

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

Mario Becerra Peter Goos October 22nd, 2021 28th Annual Meeting of the RSSB Campus Liège-Centre of ULiège Liège, Belgium

#### 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









Quantify consumer preferences







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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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  - the wheat varieties used to make bread
  - ingredients used to make a cocktail









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- The researchers' interest is generally in one or more characteristics of the mixture

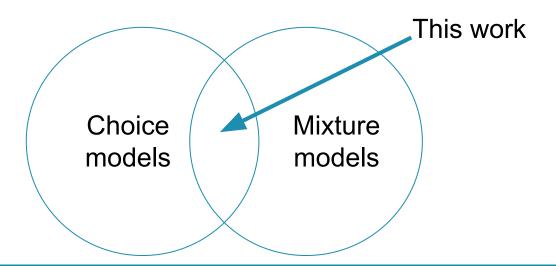


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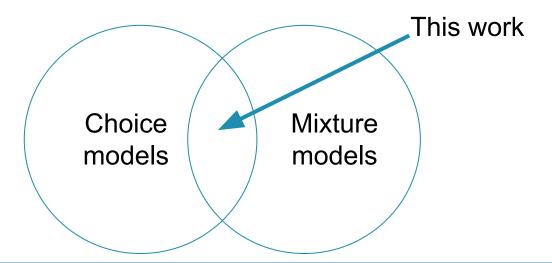
- In mixture experiments, products are expressed as combinations of proportions of ingredients
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- Choice experiments are ideal to collect data for quantifying and modeling preferences for mixtures





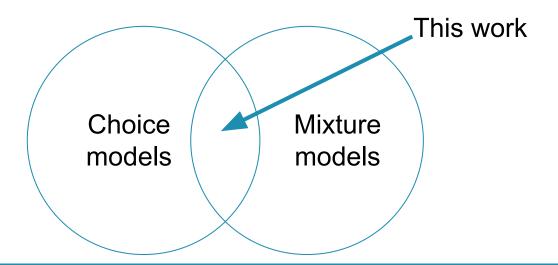


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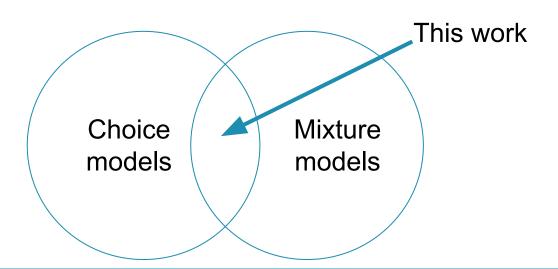




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- Preferences for cocktails involving different proportions of mango juice, lime juice, and blackcurrant syrup
- Experimental data involved the responses of sixty people, each making eight pairwise comparisons of different cocktails





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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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- In experiments with mixtures, we want to optimize the composition of the mixture to maximize consumer preference
- Precise predictions are crucial
- I-optimal designs are more suitable





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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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	Car A	Car B
BRAND	BMW	Mercedes
MILEAGE	2 miles per gallon	10 miles per gallon
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PRICE	\$20,000	\$100,000
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• The probability that a respondent chooses alternative  $j \in \{1, ..., J\}$  in choice set s is

$$p_{js} = rac{\exp\left[oldsymbol{f}^T(oldsymbol{x}_{js})oldsymbol{eta}
ight]}{\sum_{t=1}^{J}\exp\left[oldsymbol{f}^T(oldsymbol{x}_{ts})oldsymbol{eta}
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- Perceived utility modeled as

$$U_{js} = m{f}^T(m{x}_{js})m{eta} = \sum_{i=1}^{q-1}eta_i^*x_{ijs} + \sum_{i=1}^{q-1}\sum_{k=i+1}^qeta_{ik}x_{ijs}x_{kjs} + \sum_{i=1}^{q-2}\sum_{k=i+1}^{q-1}\sum_{l=k+1}^qeta_{ikl}x_{ijs}x_{kjs}x_{ljs} + arepsilon_{js}$$

# D-optimal designs



## D-optimal designs

D-optimality criterion

$$\mathcal{D} = \log \left( \det \left( \left[ oldsymbol{I}^{-1}(oldsymbol{X}, oldsymbol{eta}) 
ight) 
ight]^{rac{1}{r}} 
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Bayesian D-optimality criterion

$$\mathcal{D}_B = \log \left( \int_{\mathbb{R}^r} \left[ \det \left( oldsymbol{I}^{-1}(oldsymbol{X}, oldsymbol{eta}) 
ight) 
ight]^{rac{1}{r}} \pi(oldsymbol{eta}) doldsymbol{eta} 
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$$\mathcal{I} = \operatorname{tr}\left[\boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta})\boldsymbol{W}_{u}\right]$$

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## I-optimal designs

I-optimality criterion

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Bayesian I-optimality criterion

$$\mathcal{I}_B = \int_{\mathbb{R}^r} \operatorname{tr} \left[ \boldsymbol{I}^{-1}(\boldsymbol{X}, \boldsymbol{\beta}) \boldsymbol{W}_u \right] \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}$$

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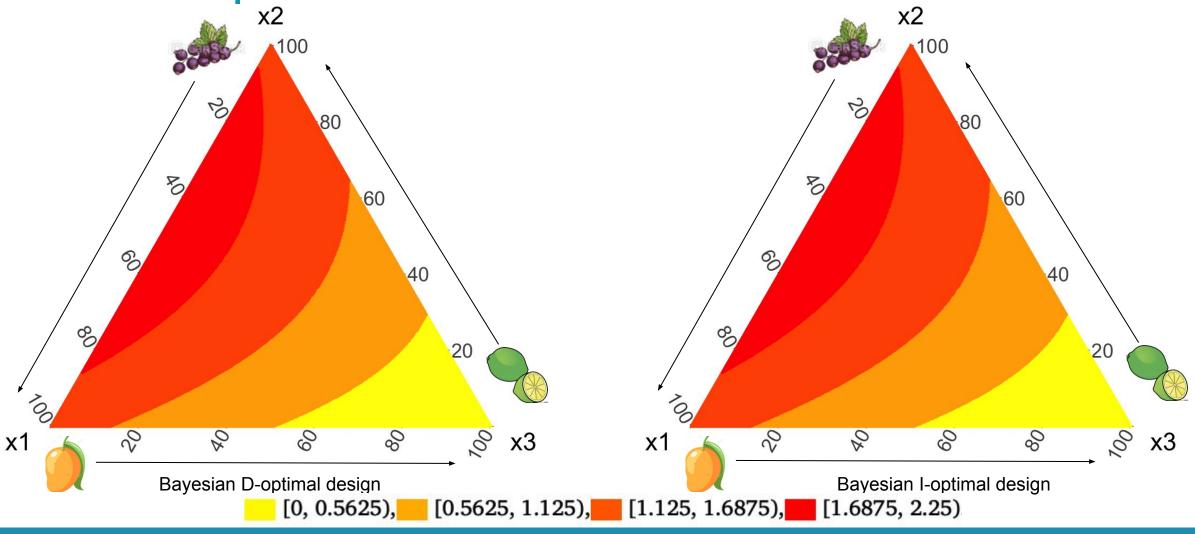


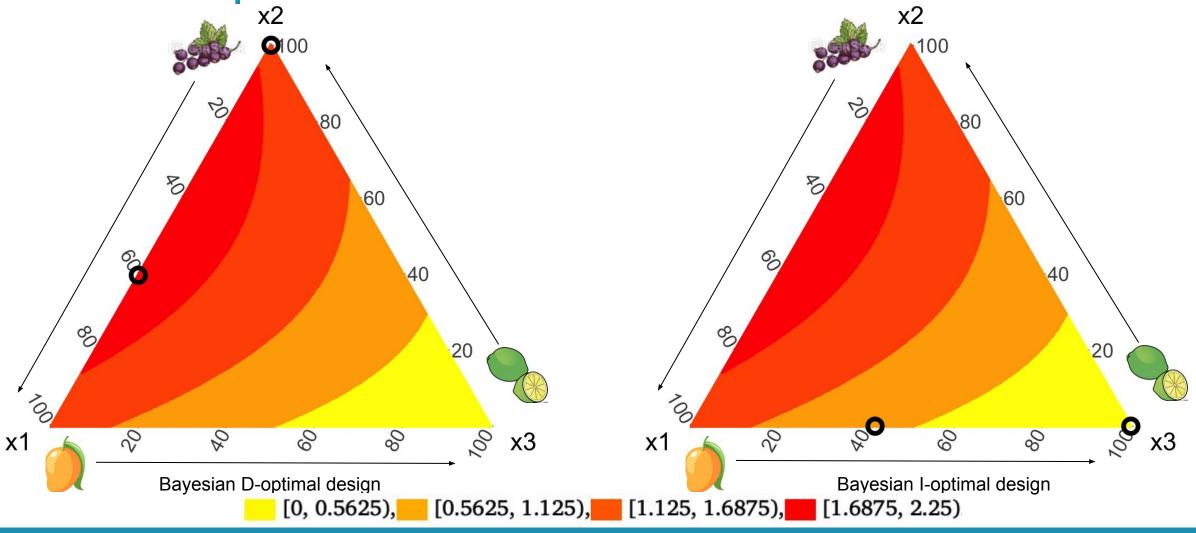
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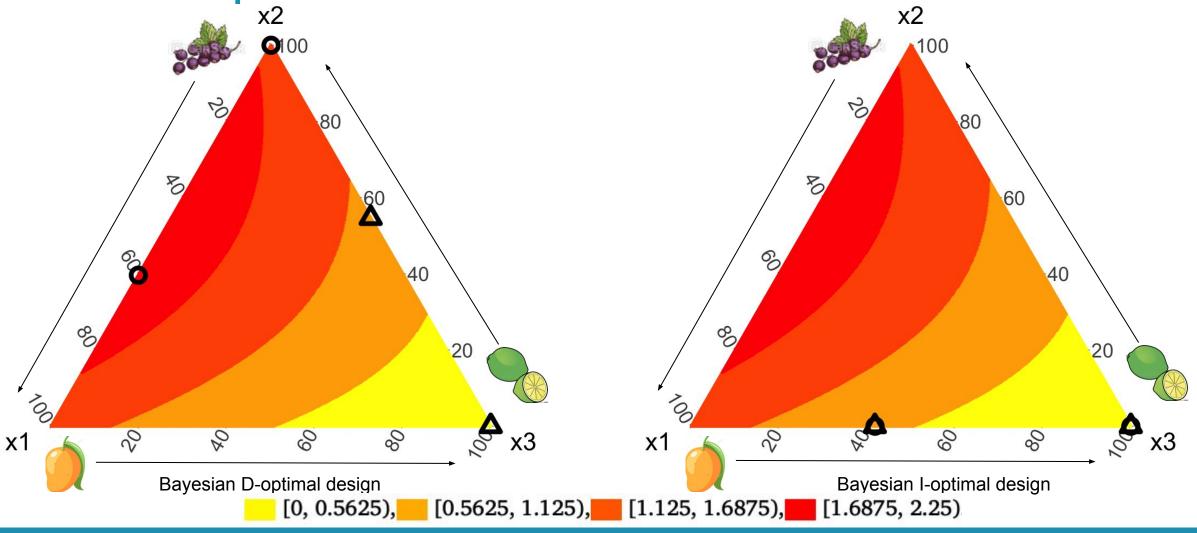


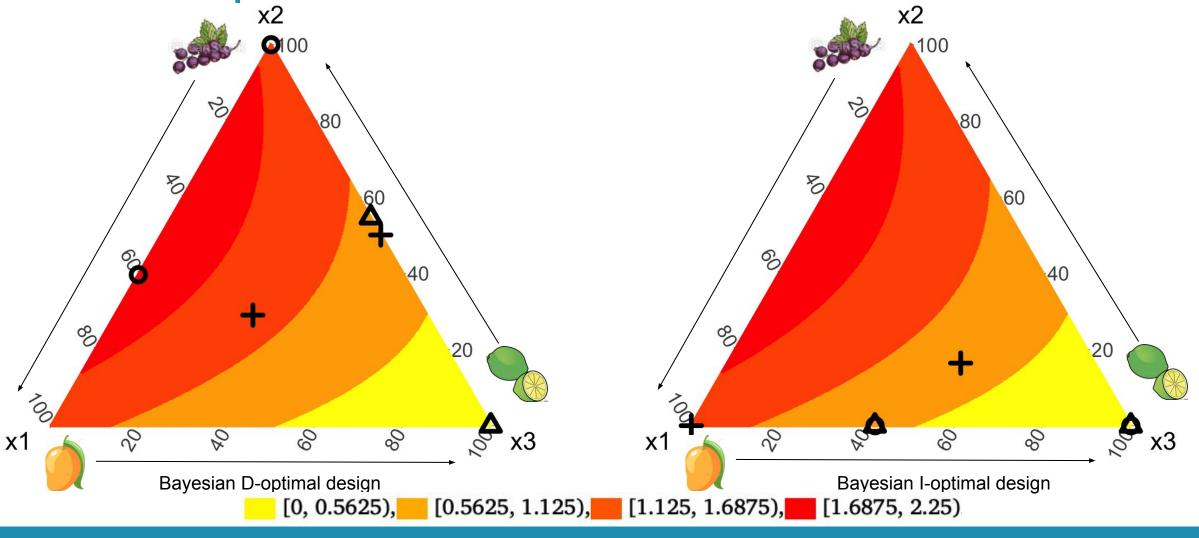
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- Ruseckaite et al. obtained a prior distribution for parameter vector β in a special-cubic Scheffé model
- We used the same prior distribution to compute Bayesian D- and I-optimal designs using a coordinate-exchange algorithm

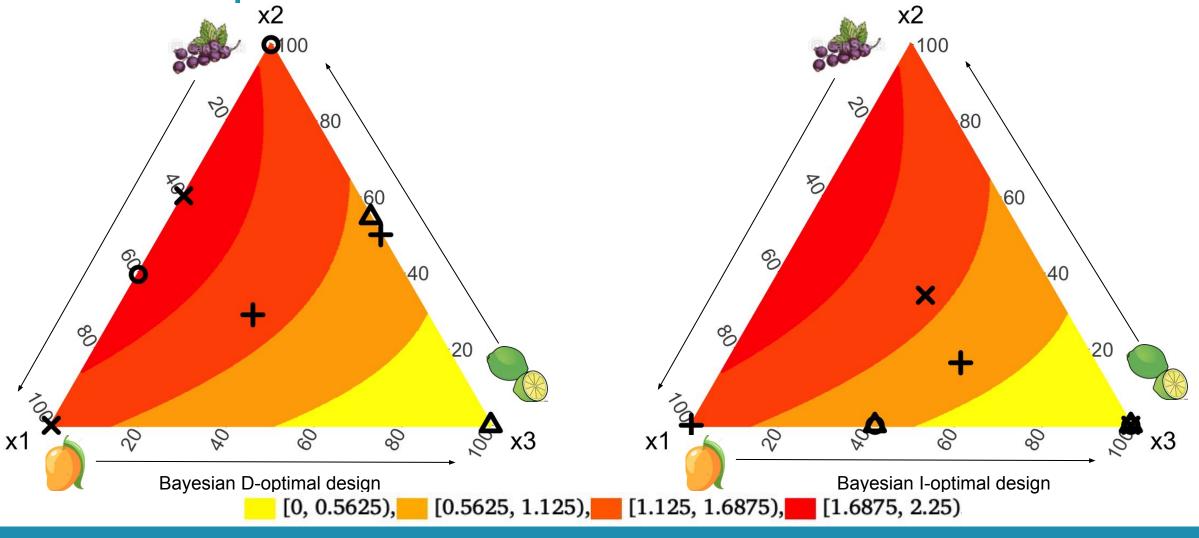


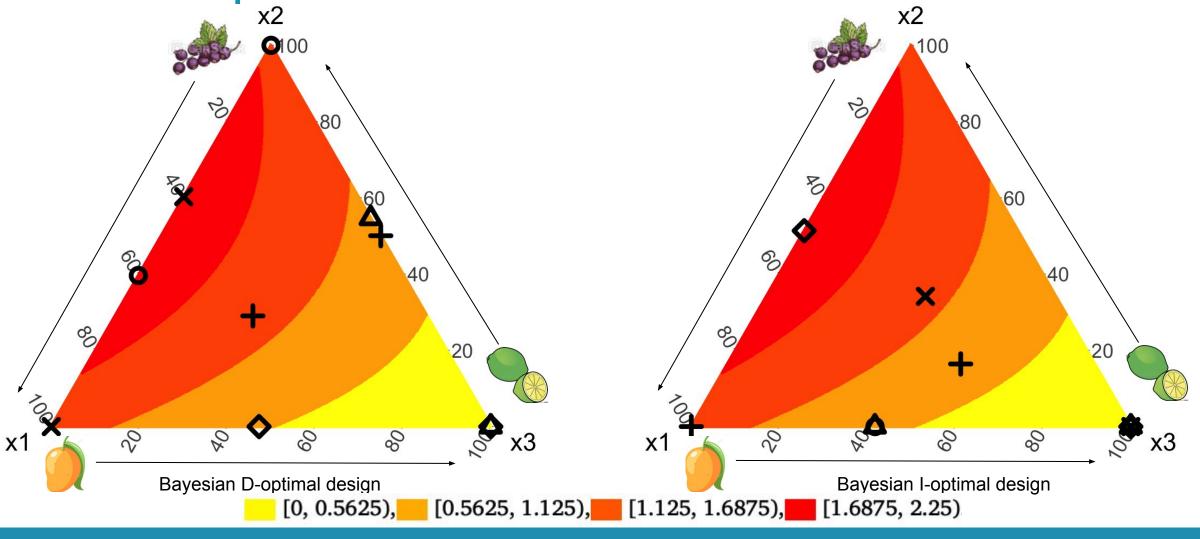


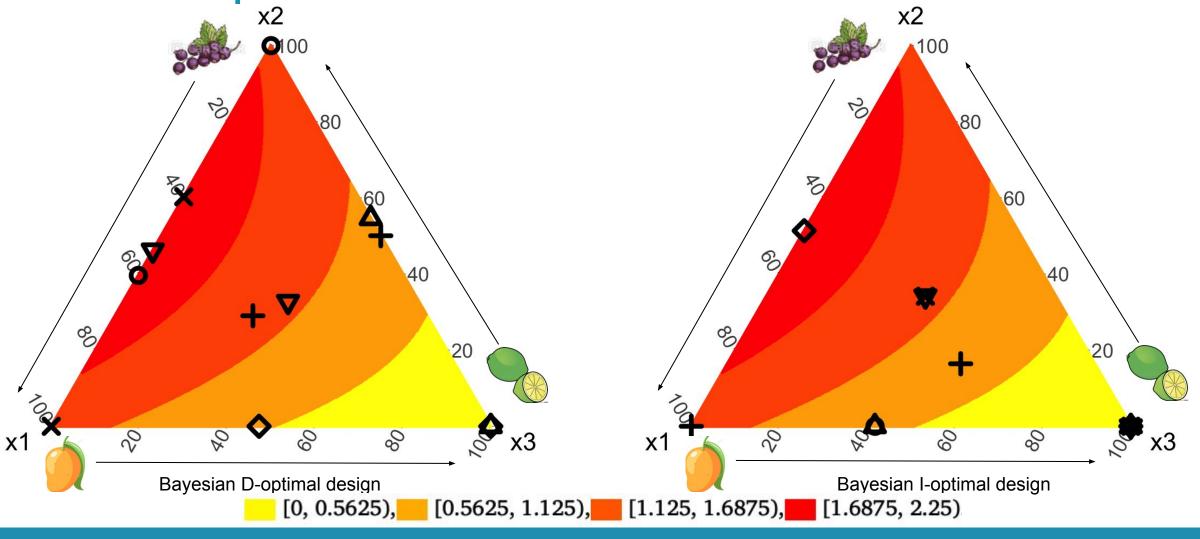


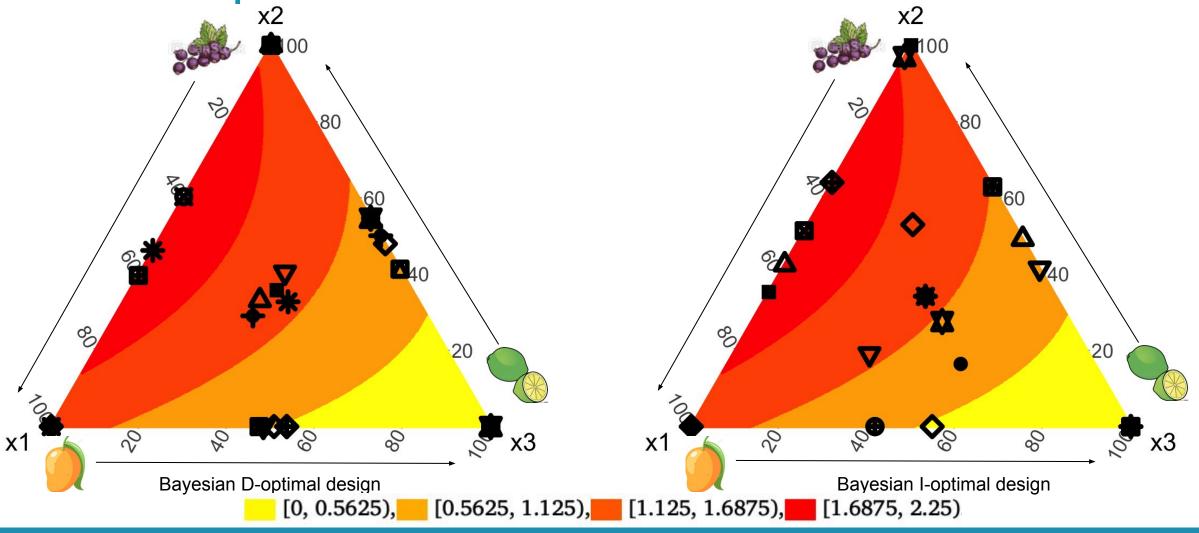


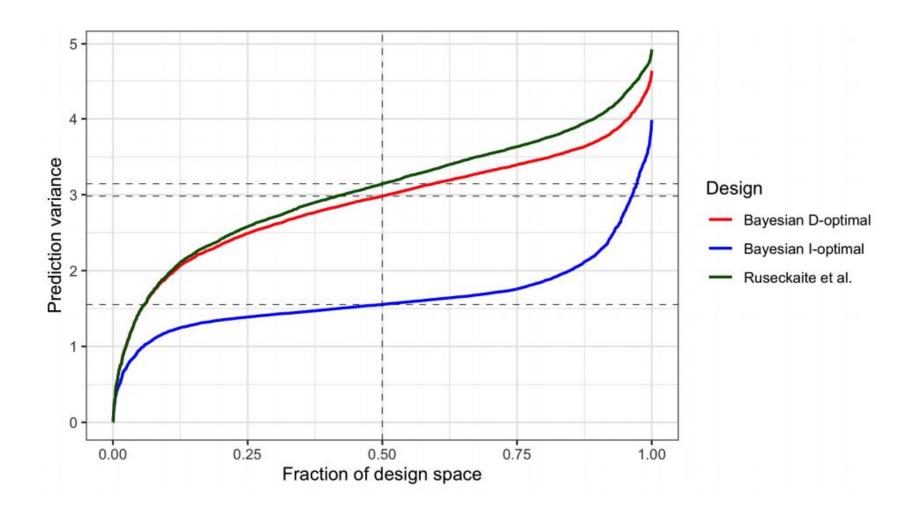














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- Add process variables
- Models that take into account possible presence of consumer heterogeneity
- Extend the work to other classes of models for data from mixture experiments



#### 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): <u>mariobecerra.github.io/</u>

