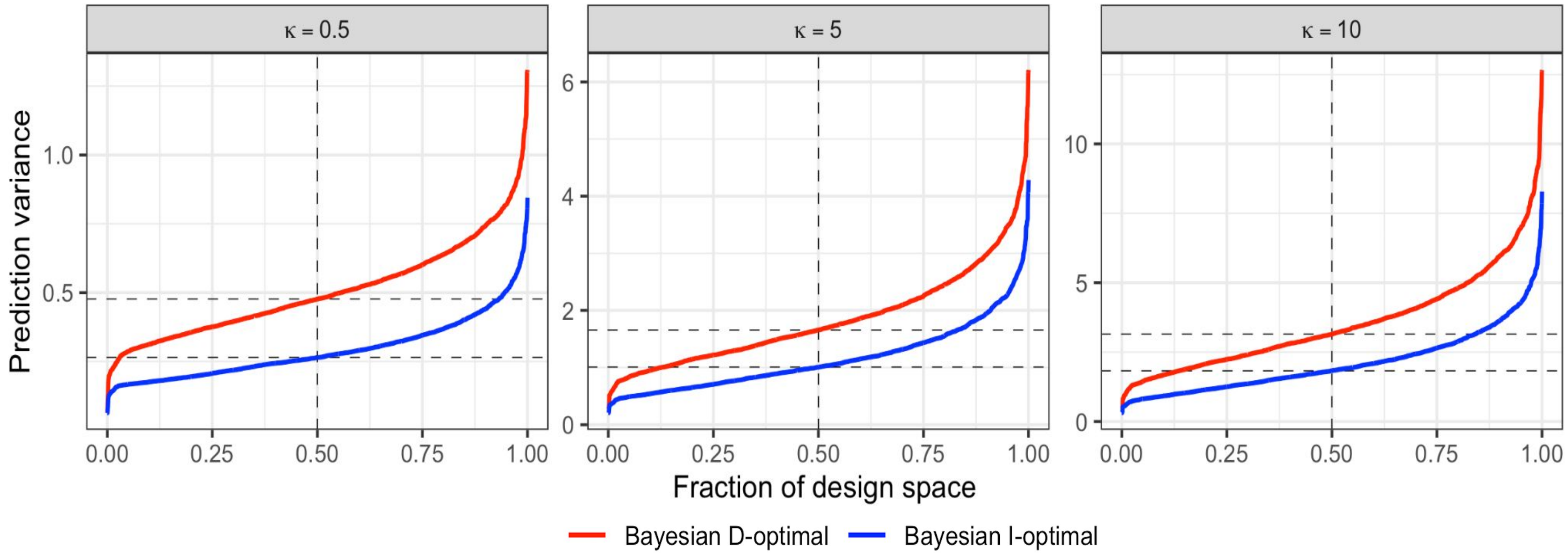
D-optimal



I-optimal



Fish patty experiment



Final remarks

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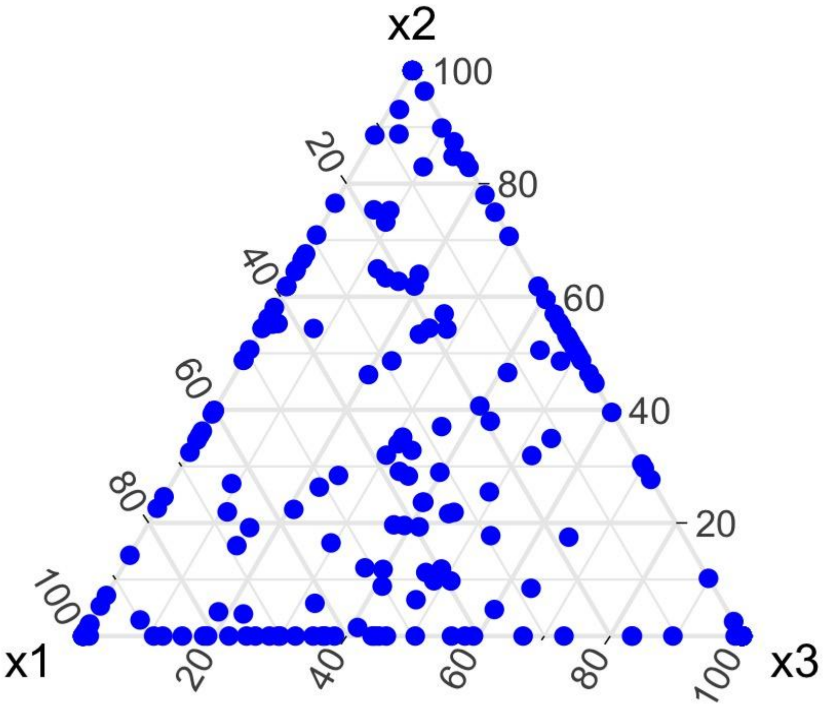
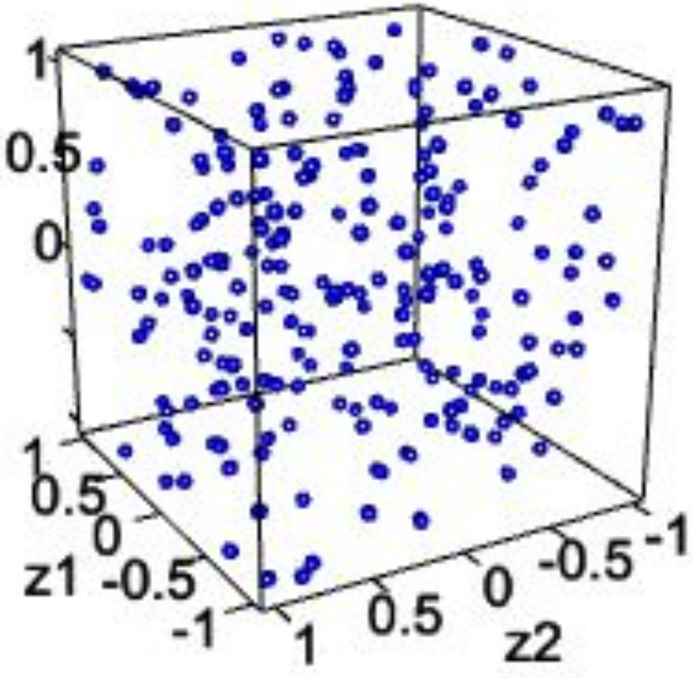

x2
100
20
80
40
60
60
40
80
20
100
x1
20
40
60
80
100
x3


1
0.5
0
1
0.5
0
z1 -0.5
-1
1
0.5
0
-0.5
-1
z2

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- Extending the algorithm to find designs with an upper bound on the number of distinct mixtures and/or an upper bound on the number of distinct choice sets
- Models that take into account possible presence of consumer heterogeneity

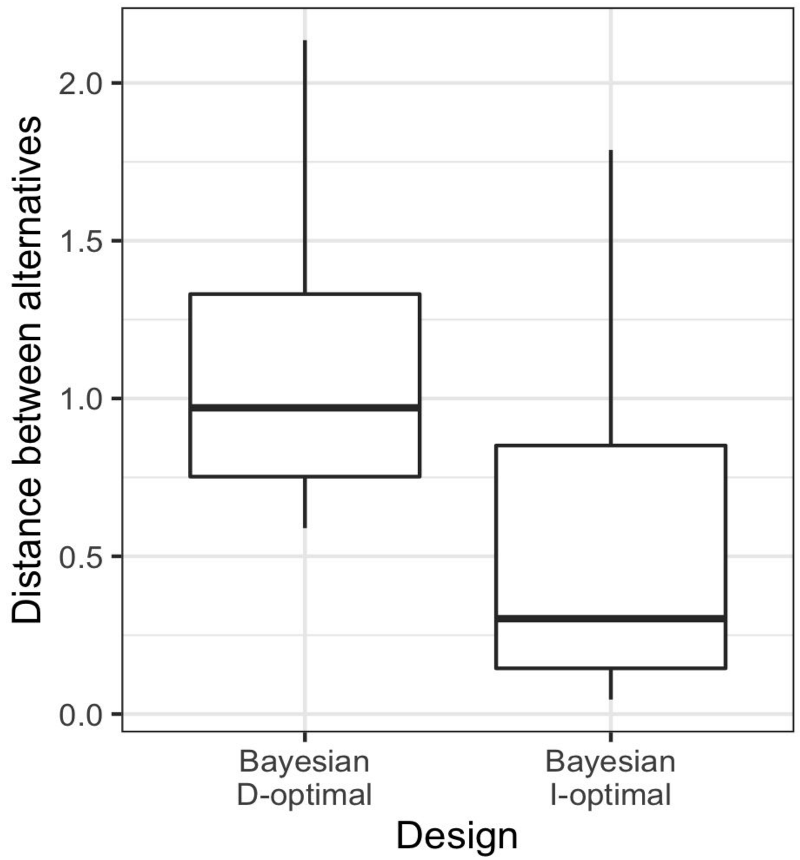
More information

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

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

Thank you

Extra: Cocktail preferences



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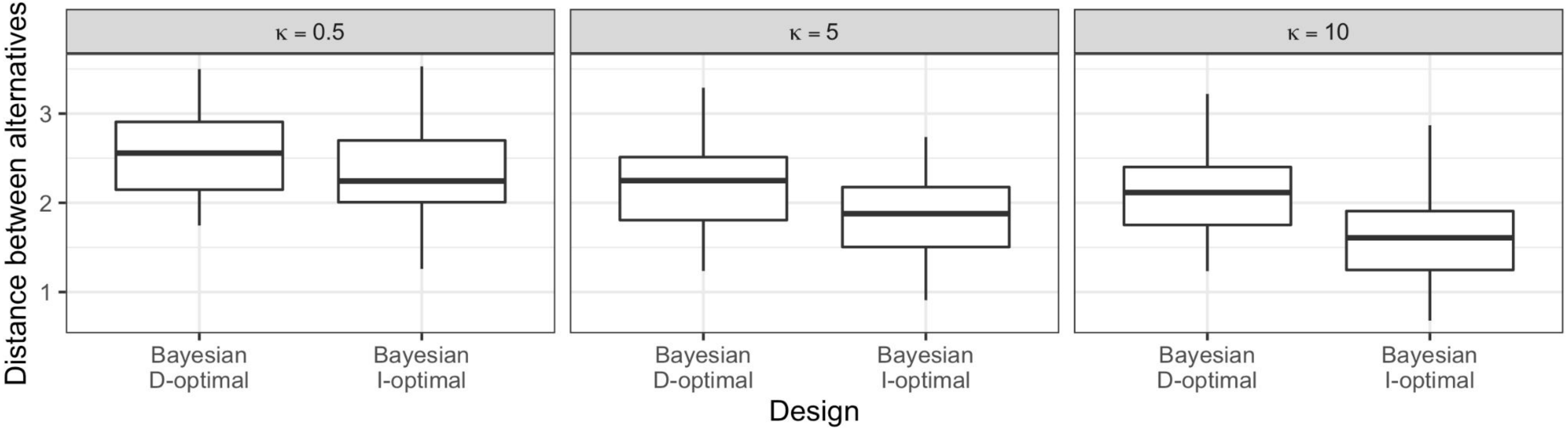


Extra: Optimal design criteria

- 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

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

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

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

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

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

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

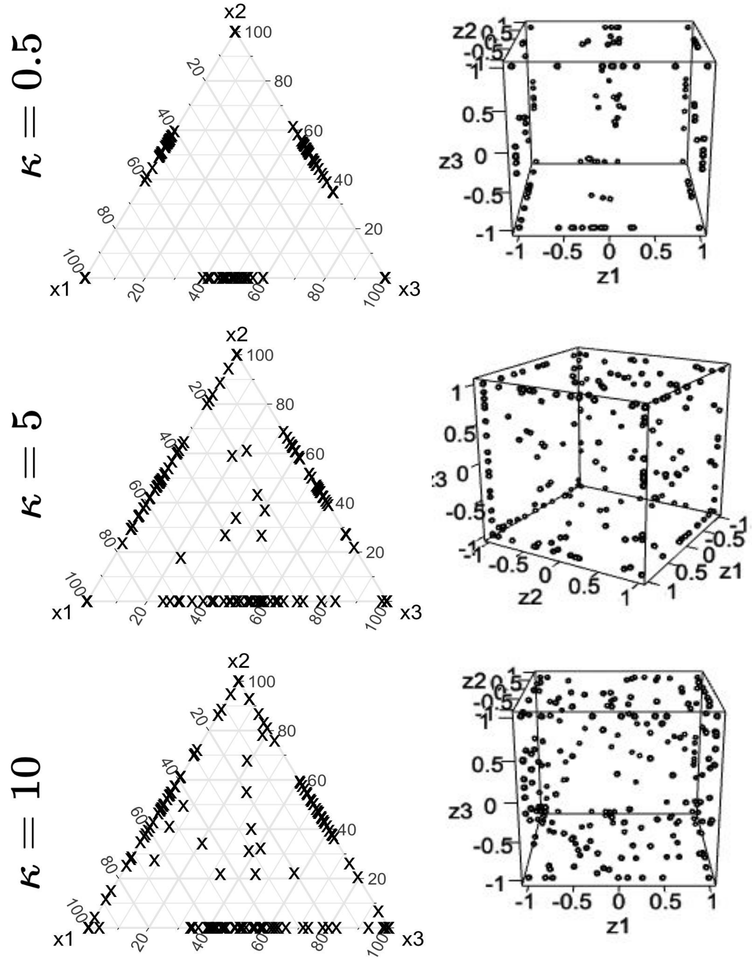
$$\boldsymbol{f}(\boldsymbol{x}_{js}) = (x_{1js}, x_{2js}, \ldots, x_{q-1,js}, x_{1js}x_{2js}, \ldots, x_{q-1,js}x_{qjs}, x_{1js}x_{2js}x_{3js}, \ldots, x_{q-2,js}x_{q-1,js}x_{qjs})^T$$

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

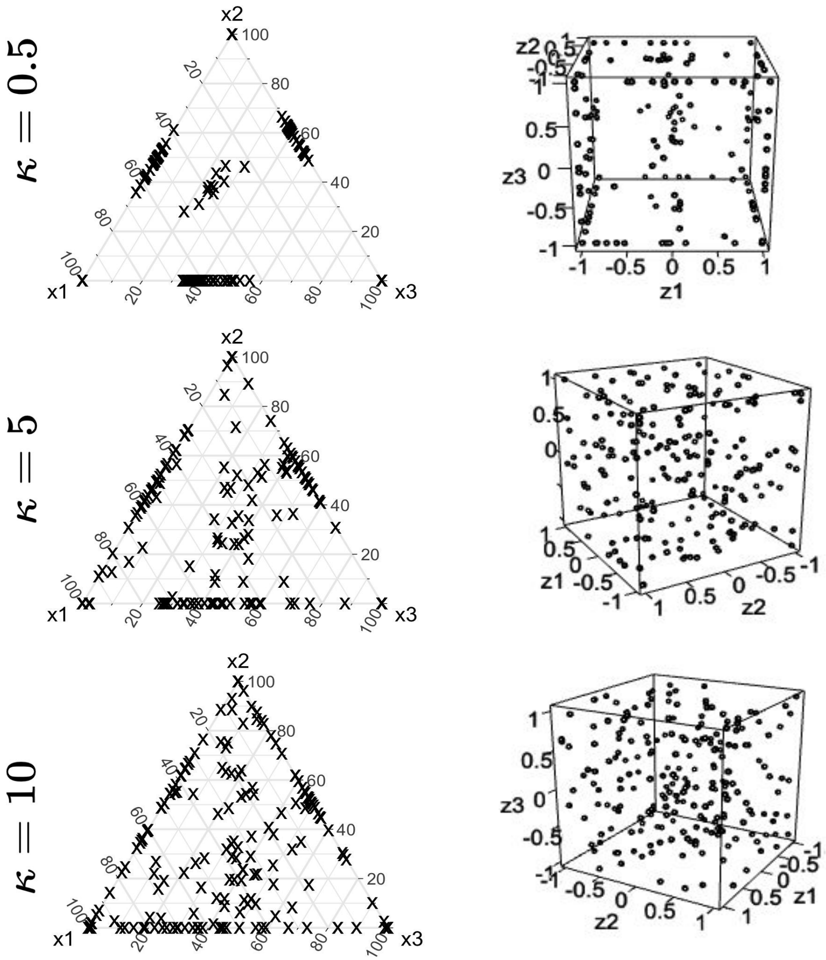
$$\boldsymbol{x}_{js} = (x_{1js}, x_{2js}, \ldots, x_{qjs})^T \qquad \boldsymbol{\beta} = (\beta_1^*, \beta_2^*, \ldots, \beta_{q-1}^*, \beta_{1,2}, \ldots, \beta_{q-1,q}, \beta_{123}, \ldots, \beta_{q-2,q-1,q})^T$$

Fish patty experiment

D-optimal



I-optimal



D-optimal designs

$$\boldsymbol{\beta} = 0$$

- D-optimality criterion

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

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→ $\boldsymbol{\beta} = 0$

→ point estimate

→ prior distribution $\pi(\boldsymbol{\beta})$

Fish patty experiment

- Experiment from the 1980s by Cornell
- Interest in firmness of patties
- Three fish species:
  - mullet
  - sheepshead

KU LEUVEN

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