## Mixed Integer Programming Approaches for Experimental Design

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Joint work with Chris Coey, Miles Lubin and Denis Saure

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#### **Experimental Design for Preference Surveys**









Feature	SX530	RX100
Zoom	50x	3.6x
Prize	\$249.99	\$399.99
Weight	15.68 ounces	7.5 ounces
Prefer		



Feature	TG-4	<b>G</b> 9
Waterproof	Yes	No
Prize	\$249.99	\$399.99
Weight	7.36 lb	7.5 lb
Prefer		<b>√</b>





Feature	TG-4	Galaxy 2
Waterproof	Yes	No
Prize	\$249.99	\$399.99
Viewfinder	Electronic	Optical
Prefer		





Parametric
Preference Model



Estimate Preference Parameter

#### **Experimental Design for Preference Surveys**





Feature	Chewbacca	BB-8
Wookiee	Yes	No
Droid	No	Yes
Blaster	Yes	No
I would buy toy		
Product Profile	$x^1$	$x^2$

$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = x^2$$

- Even evaluating "quality" of survey design may be expensive:
  - Can state-of-the-art MIP help?

#### 50+ Years of MIP = Significant Solver Speedups

- Machine-independent algorithmic improvements (on standard and solver benchmark instances):
  - CPLEX v1.2 (1991) v11 (2007): 29,000x speedup
  - Gurobi v1 (2009) v6.5 (2015): 48.7x speedup
  - Commercial, but free for academic use (Also Xpress)
- (Reasonably) effective free / open source solvers:
  - GLPK, COIN-OR (CBC) and SCIP (only for non-commercial)
- Accessible, fast and versatile 21<sup>st</sup> century tools:
  - Julia -based JuMP modelling language
- Mature and evolving effectiveness:
  - Linear MIP, second order cone MIP (MI-SOCP) and convex/conic nonlinear MIP (MI-SDP, MI-SDP+EXP)

## Case Study 1:

# Quick Linear Regression During Christmas in Viña del Mar

#### **Experimental Design for Linear Regression**

Model:  $y^i = \beta \cdot z^i + \epsilon_i, \quad \epsilon_i \sim N(0, 1)$ 

Questions: Answers:

$$Z = \left[z^{1} | \dots | z^{q}\right]^{T} \in \mathbb{R}^{q \times n} \qquad Y = \left[y_{1} | \dots | y_{q}\right]^{T}$$

(One) design goal = Min. "variance" of estimator of  $oldsymbol{eta} \in \mathbb{R}^n$ 

(One) Version of variance for OLS = D-efficiency:

Example  $\mathcal{Z}$  = Product profiles

$$\max_{Z \in \mathcal{Z}} \left( \det \left( Z^T Z \right) \right)^{1/q} \qquad x^{1,i}, x^{2,i} \in \{0,1\}^n \\ z^i = x^{1,i} - x^{2,i} \in \{-1,0,1\}^n$$

MIP = flexible  $\mathcal{Z}$  . e.g. partial profiles :  $\left\|x^{1,i}-x^{2,i}\right\|_1 \leq m$ 

#### MIP Formulations Approaches

• Traditional MI-SDP (SDP representation of  $\det^{1/q}$ ):

$$\left\{ z^{i_j} \right\}_{j=1}^k \to \max_{w} \left\{ \left( \det \left( \sum_{j=1}^k w_j z^{i_j} \cdot z^{i_j}^T \right) \right)^{1/q} : \sum_{j=1}^k w_j = q \\ w \in \mathbb{Z}_+^k \right\}$$

- MI-SOCP reformulation (Sagnol and Harman, '15)
- MI-SDP + linearization of products of binaries:

$$\max_{z^{i}, x^{1,i}, x^{2,i}} \left\{ \left( \det \left( \sum_{i=1}^{q} z^{i} \cdot z^{i}^{T} \right) \right)^{1/q} : \begin{array}{c} x^{1,i} - x^{2,i} = z^{i} \\ x^{1}, x^{2} \in \{0, 1\}^{n} \end{array} \right\}$$

MI-SDP+EXP :

$$\left(\det\left(\sum\nolimits_{i=1}^{q}z^{i}\cdot z^{i}^{T}\right)\right)^{1/q}\to \log\det\left(\sum\nolimits_{i=1}^{q}z^{i}\cdot z^{i}^{T}\right)$$

#### Solvers for Mixed Integer Conic Programming

- MI-SOCP: relatively mature + active development:
  - V., Dunning, Huchette and Lubin '16: Extended formulations. Adopted by Gurobi 6.5 (4x speedup). Also adopted in CPLEX 12.6.3 and Xpress 8.0.
- MI-SDP: only basic algorithms until:
  - Pajarito: Lubin, Yamangil, Bent and V. '16 and Coey, Lubin and V. '17. Uses generic linear-MIP and conic solver.





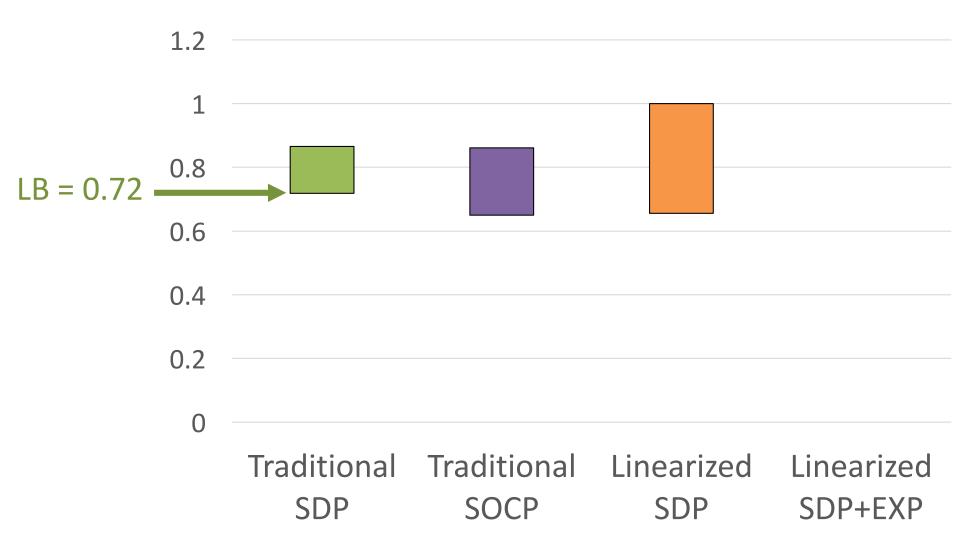


- SCIP-SDP: Gally, Pfetsch and Ulbrich '16 (harder to install).
- MI-SDP+EXP : Also Pajarito:
  - Less stable (IPM conic solver) and needs CVX/Convex.jl

#### Computational Experiment

- 12 binary features and 16 questions.
- Random k = 500 for traditional.
- SOCP = Gurobi 7
- MI-SDP = Pajarito with Gurobi 7 and Mosek 8
- MI-SDP+EXP = Pajarito with Gurobi 7 and SCS 1.1.8
- Core i7-6700K CPU @ 4.00GHz, 32GB RAM (Latest iMac)

#### Get a cup of coffee time length = 5 min



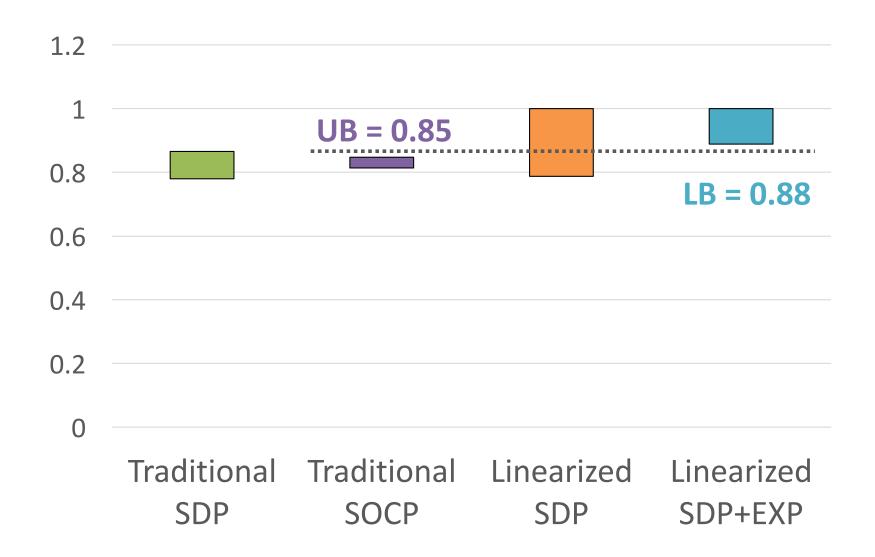
Lower Bound = Feasible Solution. e.g. Traditional SDP yields a design with D-eff = 0.72

#### Get a cup of coffee time length = 5 min

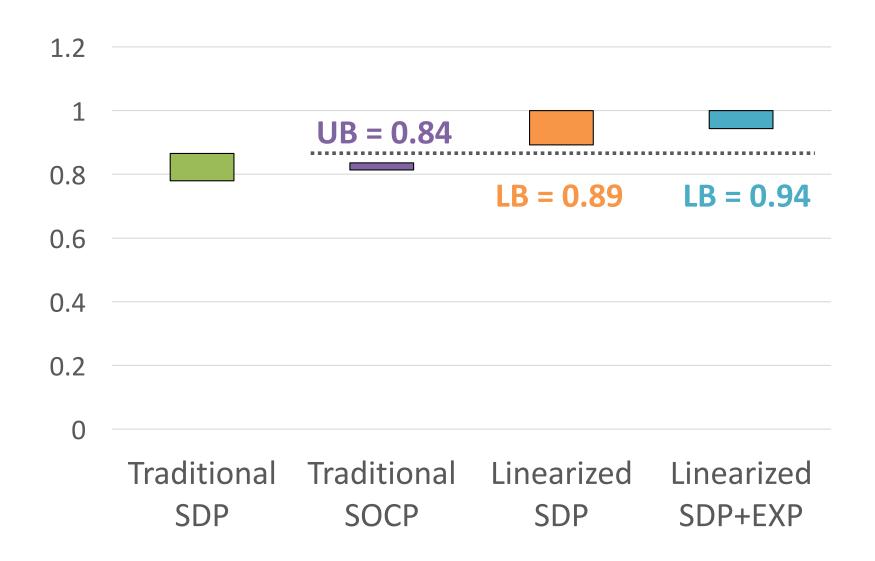


Upper Bound = Bound on best possible solution (**for model**). e.g. Any design **for traditional SDP** has D-eff ≤ 0.87

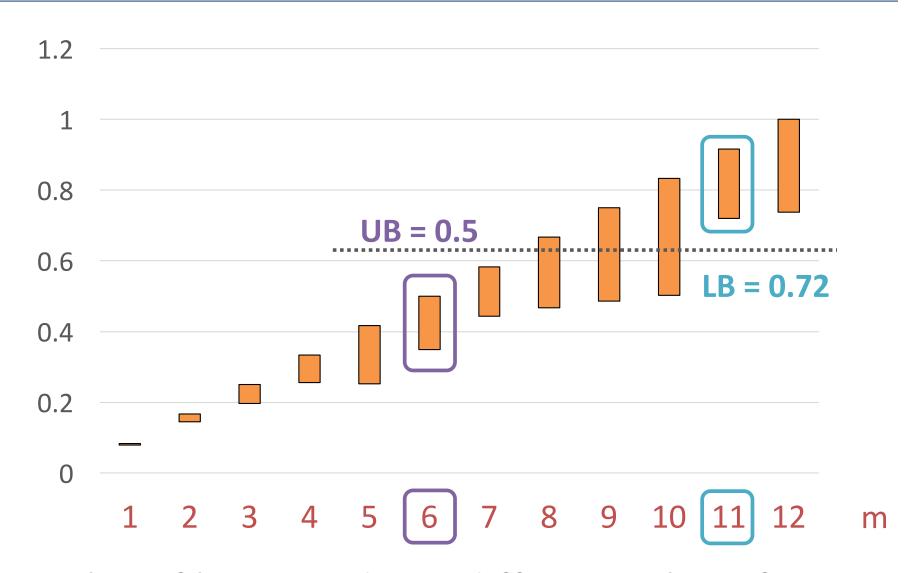
#### Going to lunch time length = 1 hour



#### Overnight time length = 16 hour

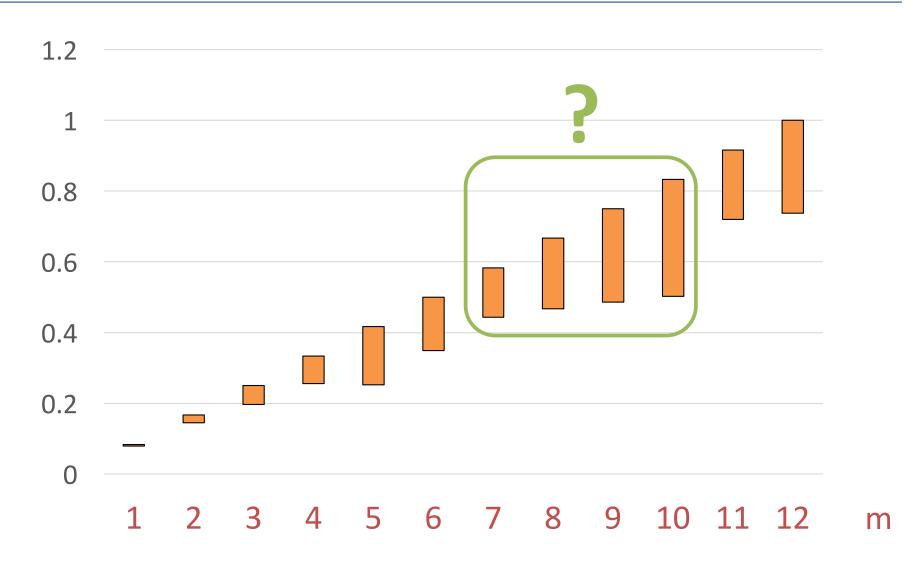


#### Application: Cost of Partial Profiles (L. SDP – 1 h)



Partial Profile: 2 products differ in only m features

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Partial Profile: 2 products differ in only m features

### Case Study 2:

Choice-Based Comparisons and

Real-Time Adaptive Logistic Regression

#### **Choice-based Conjoint Analysis**

Feature	Chewbacca	BB-8
Wookiee	Yes	No
Droid	No	Yes
Blaster	Yes	No
I would buy toy		
Product Profile	$x^1$	$x^2$

$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = x^2$$

MNL Preference Model Logistic Regression

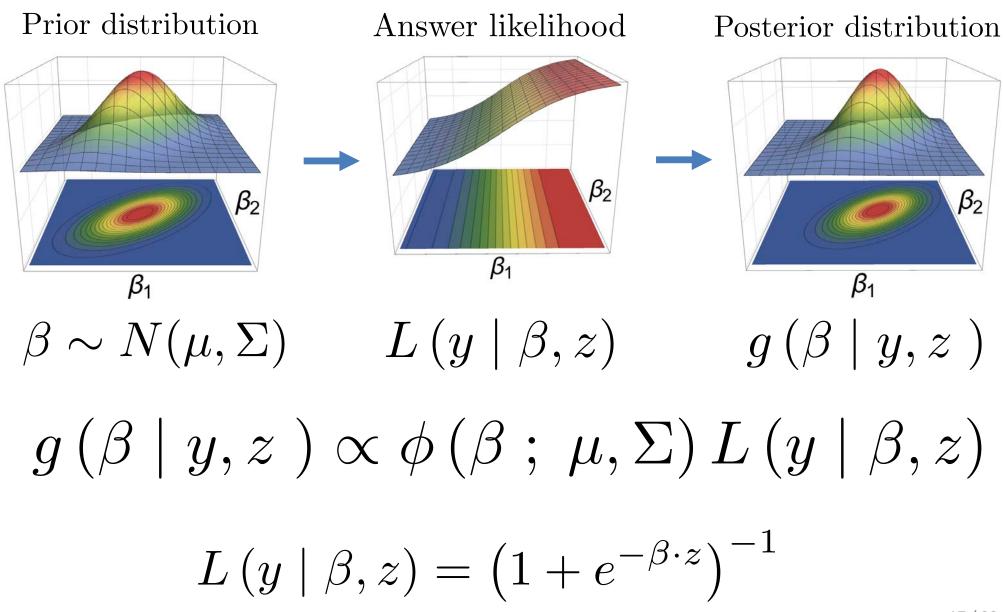
$$\beta \cdot x^1 \ge \beta \cdot x^2 \qquad \Leftrightarrow \qquad \beta \cdot z \ge 0 \quad z = x^1 - x^2$$

$$\Leftrightarrow$$

$$\beta \cdot z \ge 0$$

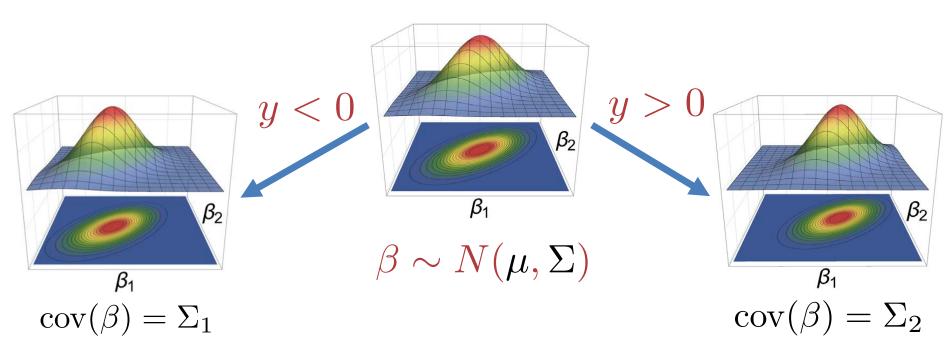
$$z = x^1 - x^2$$

#### 1-Question Bayesian Logistic Regression



#### D-Efficiency and Expected Posterior Variance

$$f(z, \mu, \Sigma) := \mathbb{E}_{y, \beta} \left\{ (\det \operatorname{cov}(\beta \mid y, z))^{1/m} \right\}$$



$$\max_{z \in \{-1,0,1\}^n} f(z,\mu,\Sigma)$$

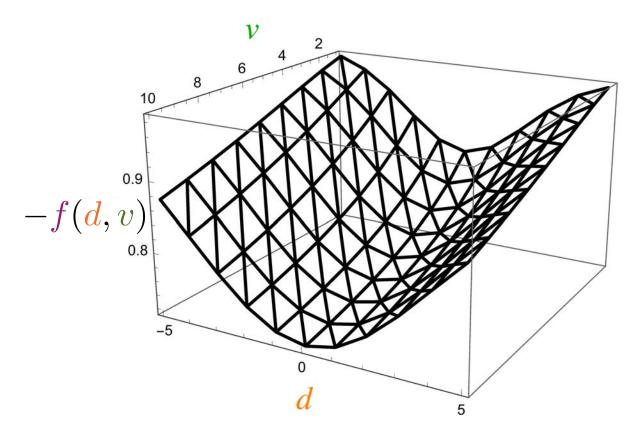
•  $f(z, \mu, \Sigma)$  is hard to evaluate, non-convex and n large

#### Reformulation from V. and Saure '16

• D-efficiency f(z) = Non-convex function f(d, v) of

mean: 
$$d := \mu \cdot z$$

variance: 
$$v := z' \cdot \sum \cdot z$$



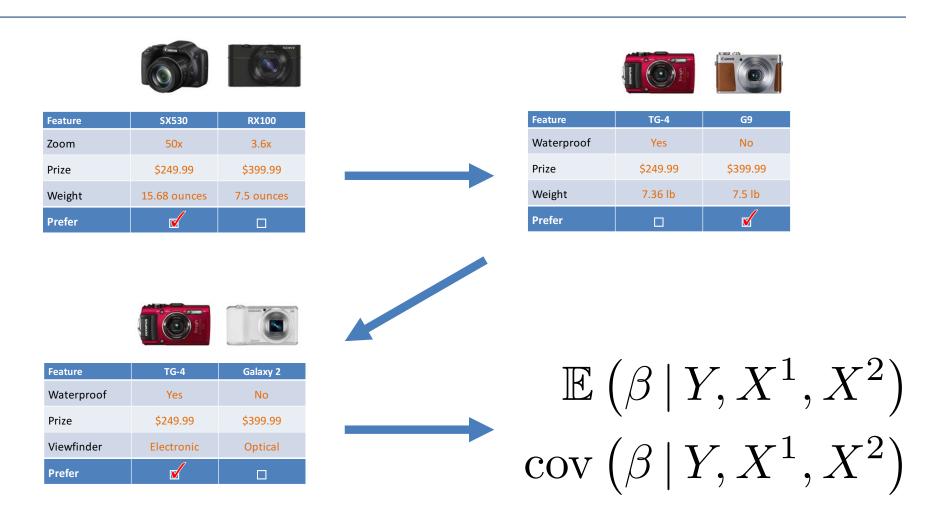
Can evaluate f(d, v) with 1-dim integral  $\odot$ 

Piecewise Linear Interpolation

Linear MIP formulation

Aligns with selection criteria from Toubia, Hauser, and Simester '04: minimize mean and maximize variance

#### MIP-based Moment-Matching Approx. Bayes

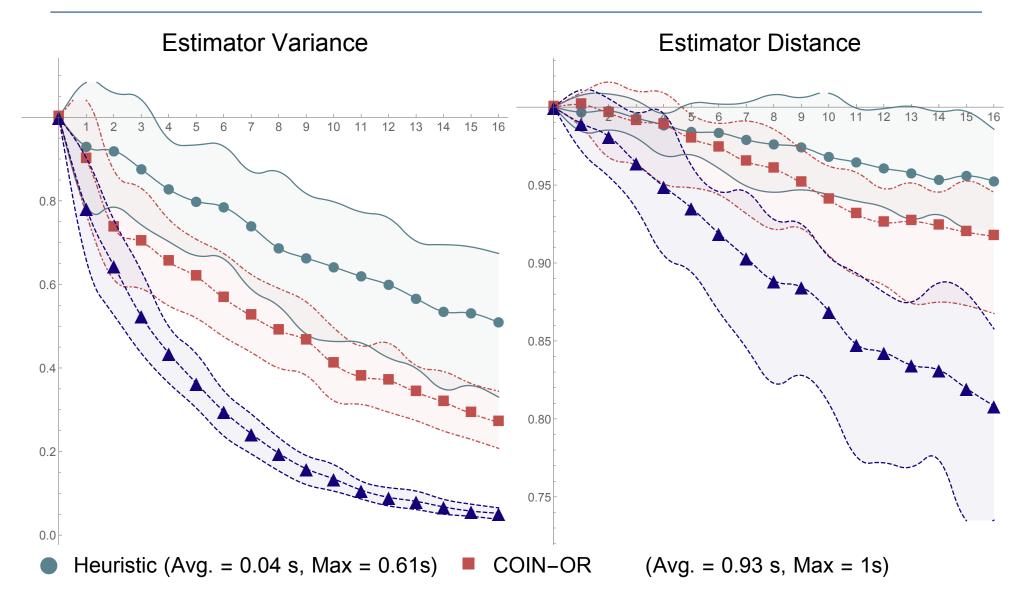


 After each answer compute posterior mean and covariance and replace with corresponding Gaussian

#### Computational Experiments

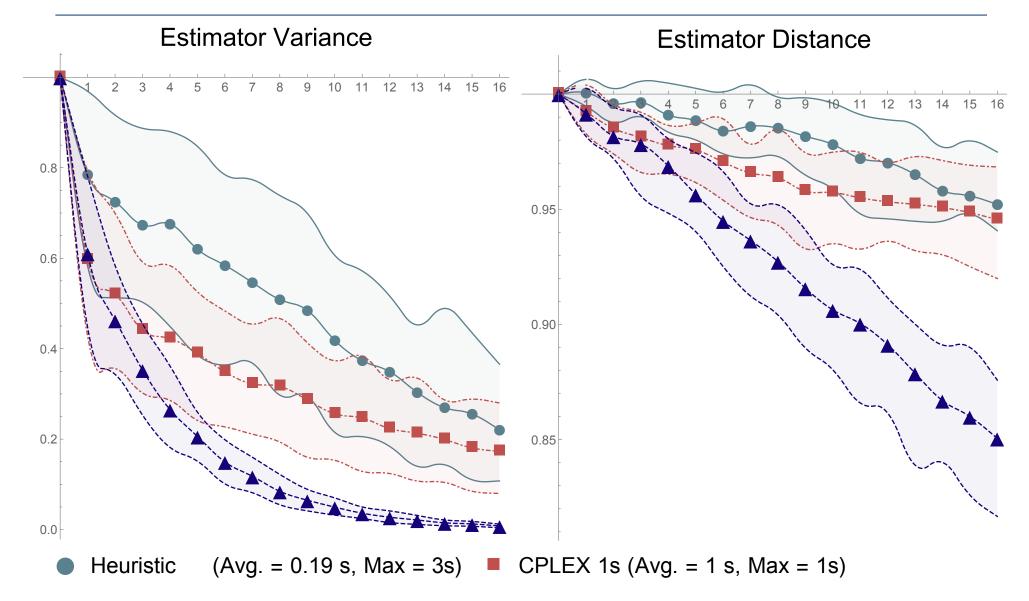
- 16 questions, 2 options, 12 and 24 features
- Simulate MNL responses with known  $\beta^*$
- Question Selection
  - Linear MIP-based using CPLEX and open source COIN-OR
  - Knapsack-based geometric Heuristic by Toubia et al.
- Time limits of 1 s and 10 s
- Metrics:
  - Estimator variance =  $\left(\det \operatorname{cov}\left(\beta \mid Y, X^{1}, X^{2}\right)\right)^{1/2}$
  - Estimator distance =  $\left\| \mathbb{E} \left( \beta \mid Y, X^1, X^2 \right) \beta^* \right\|_2$
  - Computed for true posterior with MCMC
- Slightly slower computer (~'12 iMac)

#### Results for 12 Features, 1 s time limit



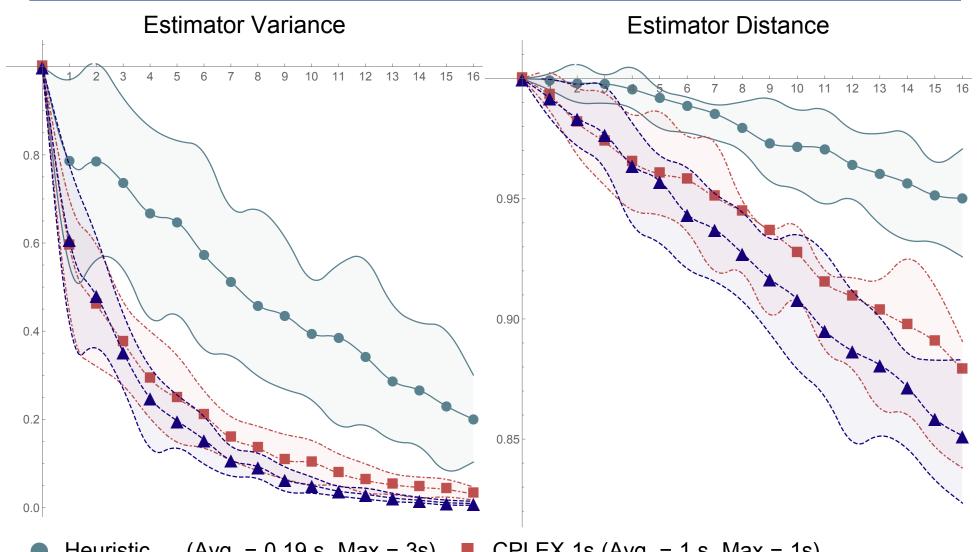
▲ CPLEX (Avg. = 0.21 s, Max = 0.48s)

#### Does it Scale? Results for 24 features



▲ CPLEX 10s (Avg. = 7.7 s, Max = 10s)

#### Some improvements for 24 features



- Heuristic (Avg. = 0.19 s, Max = 3s)■ CPLEX 1s (Avg. = 1 s, Max = 1s)
- ▲ CPLEX 10s (Avg. = 7.7 s, Max = 10s)

#### **Summary and Extensions**

- MIP for experimental design
  - Effective even for non-linear and near-real time
  - Appropriate domain expertise can be crucial for MIP'ing
  - Commercial solvers best, but free solvers reasonable
  - Integration into complex systems easy with JuMP
  - Some scalability: get the most out of "small" data
- Multi-Question Bayesian Logistic Regression:  $Z = \left\{z^i\right\}_{i=1}^q$ 
  - For many variants and approximations of "variance"

$$f(Z, \mu, \Sigma) = f\left(\left\{\mu \cdot z^i\right\}_{i=1}^q, \left\{z^{iT} \sum z^j\right\}_{i,j=1}^q\right)$$

 What kind of designs do you want to build? (future benchmark instances)