Notes on "Optimal Bayesian Design for Model Discrimination via Classification"

- Setup
  - K candidate statistical models, one of them is true
  - Models indexed by M, a random variable in $\{1, \dots, K\}$
  - For $M = m$, model is $p(y|\theta_m, m, d)$
    - $y \in \mathcal{Y}$ is data vector
    - $\theta_m \in \Theta_m$ is parameter vector
    - $d \in \mathcal{D}$ is design vector, the variables governing the experiment
  - Prior on θ_m is $p(\theta_m|m)$, given for each possible model
  - Prior on m is $p(m)$
- Picking d. Can use loss function that might depend on m, θ_m, and y, write it as

  $$l(d) = E_{\theta_m, y, M|d}[l(d, \theta_m, y, M)].$$

  Optimal d is $d^* = \arg\min_{d \in \mathcal{D}} l(d)$. We want to use an l that captures entropy around the distribution of M (which we then minimize). So we want to pick a d, which produces data y, that leads to the most information about the distribution of M. This will help us pick the correct model.
- Choice of loss function.
  - Shannon entropy (MD stands for multinomial deviance).

    $$l_{MD} : \begin{cases} \mathcal{D} \times \mathcal{Y} \to [0, \infty) \\ (d, y) \mapsto -\sum_{m=1}^{K} p(m|y, d) \log p(m|y, d) \end{cases}.$$

    y is observed after the experiment, so we don't actually know l_{MD}. So we'll integrate it out: they rewrite l_{MD} as

    $$\begin{aligned} l_{MD}(d) &= -\int_y p(y|d) \sum_{m=1}^{K} p(m|y, d) \log p(m|y, d) dy \\ &\overset{\text{Bayes' Rule}}{=} -\sum_{m=1}^{K} p(m) \int_y p(y|m, d) \log p(m|y, d) dy. \end{aligned} \tag{1}$$

  - 0-1 loss. Use a loss matrix for all combinations of true and selected models:

    $$\begin{aligned} l_{01}(d) &= \int_y p(y|d) \sum_{m=1}^{K} p(m|y, d)\{1 - I[\widehat{m}(y|d) = m]\} dy \\ &= \int_y p(y|d)\{1 - p[\widehat{m}(y|d)|y, d]\} dy. \end{aligned} \tag{2}$$

The loss functions above can be hard to compute analytically, so we can use Monte Carlo integration, by sampling from $p(m|y,d)$. Some common issues:

- Need to draw a lot of samples from $p(m|y,d)$
- $p(m|y,d)$ is not always available and needs to be estimated
- The likelihood $p(y|\theta_m, m, d)$ is intractable
- Need a lot of data/Monte Carlo samples for reasonable accuracy

Some remedies:

- using conjugate priors so integrals can be computed analytically
- quadrature
- sequential Monte Carlo (only applicable to sequential experimental designs, where design space is small)
- Gaussian-based posterior approximation
- ABC

Some shortcomings of ABC are addressed by classification method.

• Classification approach.