KU LEUVEN

Bayesian D- and I-optimal designs for choice experiments with mixtures using a multinomial logit model

Mario Becerra
Peter Goos

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
6. Conclusions and future work

Discrete choice experiments

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- Example: a customer responding whether they prefer to buy product A, B or C
- Models assume a latent utility function used to derive the probability of each respondent making each decision

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  - ingredients used to make a cocktail

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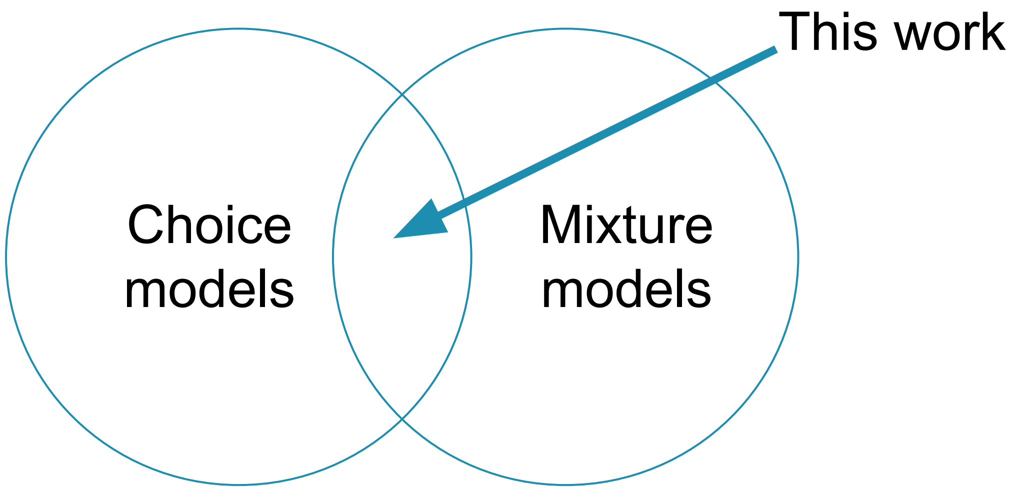
- For us, the characteristic of interest is the **preference** of respondents
- Choice experiments are ideal to collect data for quantifying and modeling preferences for mixtures

Choice experiments with mixtures



Choice experiments with mixtures

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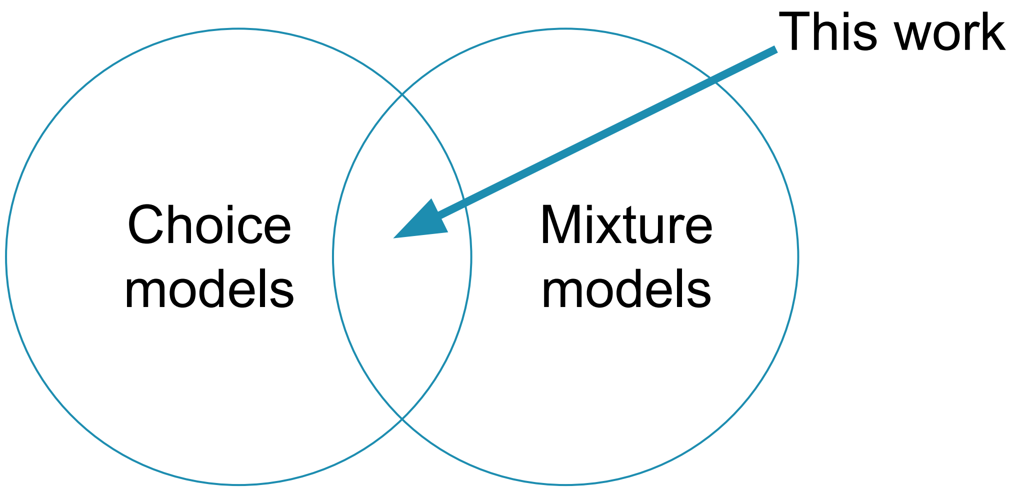

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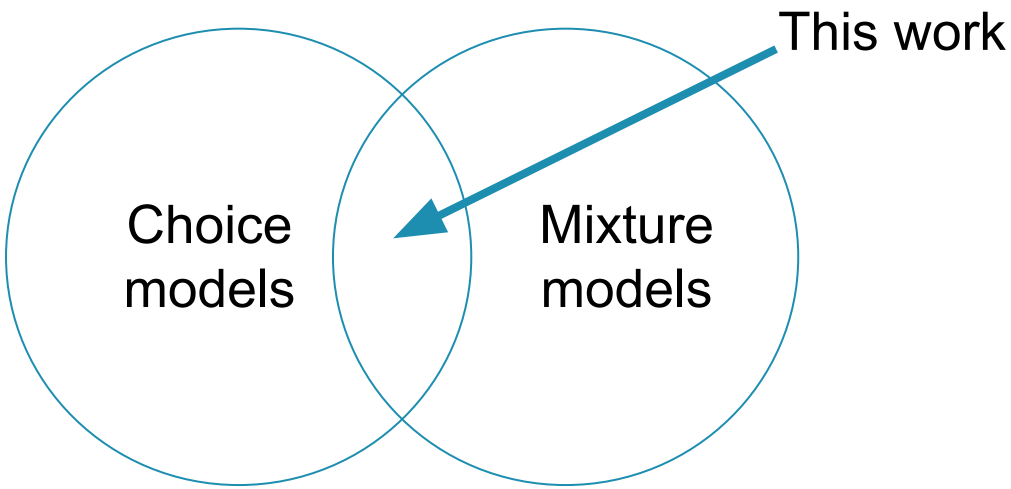

Choice experiments with mixtures

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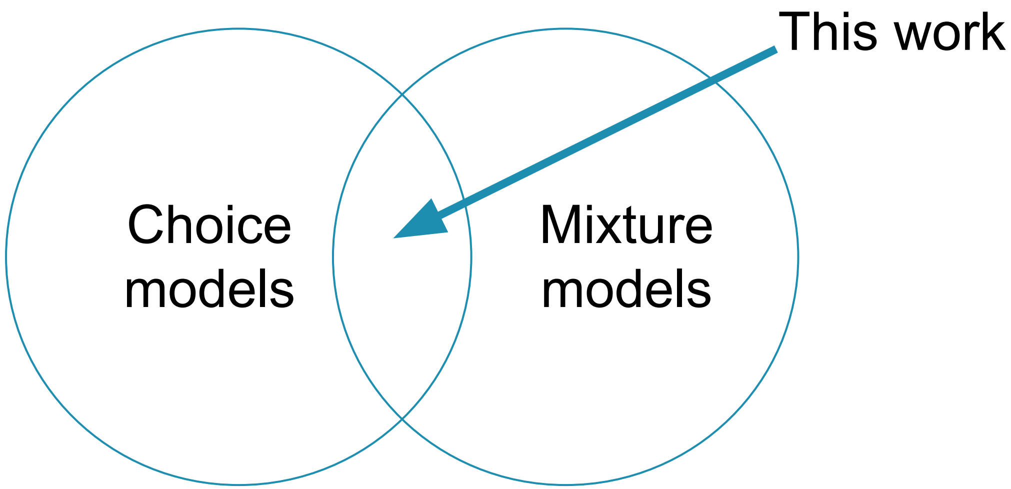
- Preferences for cocktails involving different proportions of mango juice, lime juice, and blackcurrant syrup
- Experimental data involved the responses of sixty people, each making eight pairwise comparisons of different cocktails



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- Optimal design of experiments is the branch of statistics that deals with the construction of efficient experimental designs

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- I-optimal designs are more suitable

Models for data from mixture experiments

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- Each mixture is described as a combination of *q* ingredient proportions, with the constraint that these proportions sum up to one
- Dedicated models are needed to avoid perfect collinearity
- Special-cubic Scheffé model:

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

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- 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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- Perceived utility modeled as

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

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

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- We used the same prior distribution to compute Bayesian D- and I-optimal designs using a coordinate-exchange algorithm

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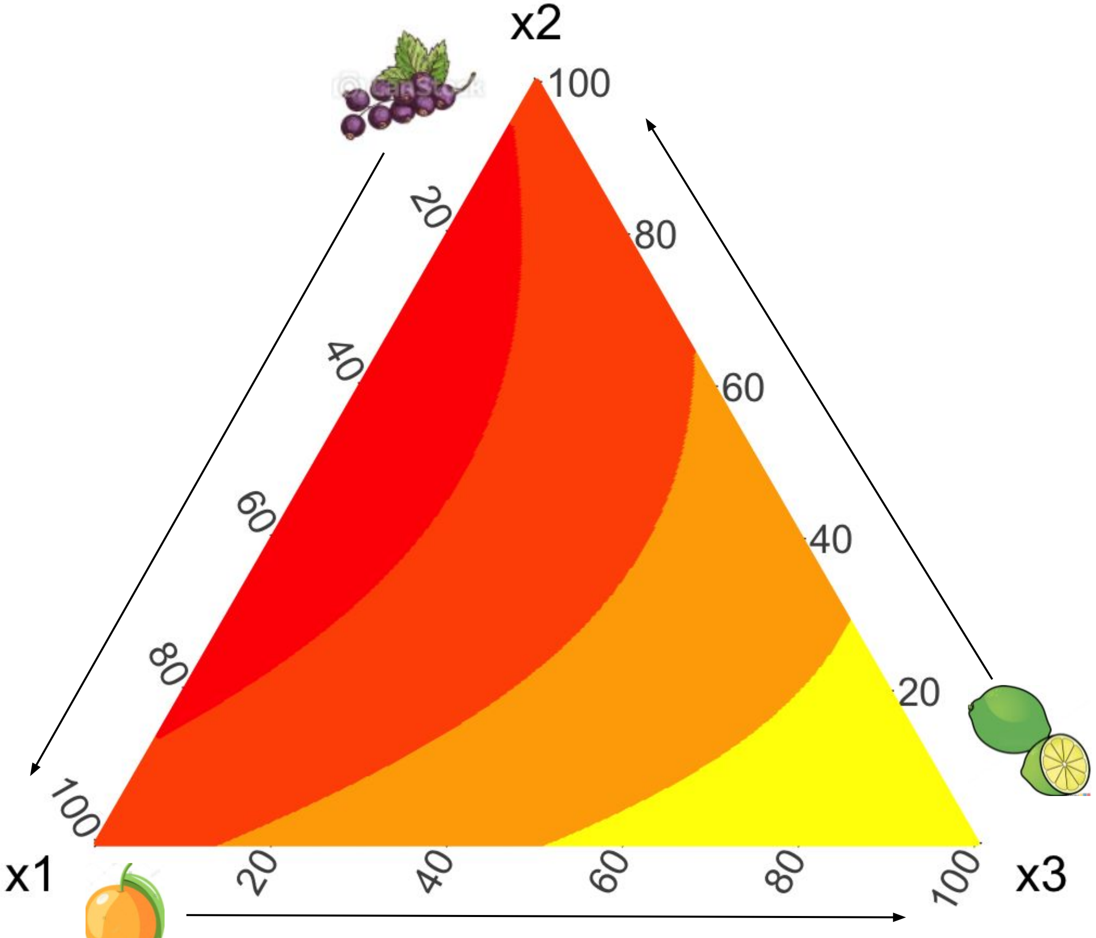

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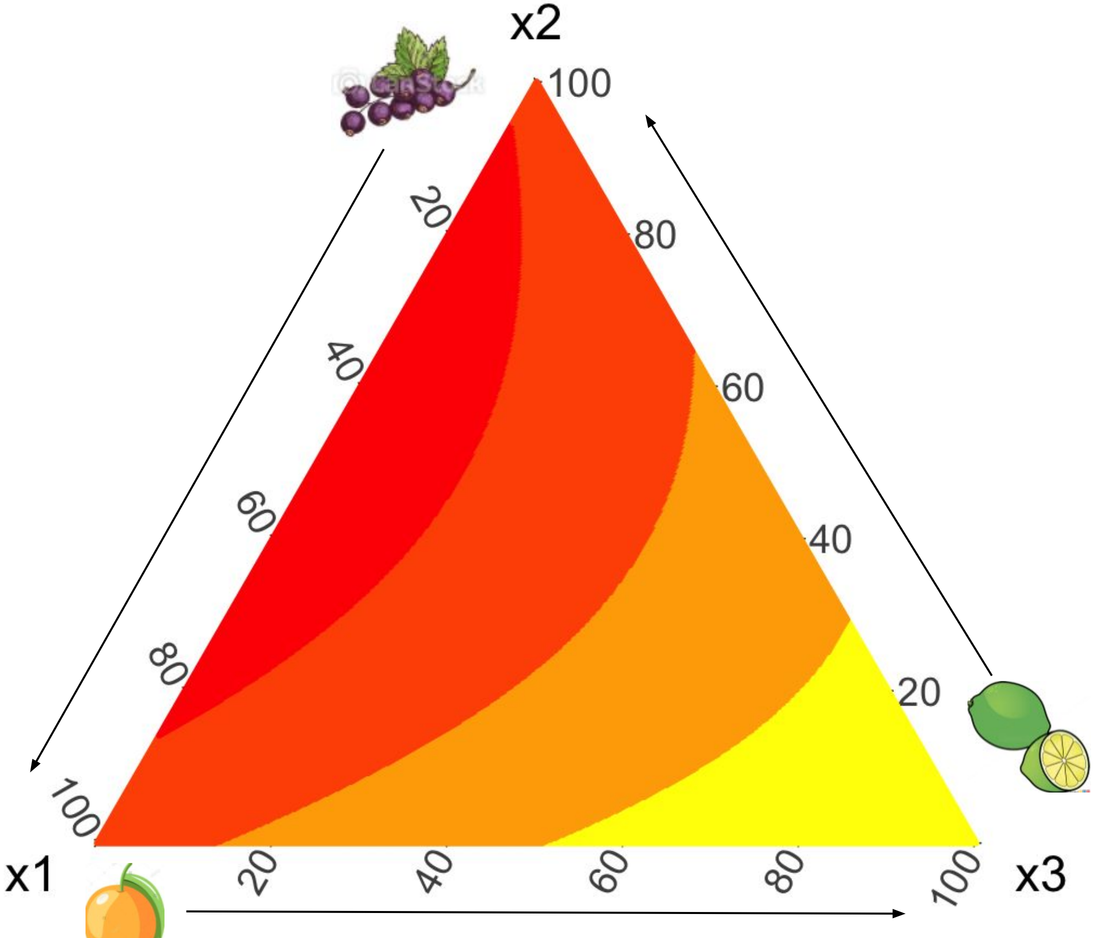

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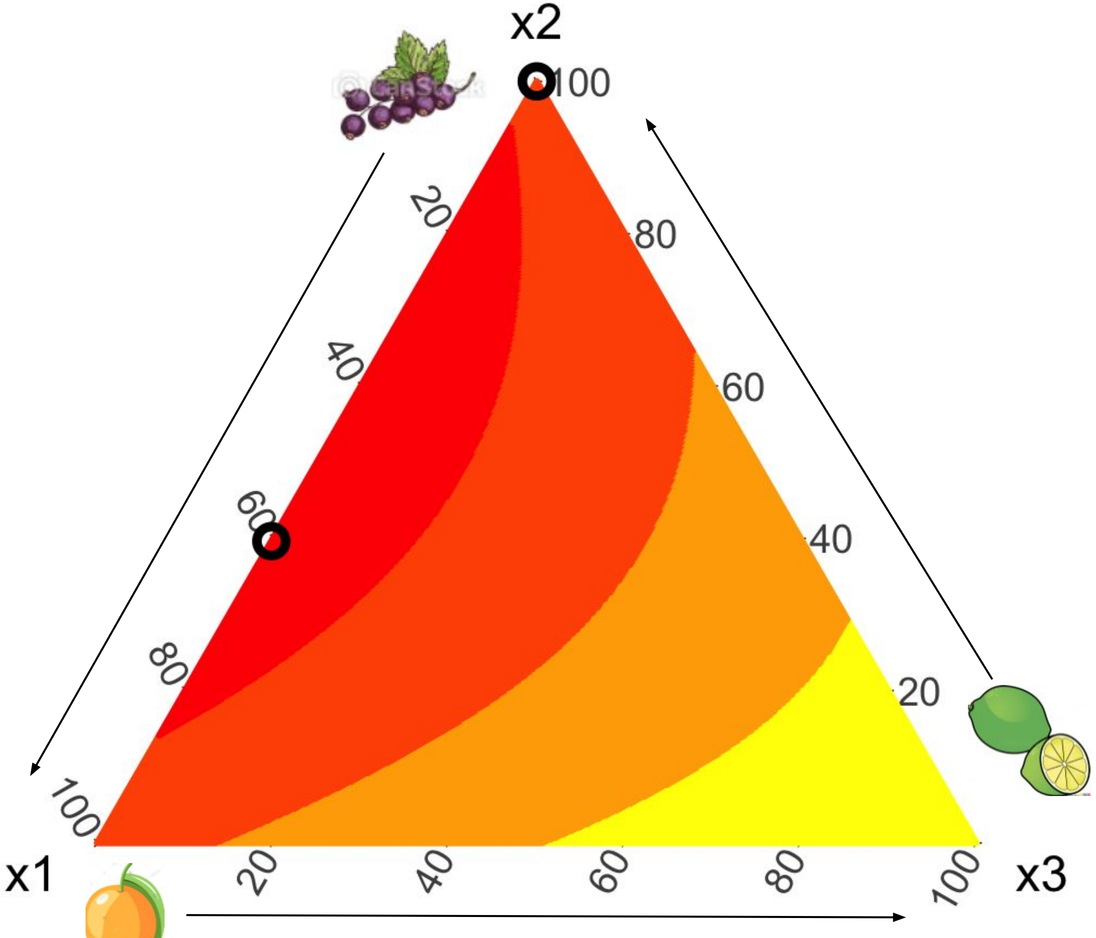

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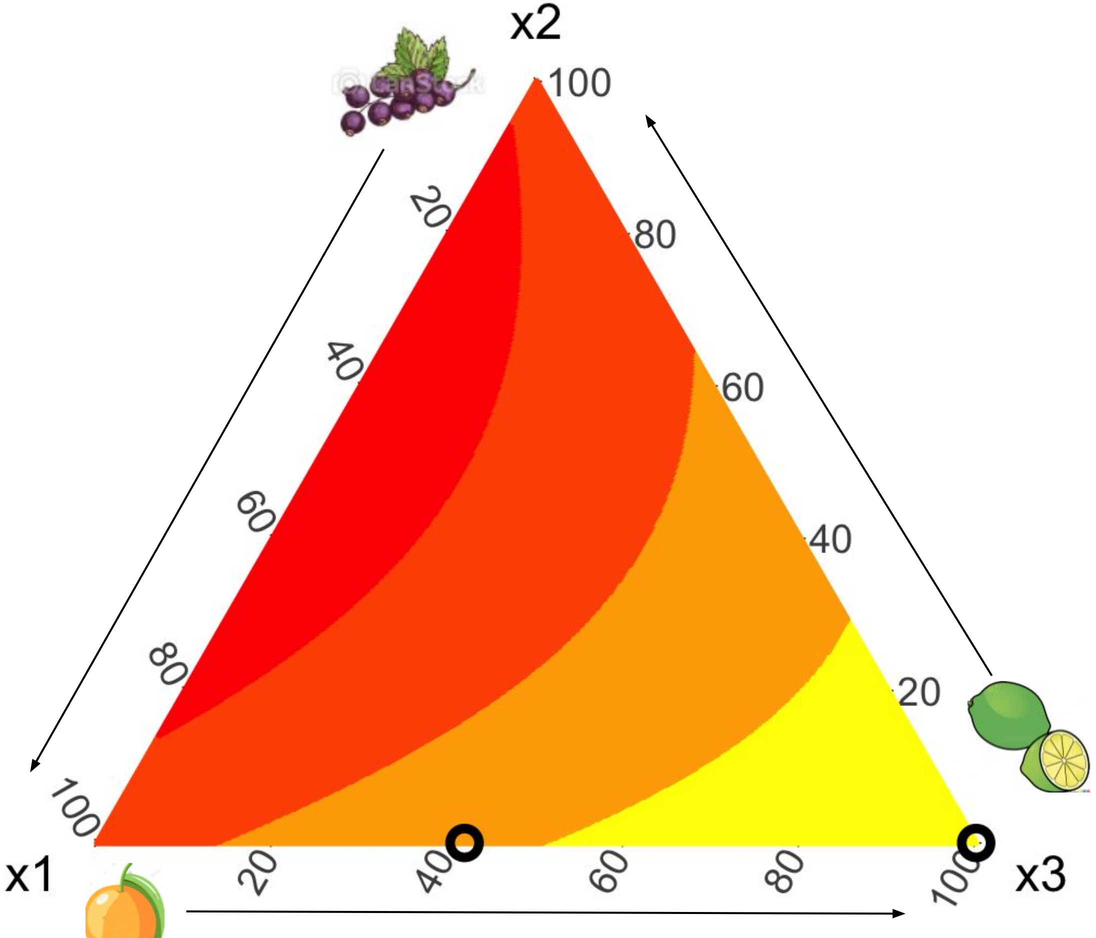

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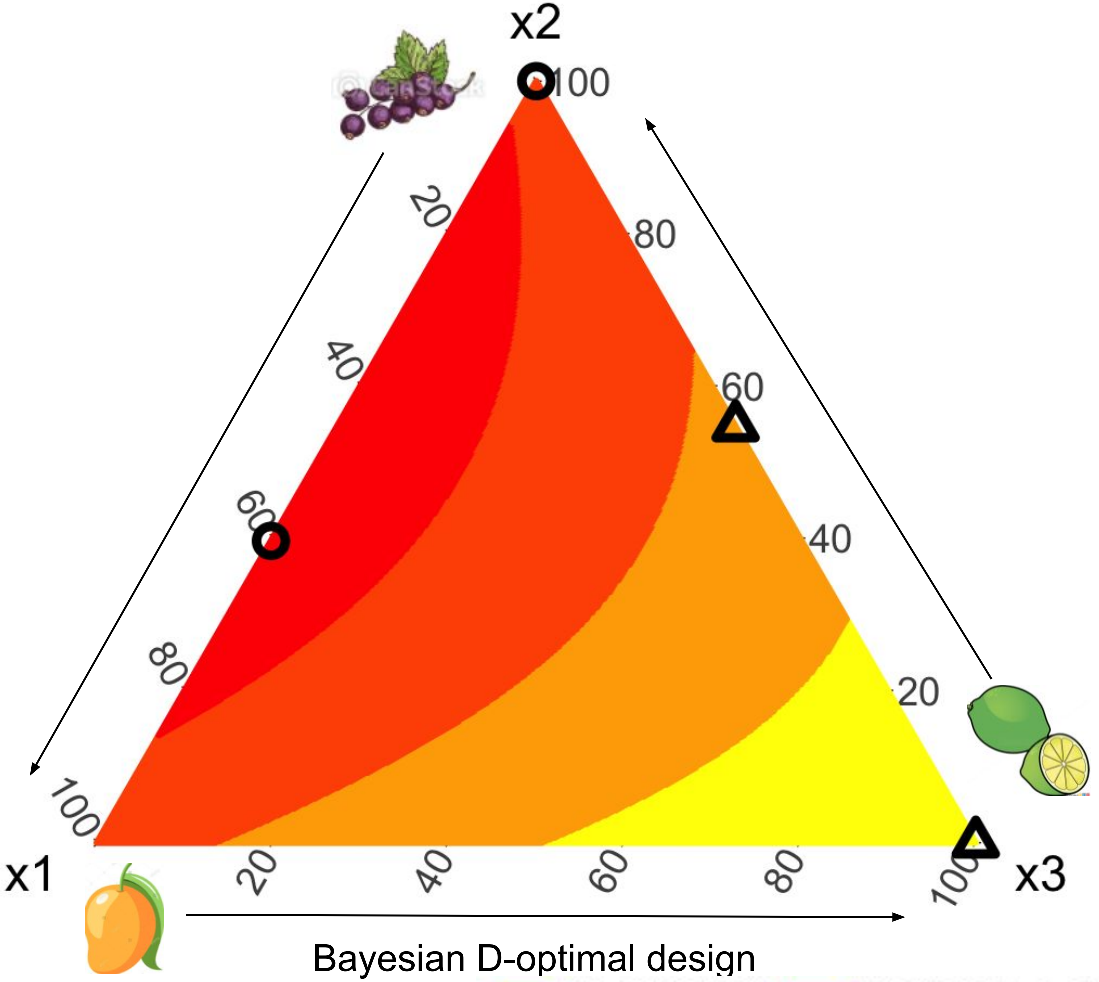

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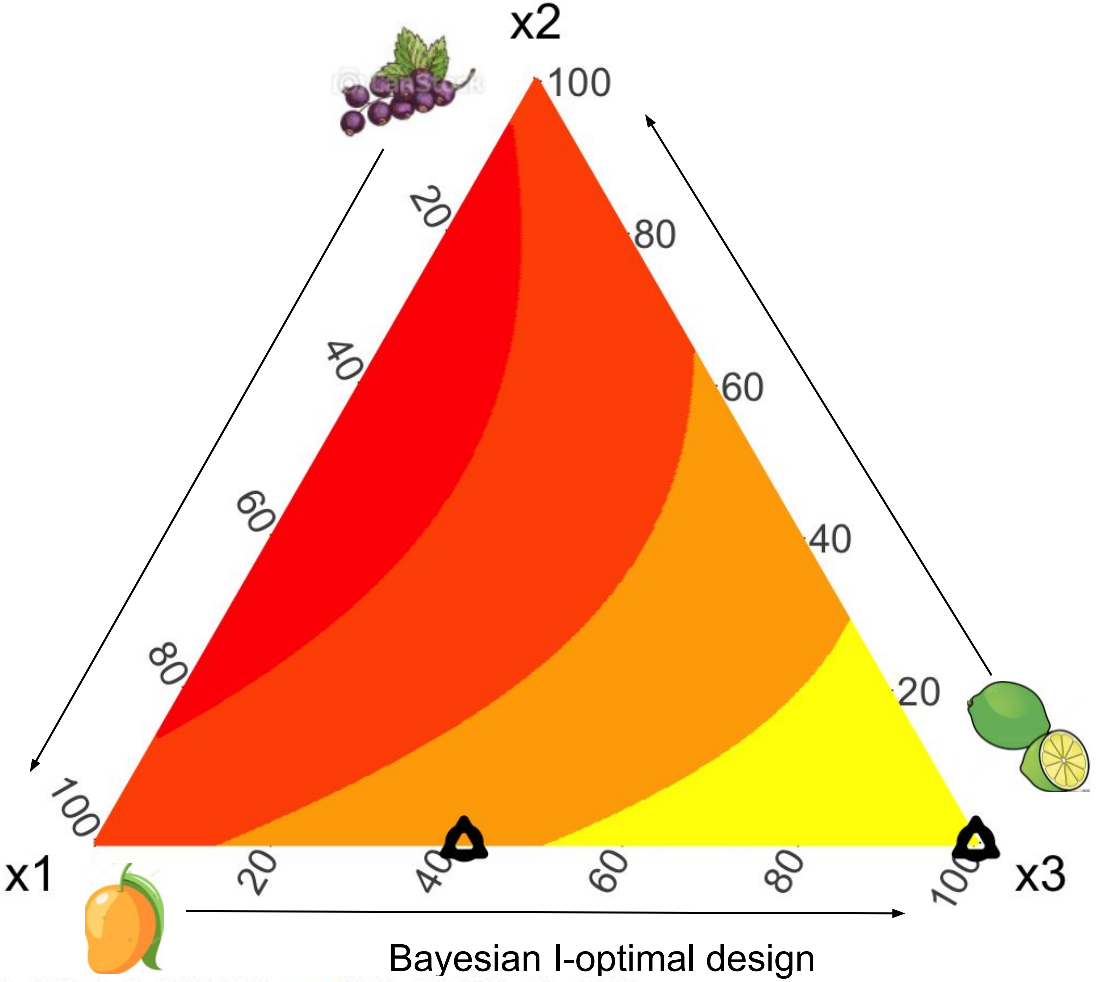

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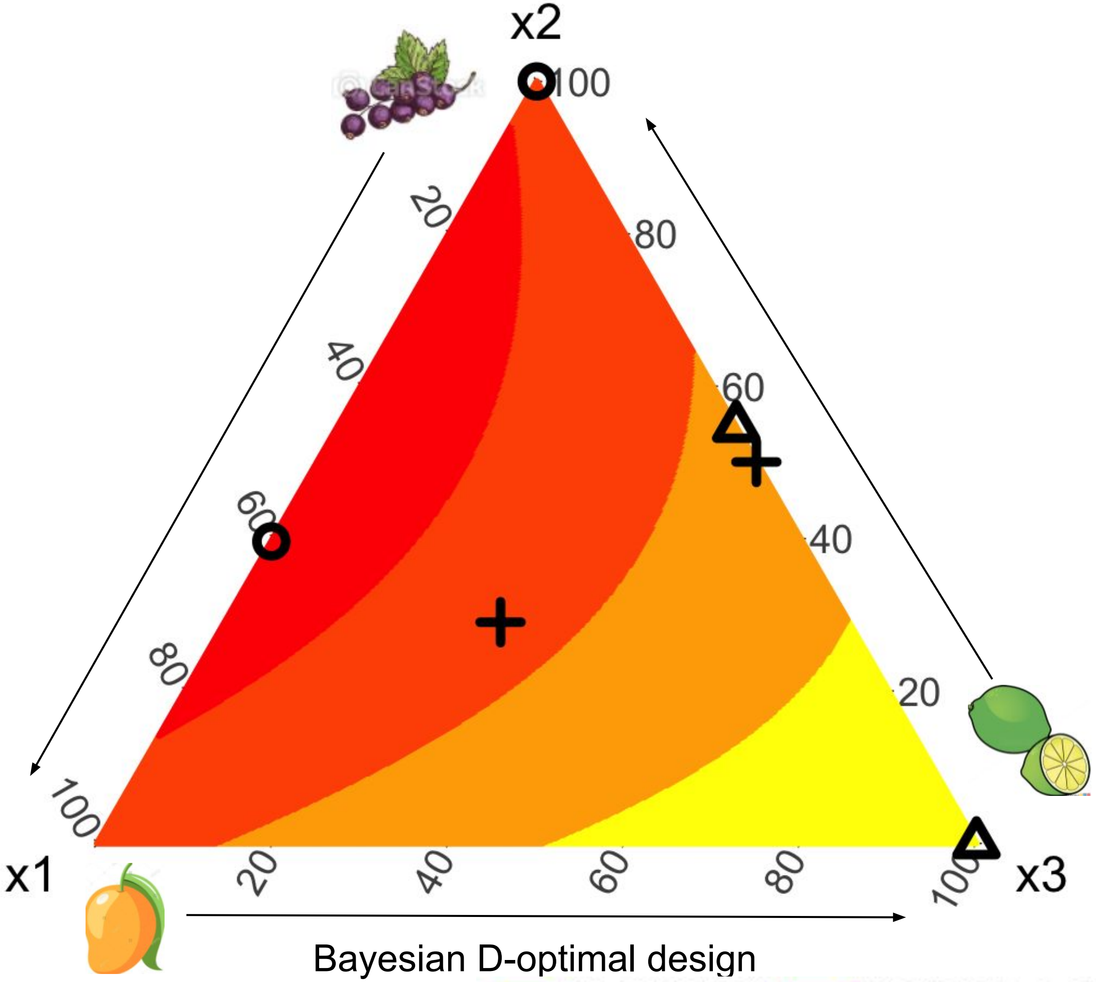

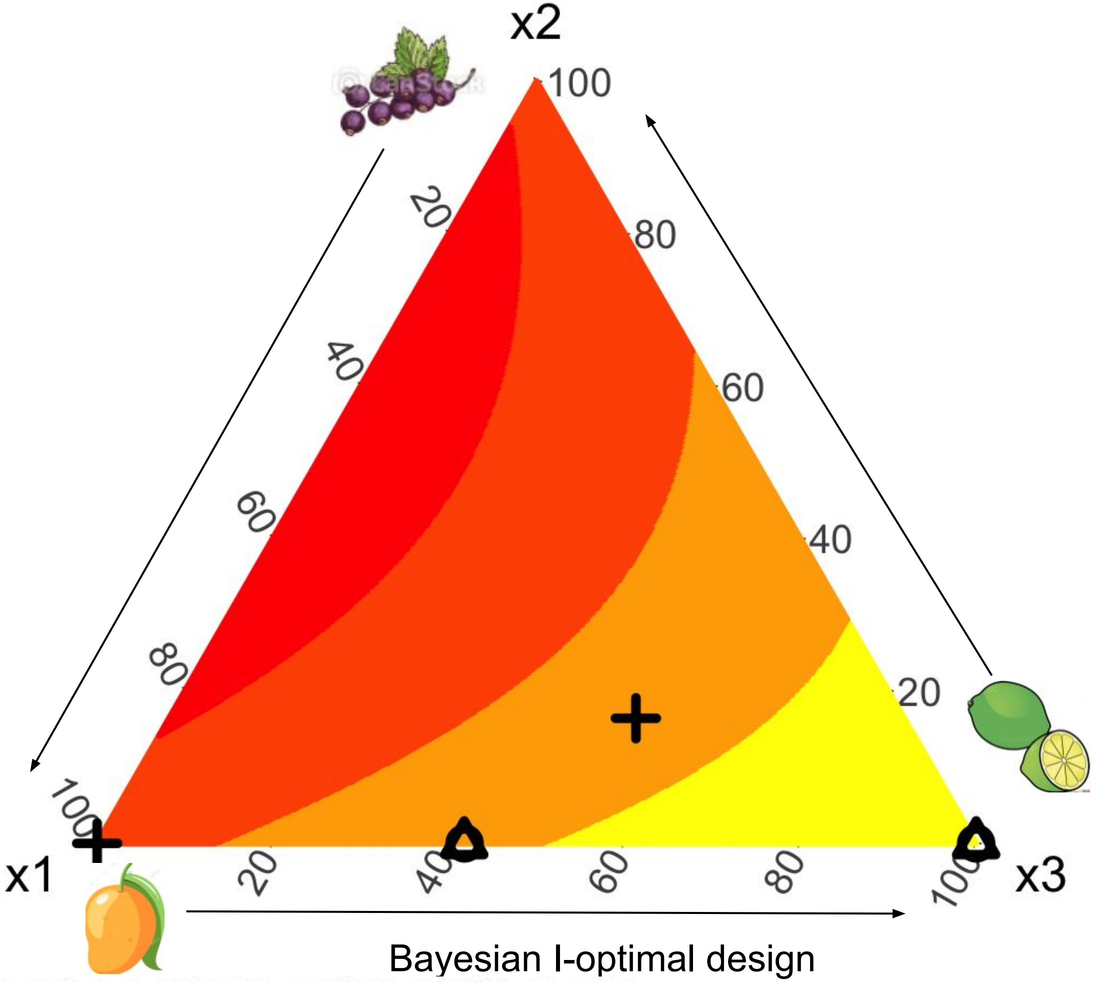

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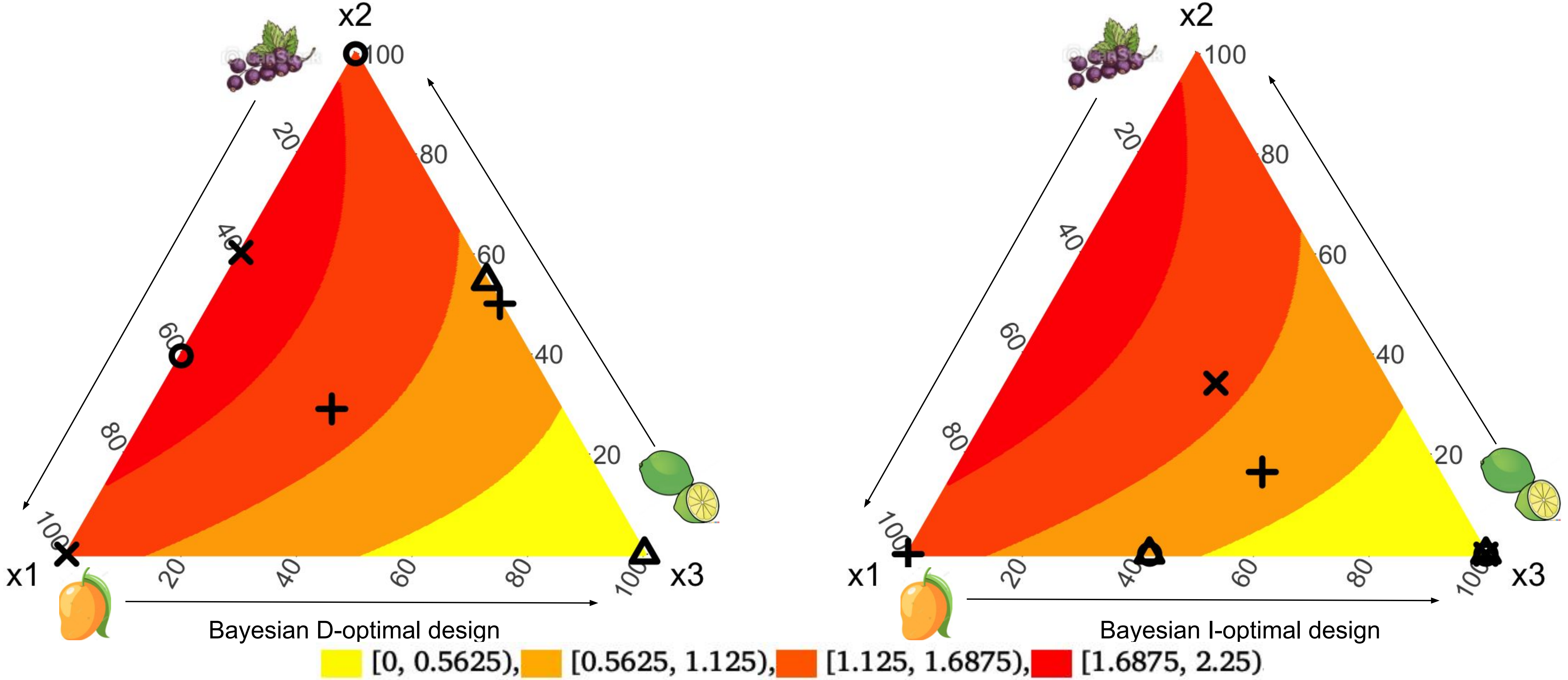

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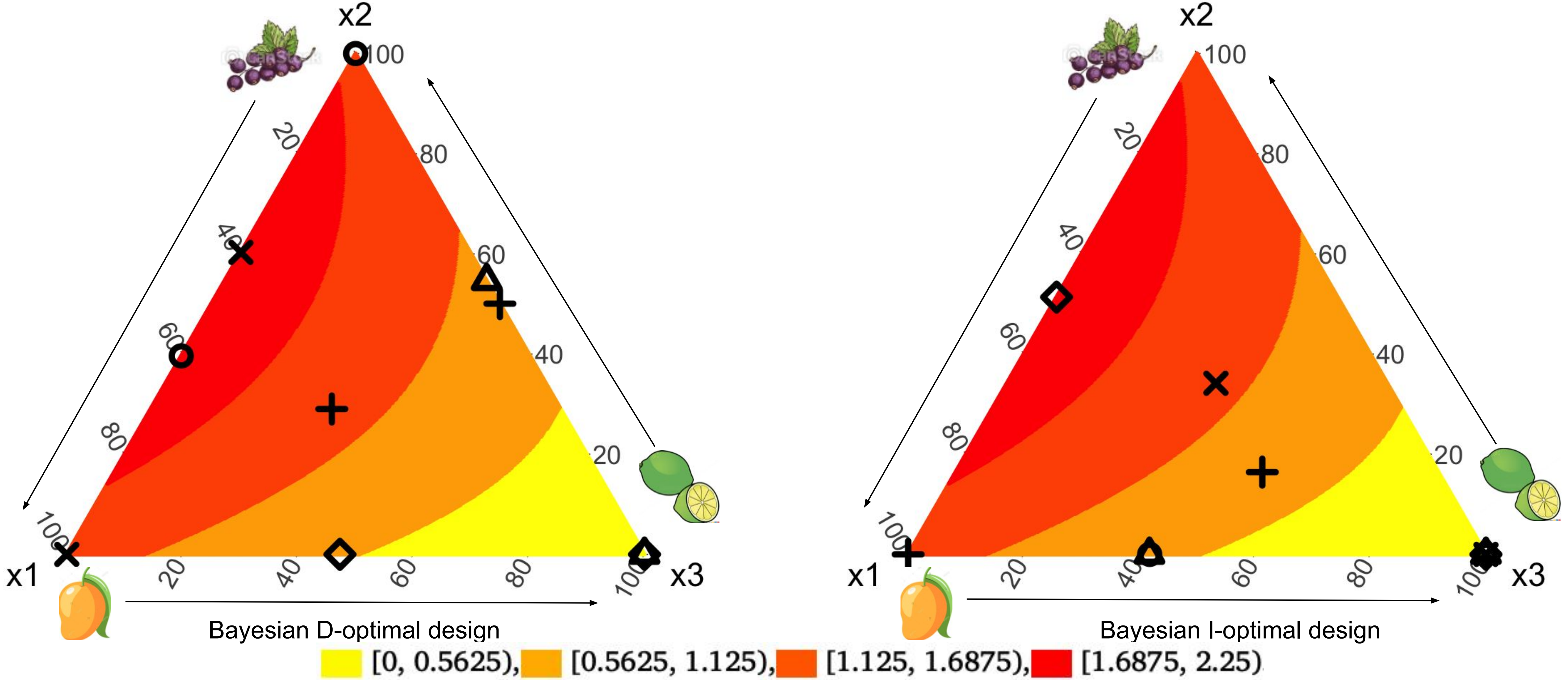

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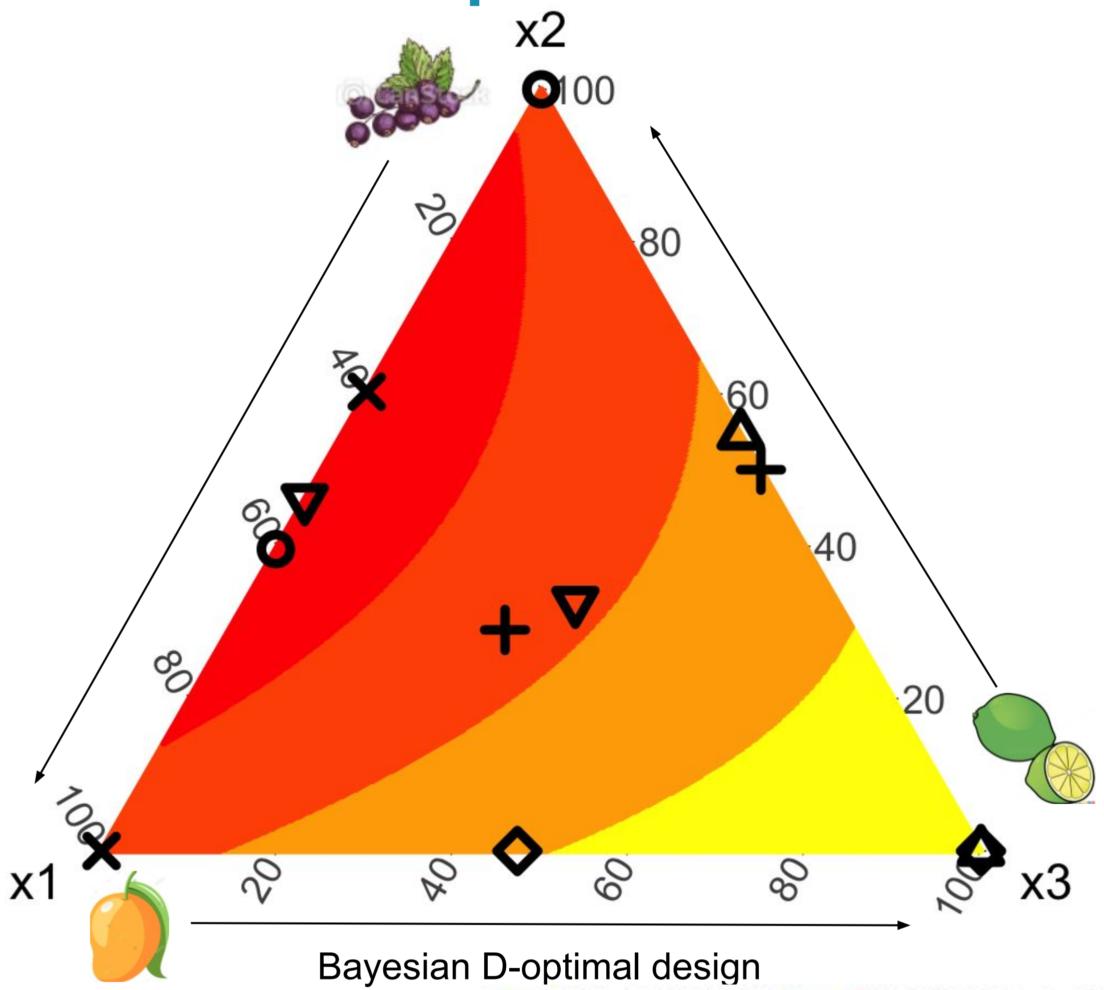

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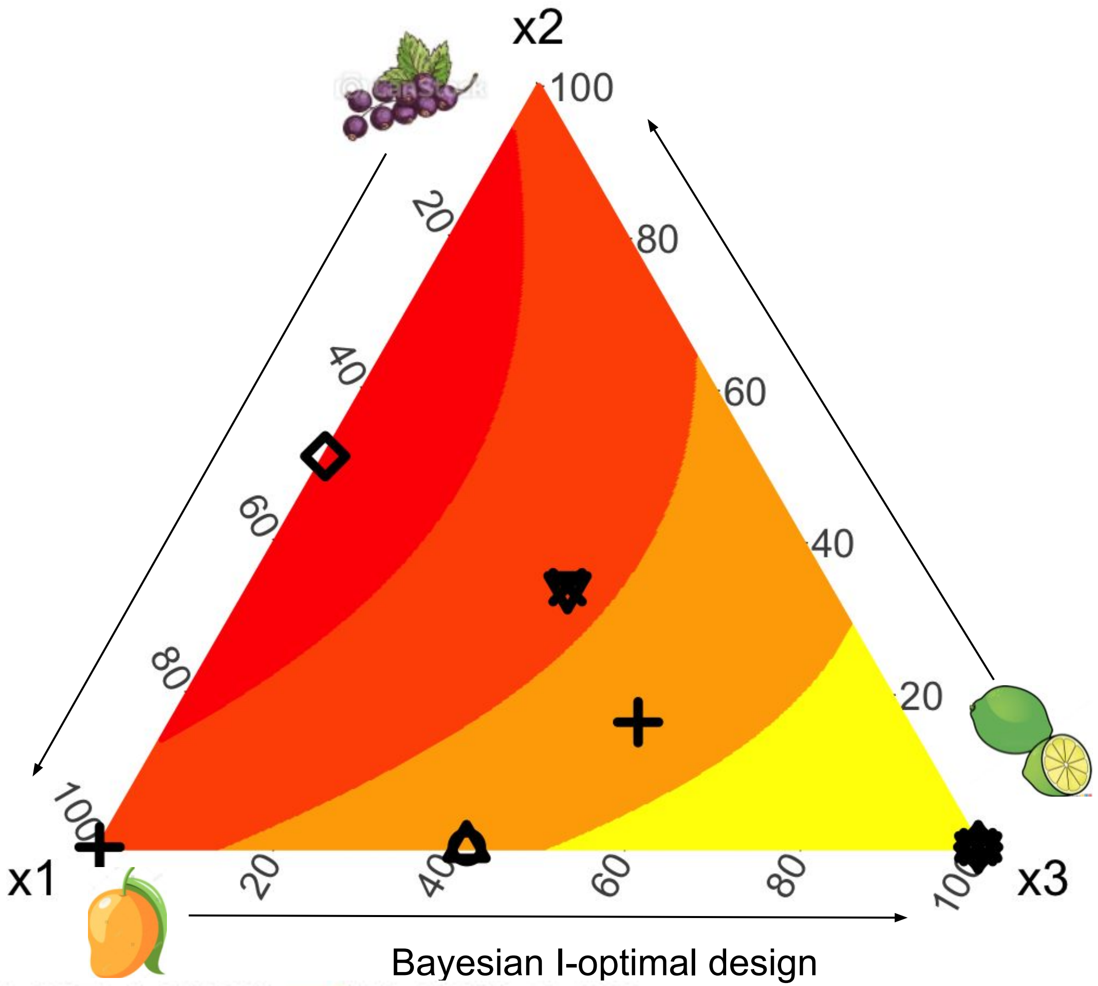

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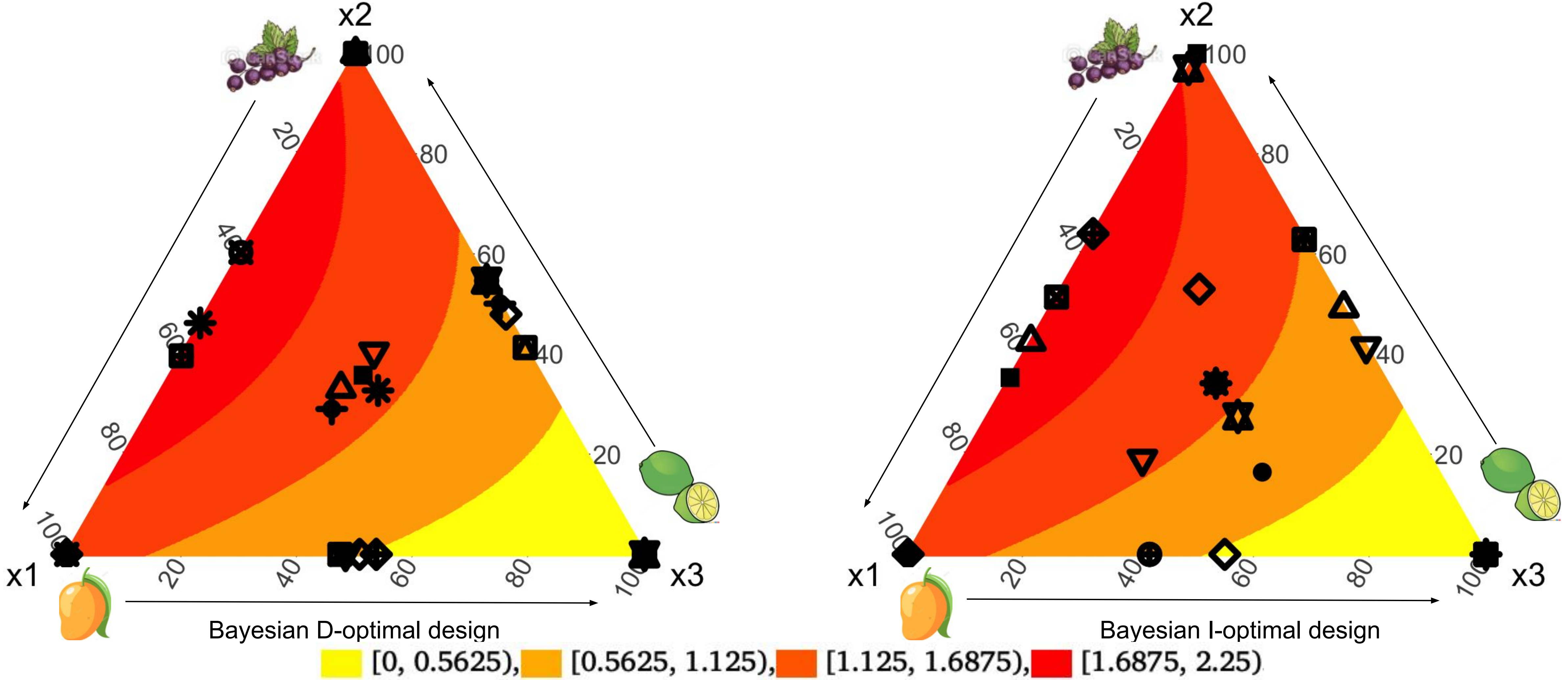

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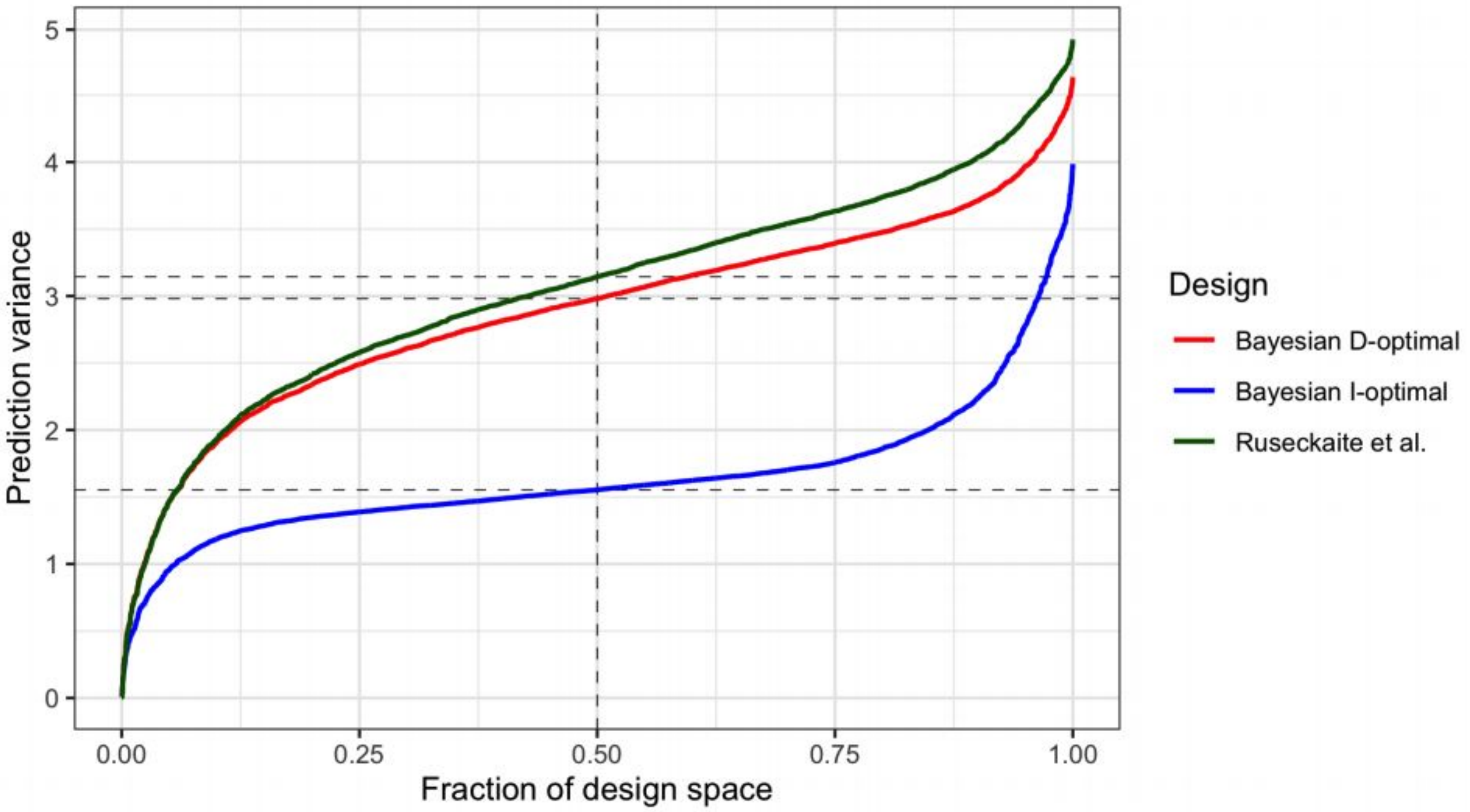

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- Extend the work to other classes of models for data from mixture experiments

More information

- Becerra, Mario, 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: 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

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

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

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

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

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

Extra: D-optimal designs

- D-optimality criterion

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

- Bayesian D-optimality criterion

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

- Numerical approximation to Bayesian D-optimality criterion

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

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

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

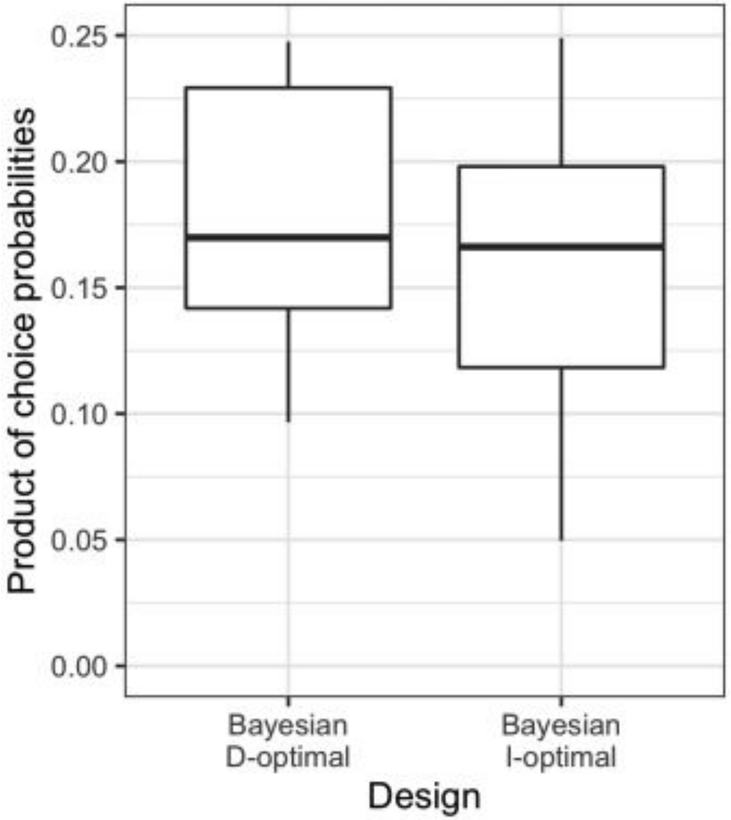
$$\boldsymbol{f}(\boldsymbol{x}_{js}) = (x_{1js}, x_{2js}, \ldots, x_{q-1,js}, x_{1js}x_{2js}, \ldots, x_{q-1,js}x_{qjs}, x_{1js}x_{2js}x_{3js}, \ldots, x_{q-2,js}x_{q-1,js}x_{qjs})^T$$

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

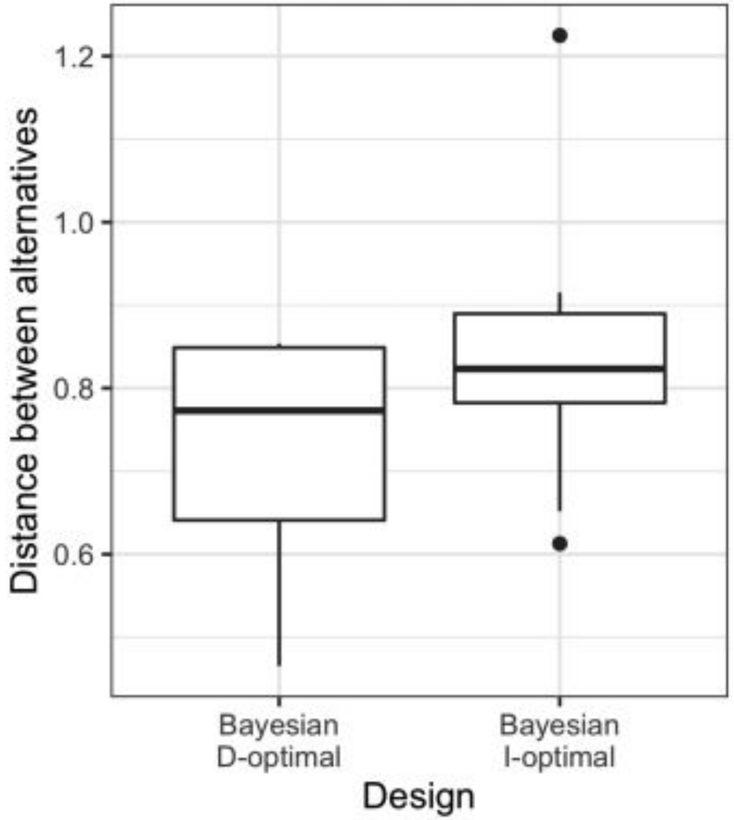
$$\boldsymbol{x}_{js} = (x_{1js}, x_{2js}, \ldots, x_{qjs})^T$$

$$\boldsymbol{\beta} = (\beta_1^*, \beta_2^*, \ldots, \beta_{q-1}^*, \beta_{1,2}, \ldots, \beta_{q-1,q}, \beta_{123}, \ldots, \beta_{q-2,q-1,q})^T$$

Extra results: cocktail preferences

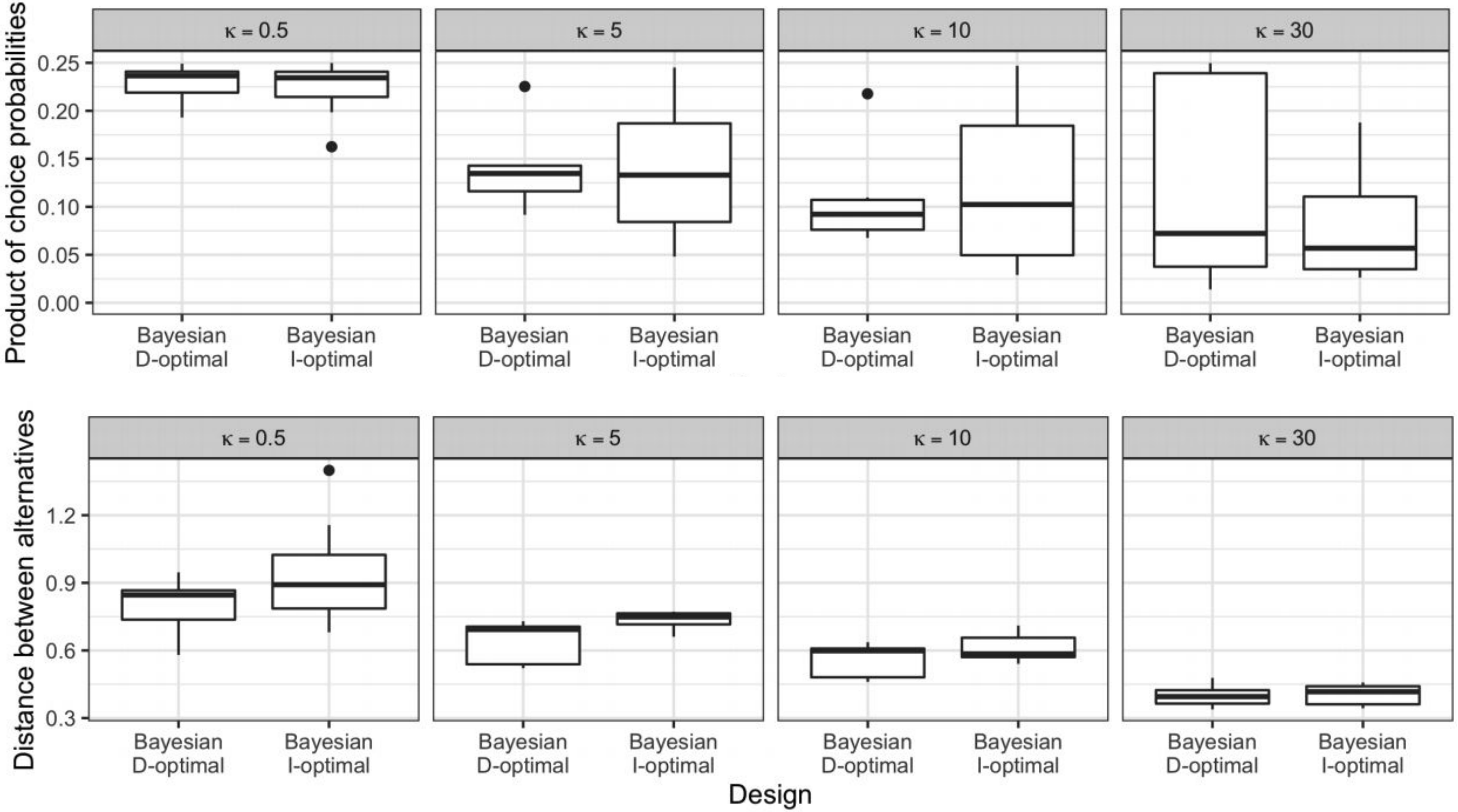


(a) Utility balance



(b) Euclidean distances

Extra results: artificial sweetener experiment



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- Varying levels of uncertainty in parameter vector parameter. Values κ = 0.5, 5, 10 and 30.

$$\mathbf{\Sigma}_0' = \begin{pmatrix} 2\kappa & \kappa & 0 & 0 & 0 & 0 \\ \kappa & 2\kappa & 0 & 0 & 0 & 0 \\ 0 & 0 & \kappa & 0 & 0 & 0 \\ 0 & 0 & 0 & \kappa & 0 & 0 \\ 0 & 0 & 0 & 0 & \kappa & 0 \\ 0 & 0 & 0 & 0 & 0 & \kappa \end{pmatrix}$$

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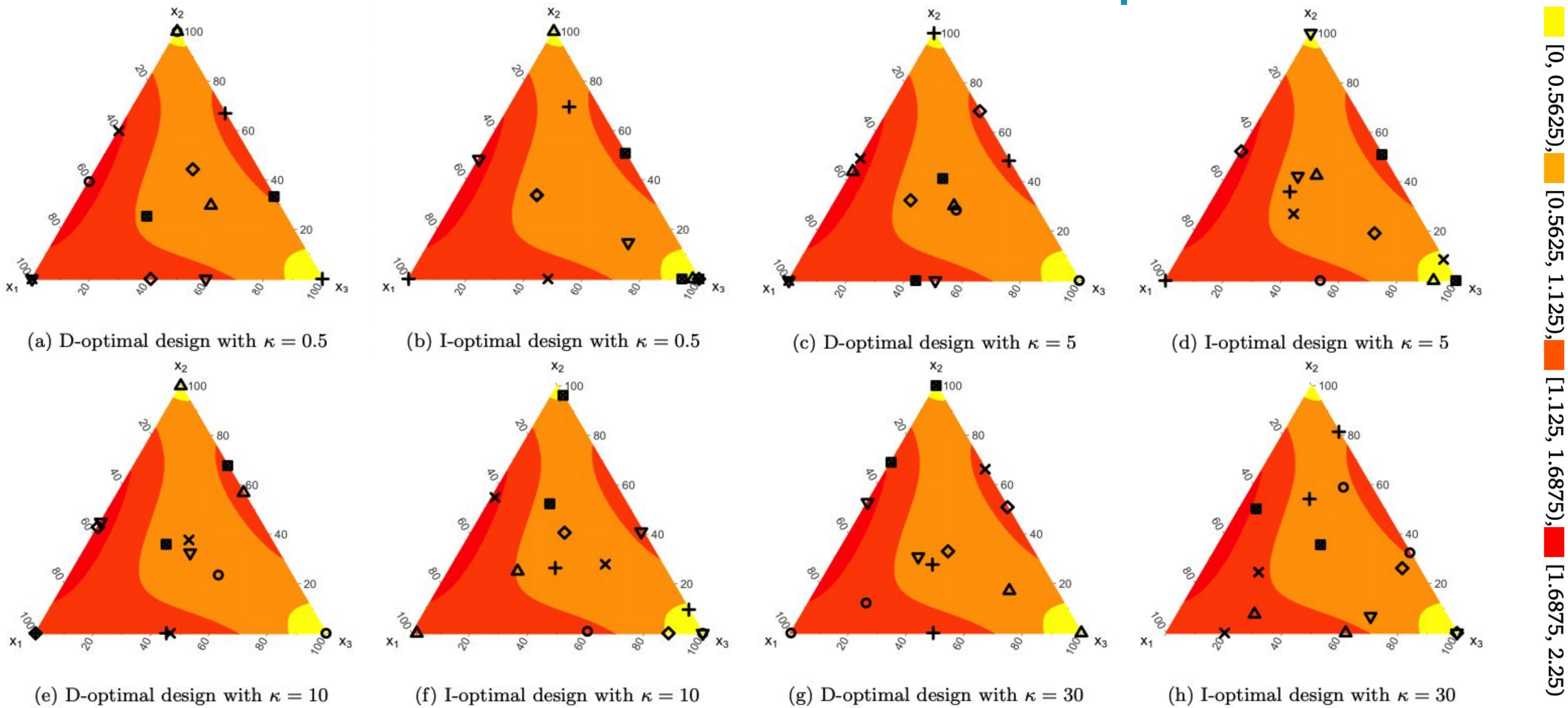

(a) D-optimal design with $\kappa = 0.5$

(b) I-optimal design with $\kappa = 0.5$

(c) D-optimal design with $\kappa = 5$

(d) I-optimal design with $\kappa = 5$

(e) D-optimal design with $\kappa = 10$

(f) I-optimal design with $\kappa = 10$

(g) D-optimal design with $\kappa = 30$

(h) I-optimal design with $\kappa = 30$

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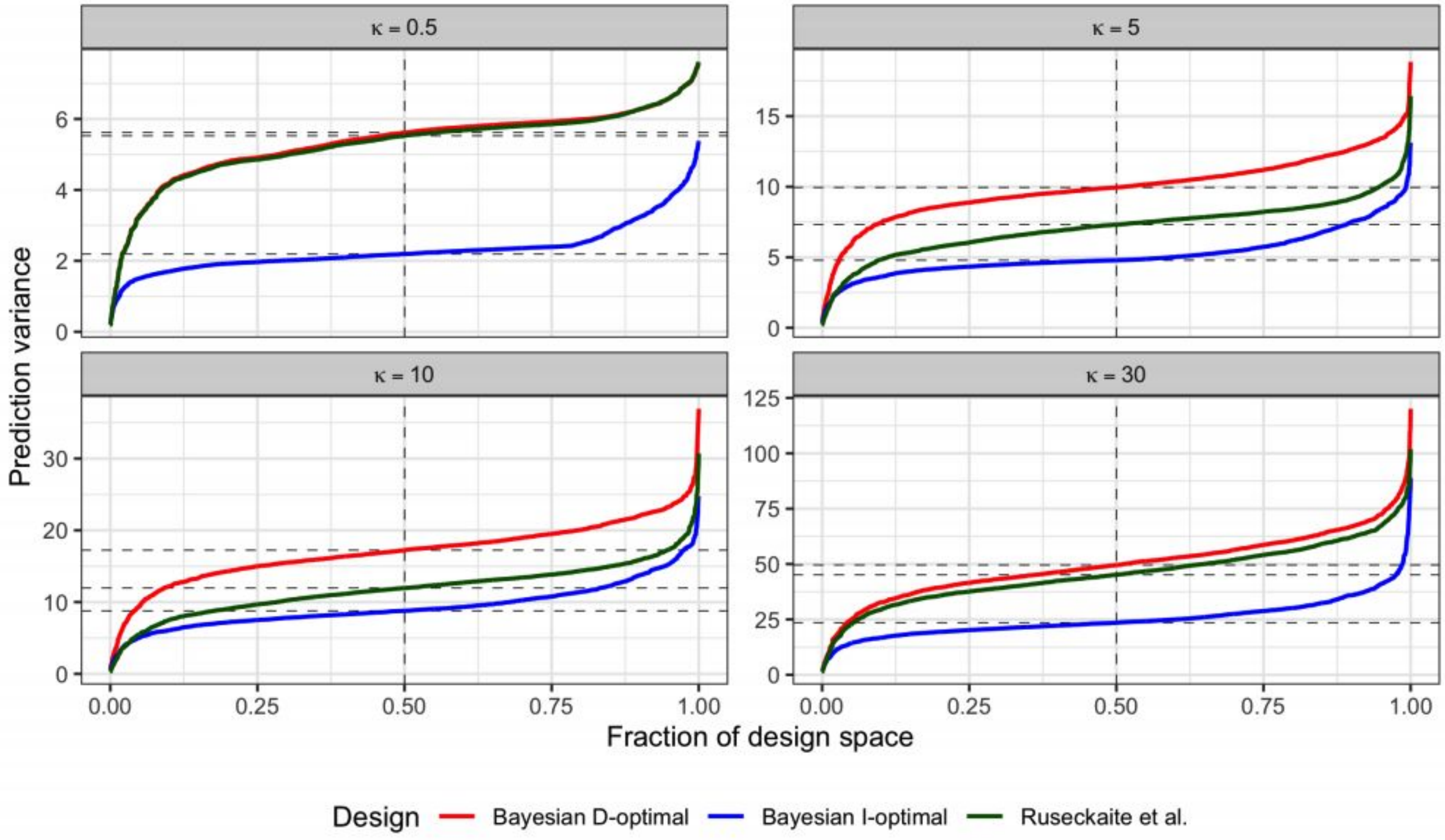

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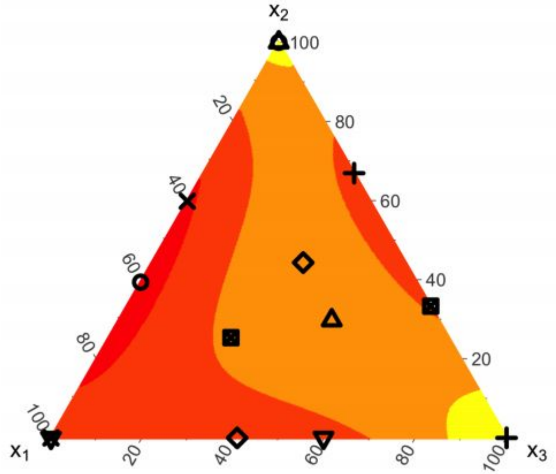
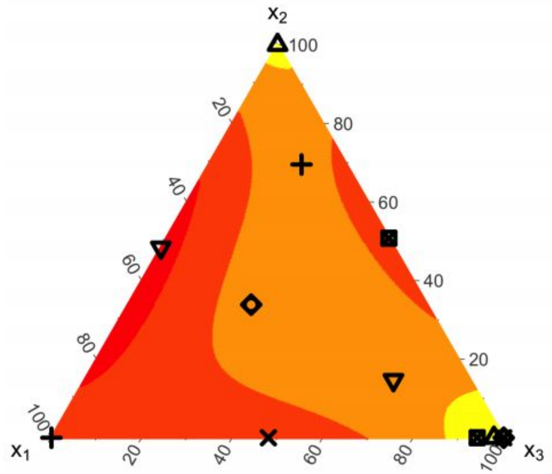
- Original response: intensity of sweetness aftertaste
- Ruseckaite et al. obtained a prior distribution for parameter vector $\boldsymbol{\beta}$ in a special-cubic Scheffé model with varying levels of uncertainty

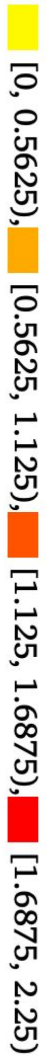
Artificial sweetener experiment



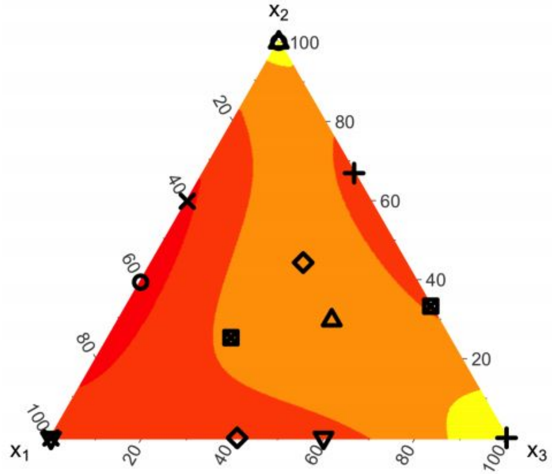
Bayesian D-optimal design with low uncertainty



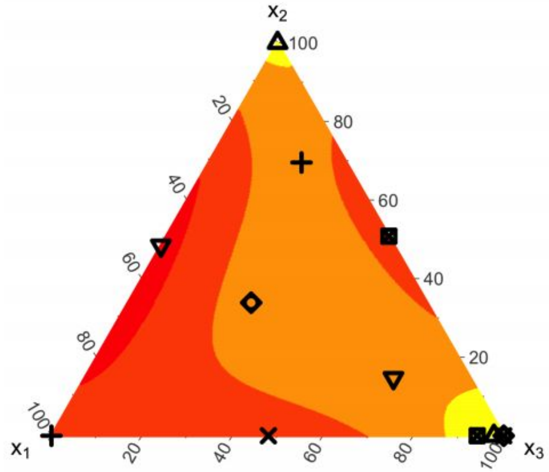
Bayesian D-optimal design with high uncertainty



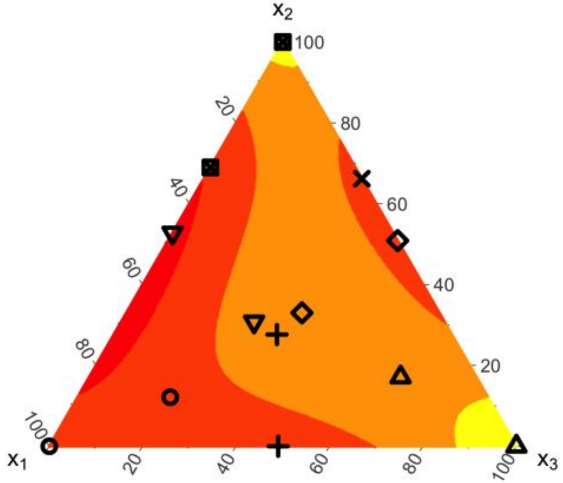
Artificial sweetener experiment



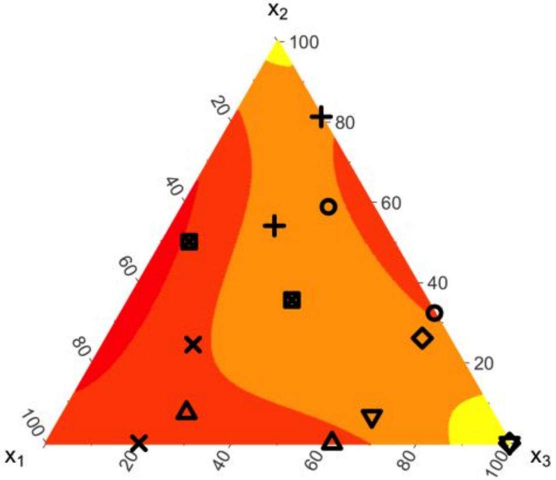
Bayesian D-optimal design with low uncertainty



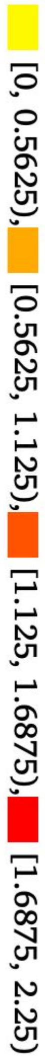
Bayesian D-optimal design with high uncertainty



Bayesian I-optimal design with low uncertainty



Bayesian I-optimal design with high uncertainty



Artificial sweetener experiment