Robust Optimal Experimental Design for Functional Response Experiments

Dr Christopher Drovandi

School of Mathematical Sciences
ARC Centre of Excellence for Mathematical and Statistical Frontiers (ACEMS)
Queensland University of Technology

Collaborators: Jeff Zhang
Functional response models are important in understanding predator-prey interactions.

Optimal Design for Functional Response

In functional response experiments, the number of prey $N$ used for each observation in the experiment can sometimes be controlled.

**Aim:** Under some assumed functional response model, determine the optimal number of prey to use for each of $K$ observations in the experiment to learn about model parameters.
Case Study - Data

An experiment involving the freshwater predator *Notonecta glauca* (an aquatic insect) preying on *Asellus aquaticus* (a small crustacean resembling a woodlouse)

Original data from Hassell et al 1977: individual sample values (·), sample means (○—○—○) for each value of $N$. 
Case Study - Model

Take model from Fenlon and Faddy 2006. Modified Gompertz equation for the mean response:

\[ E[n] = a(e^{-b \exp(-cN)} - e^{-b}), \]  

where \( n \) is the number of prey consumed and \((a, b, c)\) are model parameters. Beta-binomial model is used

\[ p(n; N, \alpha, \beta) = \binom{N}{n} \frac{B(n + \alpha, N - n + \beta)}{B(\alpha, \beta)}. \]  

Link with the Gompertz equation via

\[ \mu = \frac{\alpha}{\alpha + \beta} = \frac{a}{N}(e^{-b \exp(-cN)} - e^{-b}) \] and

\[ \lambda = \frac{1}{\alpha + \beta}, \]

where \( \lambda \) is the overdispersion parameter. We define this model as the Beta-Binomial-Gompertz (BBG) model.
Design problem: If we were to design this experiment under the assumption of the BBG model, what is the optimal $N = (N_1, \ldots, N_K)$, where $N_i$ is the number of prey for experiment $i$, to use to learn about $\theta = (a, b, c)$. 
Optimal Experimental Design

Select values of controllable variables of an experiment to achieve experimental goals as quickly as possible and minimise costs.

Define some utility function, $u(N, \theta)$, which encodes the goal of experiment and perhaps costs.

Here we are interested in precise estimation of $\theta$. A common utility is this case:

$$u(\theta, N) = \det [I(\theta, N)].$$

We seek the design that maximises the utility function

$$N^*_\theta = \arg \max_{N \in \mathcal{N}} u(\theta, N),$$

so-called D-optimal design. (no optimisation details here)
Robust Optimal Design

\( N^*_\theta \) is only optimal for parameter value, \( \theta \), which is unknown. Called locally optimal design.

A robust design should perform relatively well for a range or distribution \( p(\theta) \) (sometimes called a ‘prior’) of parameter values; as long as the “true” underlying parameter value lies within the specified range.
The most common approach to robust design is the pseudo-Bayesian approach (Walter and Pronzato 1987):

\[ u_p(N) = \frac{1}{J} \sum_{j=1}^{J} \log u(N, \theta^j), \] (3)

Another method is the maximin approach (e.g. Dette et al 1997). First, we define the efficiency of design \( N \) as

\[ E(N, \theta) = \frac{u(N, \theta)}{u(N^*_\theta, \theta)} \]

where \( u(N^*_\theta, \theta) \) is the maximum local utility value based on the parameter \( \theta \). The maximin utility is then given by

\[ u_m(N) = \min_{j=1,\ldots,J} E(N, \theta_j). \]
Some New Utilities for Robust Design

The pseudo-Bayesian utility may not necessarily guard against obtaining low efficiencies for some $\theta$ values.

(1) Thus we consider mean minus standard deviation

$$u_{ps}(N) = u_p(N) - \text{sd}([\log u(N, \theta_j)]_{j=1}^{J}).$$

(2) Use efficiencies instead of log to put utility values on the same scale:

$$u_{pe}(N) = \frac{1}{J} \sum_{j=1}^{J} E(N, \theta_j).$$

(3) Finally use standard deviation to guard against low efficiencies.

$$u_{pes}(N) = u_{pe}(N) - \text{sd}([E(N, \theta_j)]_{j=1}^{J}).$$
The approach of Dror and Steinberg (2006) obtains a locally optimal designs for each $\theta_j$ for $j = 1, \ldots, J$ then ‘clusters’ all the local designs to obtain a robust design.

We develop an analogous approach for our integer valued design. Denote the concatenation (sorted from smallest to largest) of all the $J$ locally optimal designs as $N_c = \text{sort}(N_{\theta_1}^*, \ldots, N_{\theta_J}^*)$ which is of length $M = J \times K$. Then, we construct our robust design of size $K$ by systematically resampling $K$ values from $N_c$.

Fast and embarrassingly parallel.
We assume that a pilot experiment is conducted with one observation taken at each of the (eleven) prey levels.

Run Markov chain Monte Carlo to obtain posterior conditional on pilot data. Thin the sample to obtain 100 ‘prior’ samples for the robust experimental design.

We repeat the previous step so that we have a ‘prior’ sample to determine an optimal design and an independent ‘prior’ sample to test the optimal designs found from different utilities.
Results

Boxplots of the D-efficiencies obtained for different designs based on (a) prior samples A and (b) prior samples B. The results are based on the BBG model.

Christopher Drovandi
Biometrics by the Border
Conclusions

Developed optimal design approach for integer-valued designs, beta-binomial regression model and developed some new robust utilities that are generally applicable.

It is possible to test the performance on different utilities prior to performing experiment. Good to have many robust utility tools in the toolkit.

Future work:

- Include model structure uncertainty.
- Apply to other integer-valued design problems.
- Develop a sequential design approach.


Email: c.drovandi@qut.edu.au

Twitter: @chris_drovandi

Website: https://chrisdrovandi.weebly.com/