

- "Bayesian Workflow", Prof. Andrew Gelman, et al.
 - 1. Specify Model
 - Motivated by Exploratory Analysis leveraging visualizations
 - Weakly informative Priors
 - 2. Perform Prior Predictive Checking
 - Facilitated by visualizations
 - 3. Estimate Posterior (Fit Model)
 - Performed by Markov Chain Monte Carlo simulation
 - 4. Validate Computation
 - Diagnostic checking
 - 5. Evaluate Model
 - Leverage Posterior Predictive Checking
 - 6. Compare Models
 - 7. Apply Model
 - · Decision Making, etc.

Bayesian workflow*

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Bob Carpenter[¶] Yuling Yao[†] Lauren Kennedy [|] Jonah Gabry[†]
Paul-Christian Bürkner** Martin Modrák^{††}

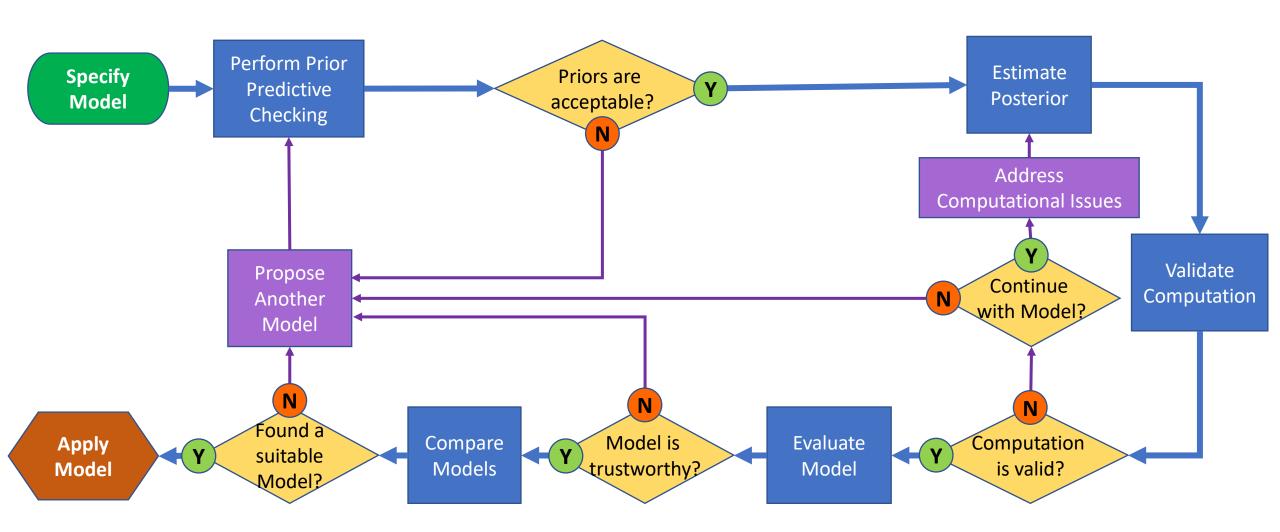
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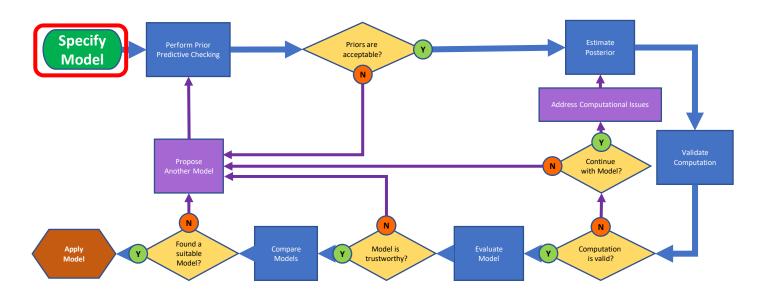
Abstract

The Bayesian approach to data analysis provides a powerful way to handle uncertainty in all observations, model parameters, and model structure using probability theory. Probabilistic programming languages make it easier to specify and fit Bayesian models, but this still leaves us with many options regarding constructing, evaluating, and using these models, along with many remaining challenges in computation. Using Bayesian inference to solve real-world problems requires not only statistical skills, subject matter knowledge, and programming, but also awareness of the decisions made in the process of data analysis. All of these aspects can be understood as part of a tangled workflow of applied Bayesian statistics. Beyond inference, the workflow also includes iterative model building, model checking, validation and troubleshooting of computational problems, model understanding, and model comparison. We review all these aspects of workflow in the context of several examples, keeping in mind that in practice we will be fitting many models for any given problem, even if only a subset of them will ultimately be relevant for our conclusions.

..but not a linear process

(adapted from Fig. 1, Gelman et al.)





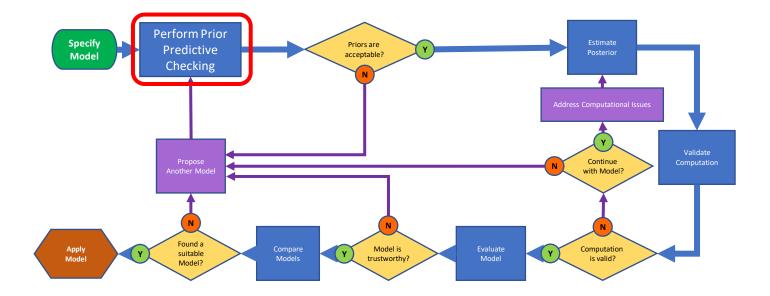
1. Specify Model

Just as with the simple Mosaic plot examples, this gives us the joint distribution, but as a simulator rather than a 2D plot. And applying Bayes Rule is, again, as simple as selecting the generated hypotheses (parameter values) that coincide with the same generated success rates as the evidence, in this case n.

Problem Statement

- We wish to estimate the success rate π of our promotional ad campaign amongst our target population. We have data from a small test amongst N=16 customers, in which we succeeded with n=6.
- Generative Model
 - Base Model: $n \sim \text{Binomial}(N, \pi)$; prior $p(\pi)$
- Weakly Informative Priors
 - Previous experience tells us that typically π ~0.30 and almost always our campaigns have π <0.80; we'll use π ~ Beta(α , β) and set the hyperparams assuming μ =0.30 and let 97.5%-ile = 0.80; so use α =0.96, β =2.24

^{*}Adapted from Rasmus Baath: "Bayesian Analysis Tutorial, Part 1: What"; YouTube (2017).



Bayesian Workflow

2. Perform

Prior

Predictive

Checking

- Simulate Response Data & Assess How Plausible They Are
 - I follow the advice of Gelman & colleagues* in picking "weakly informative" priors. These are priors that when used in generating "fake" data (i.e., simulating from the joint distn.) yield predictions of the responses that are at least plausible, even if not entirely likely.
- In Practice
 - I do Bayesian Analysis in R using <u>package `brms`</u> (Bayesian Regression Modeling with Stan).

- Gelman et al. "The Prior Can Often Only Be Understood in the Context of the Likelihood"
- Gabry et al. "Visualization in Bayesian Workflow"

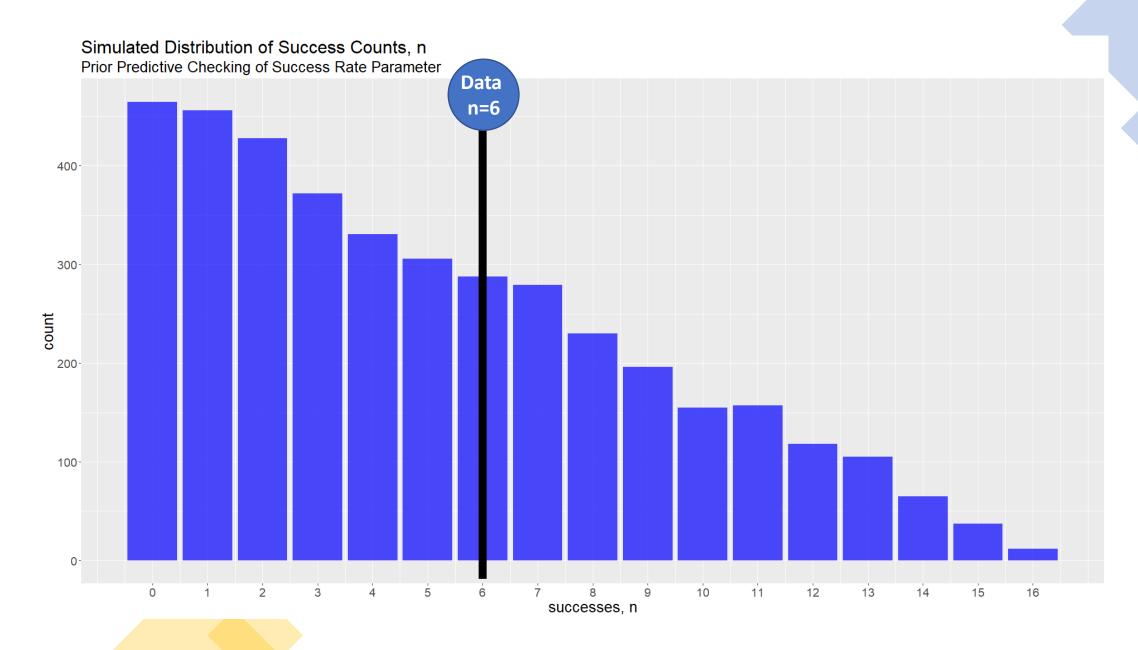
^{*}See the papers at these 2 links:

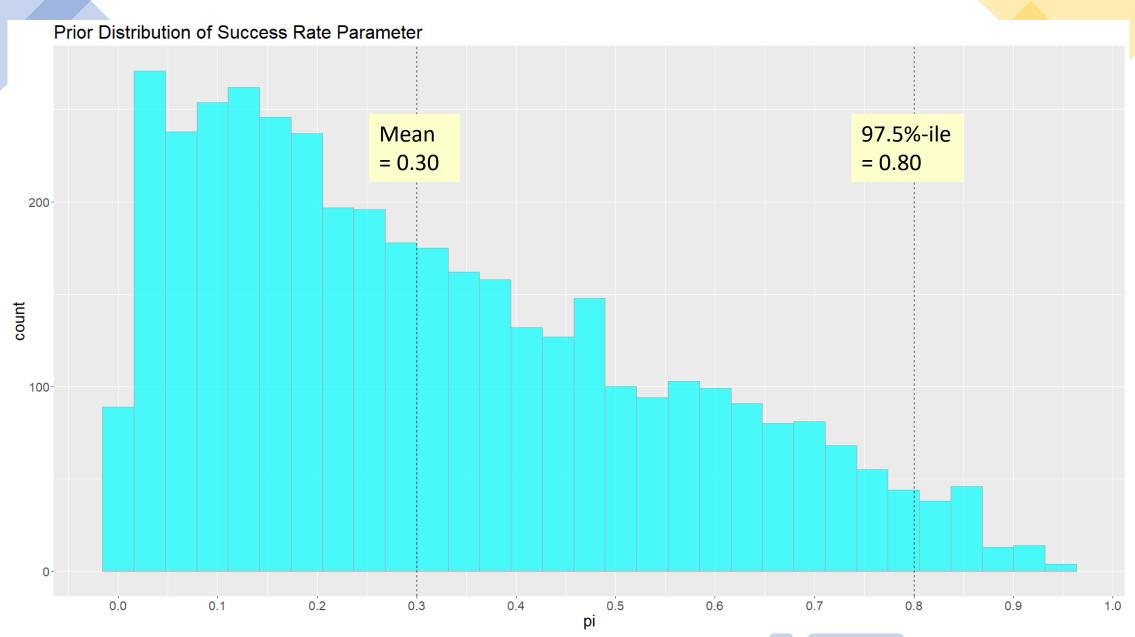
Prior Predictive Checking

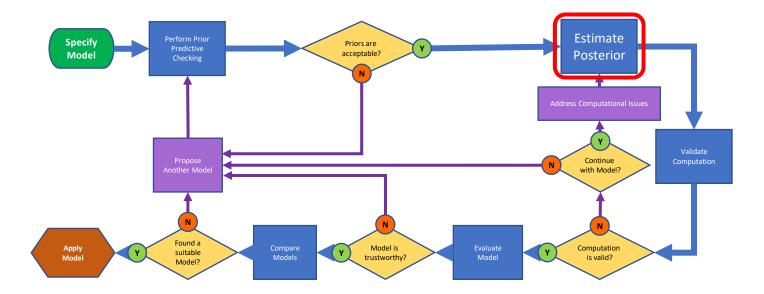
```
> library(magrittr)
> library(tidyverse)
> library(brms)
> df <- tibble(n=6,N=16)</pre>
> sim beta <- brm(</pre>
          formula = n | trials(N) ~ 1,
         family = binomial(link="identity"),
          data
                 = df
          prior = set prior(prior="beta(0.96,2.24)",class="Intercept"),
          sample prior = "only"
> sim beta
Family: binomial
 Links: mu = identity
Formula: n | trials(N) ~ 1
  Data: df (Number of observations: 1)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000
Population-Level Effects:
          Estimate Est.Error 1-95% CI u-95% CI Rhat Bulk ESS Tail ESS
                        0.23
                                 0.02
                                          0.82 1.01
                                                          454
Intercept
              0.32
                                                                   871
Samples were drawn using sampling (NUTS). For each parameter, Bulk ESS
and Tail ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

Prior Predictive Checking

```
> predict(sim_beta, summary = FALSE) %>% # generate success counts n as "fake" responses
  table() %>% # tabulate as frequency at each discrete count value
{
    tibble(n=as.integer(names(.)),p=c(.[]))
} %>%
{
    ggplot(.,aes(x=n,y=p)) +
        geom_col(fill="blue",alpha=0.7) +
        labs(
            title="Simulated Distribution of Success Counts, n",
            subtitle = "Prior Predictive Checking of Success Rate Parameter",
            y="count",
            x="successes, n"
        ) +
        theme(text = element_text(size=20)) +
        scale_x_continuous(breaks=(seq(0,16)))
} %>%
    print()
```







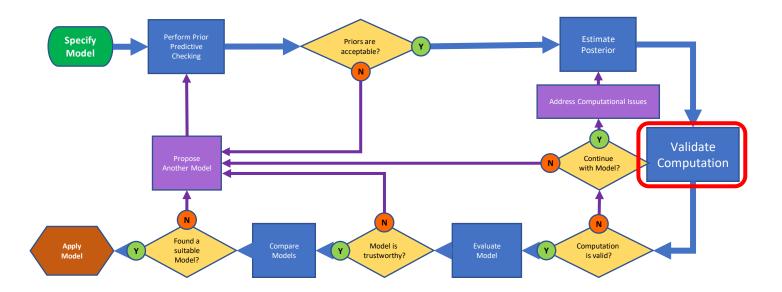
Bayesian Workflow 3. Estimate Posterior

Fitting a Model

- In Bayesian Analysis, fitting the model comes down to estimating the posterior distribution of the parameters given the data. This is conceptually like simulating responses from the joint and filtering out those simulated results that don't match the observed data for the responses and retaining the parameters of the model that generated the retained predicted responses. However, doing it that way (as rejection sampling) is only practical on simple problems. We use more advanced algorithms, like MCMC below, for modern real-world problems.
- Markov Chain Monte Carlo (MCMC) Simulation
 - The *de facto* standard in sampling from the posterior distribution is Hamiltonian Monte Carlo with the "No-U-Turn" Sampler (HMC-NUTS) as implemented in the <u>Stan probabilistic programming language</u>.

Estimating Posterior

```
> mod beta <- update(sim beta,sample prior="no")</pre>
> mod beta
 Family: binomial
 Links: mu = identity
Formula: n | trials(N) ~ 1
   Data: df (Number of observations: 1)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000
Population-Level Effects:
          Estimate Est.Error 1-95% CI u-95% CI Rhat Bulk ESS Tail ESS
                                                        1537
Intercept
              0.36
                        0.11
                                 0.17
                                          0.58 1.00
                                                                  1770
Samples were drawn using sampling (NUTS). For each parameter, Bulk ESS
and Tail ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
Warning message:
There were 6 divergent transitions after warmup. Increasing adapt delta above 0.8 may help.
See http://mc-stan.org/misc/warnings.html#divergent-transitions-after-warmup
> plot(mod beta)
```



4. Validate Computation

Assessing Convergence

 Before we evaluate the model for its predictive or explanatory ability, we must be sure we have achieved valid computation, i.e. the simulation converged to the actual posterior probability distribution.

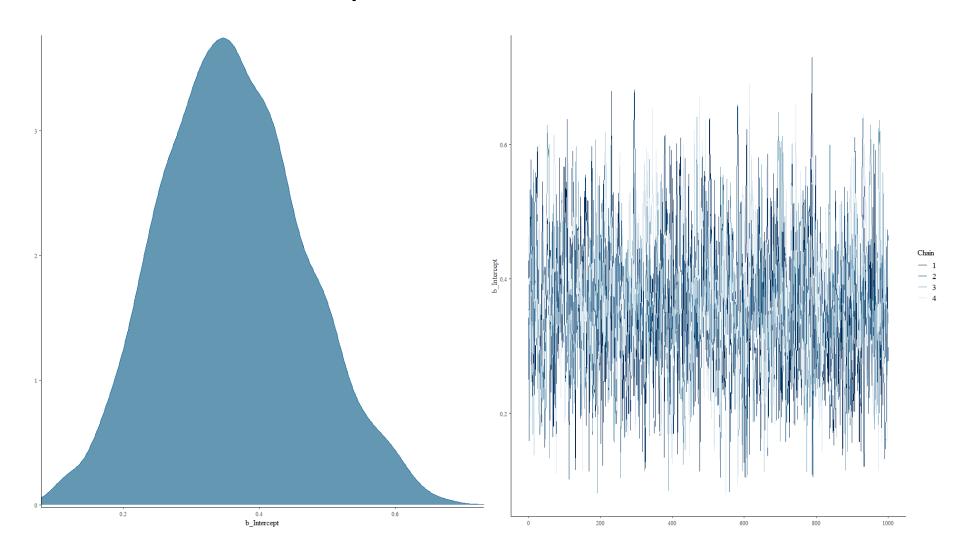
Diagnostics

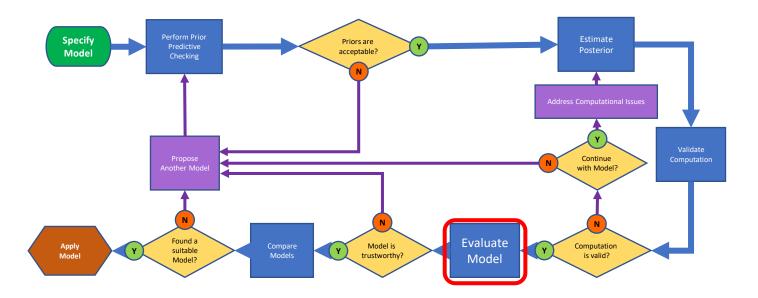
• Stan and the R packages based upon it provide us with a wealth of diagnostics, which we use to validate the computation. See the explanations & tips here: "Brief Guide to Stan's Warnings: Runtime Warnings".

Checking Diagnostics & Warnings

```
> mod beta <- update(sim beta,sample prior="no")</pre>
> mod beta
 Family: binomial
 Links: mu = identity
Formula: n | trials(N) ~ 1
   Data: df (Number of observations: 1)
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> plot(mod beta)
```

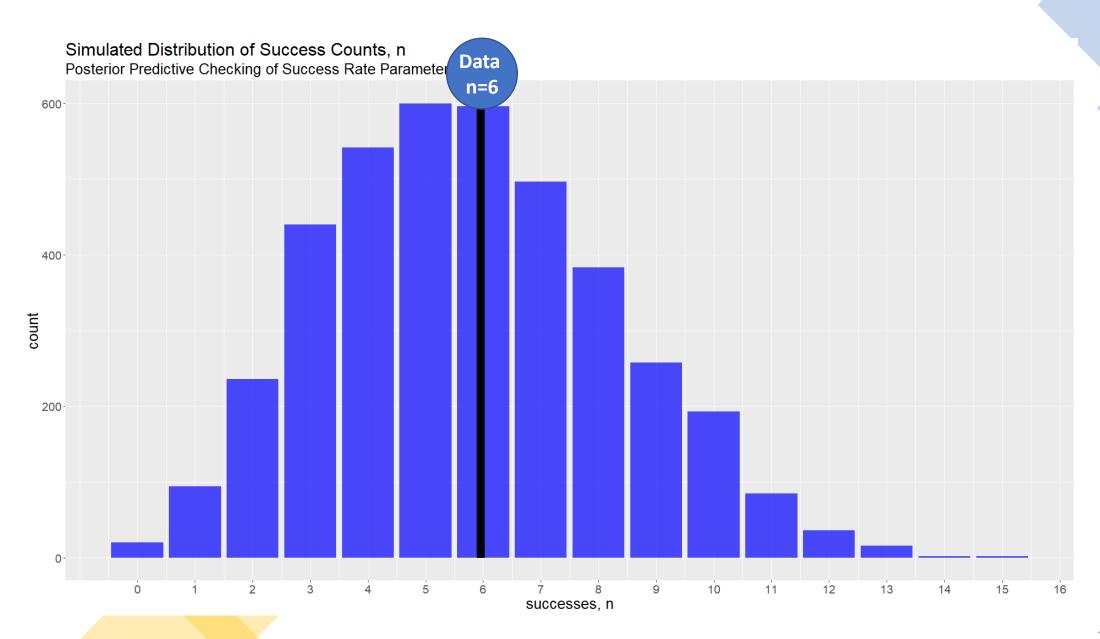
Posterior Density & Monte Carlo Trace Plot for success rate parameter π

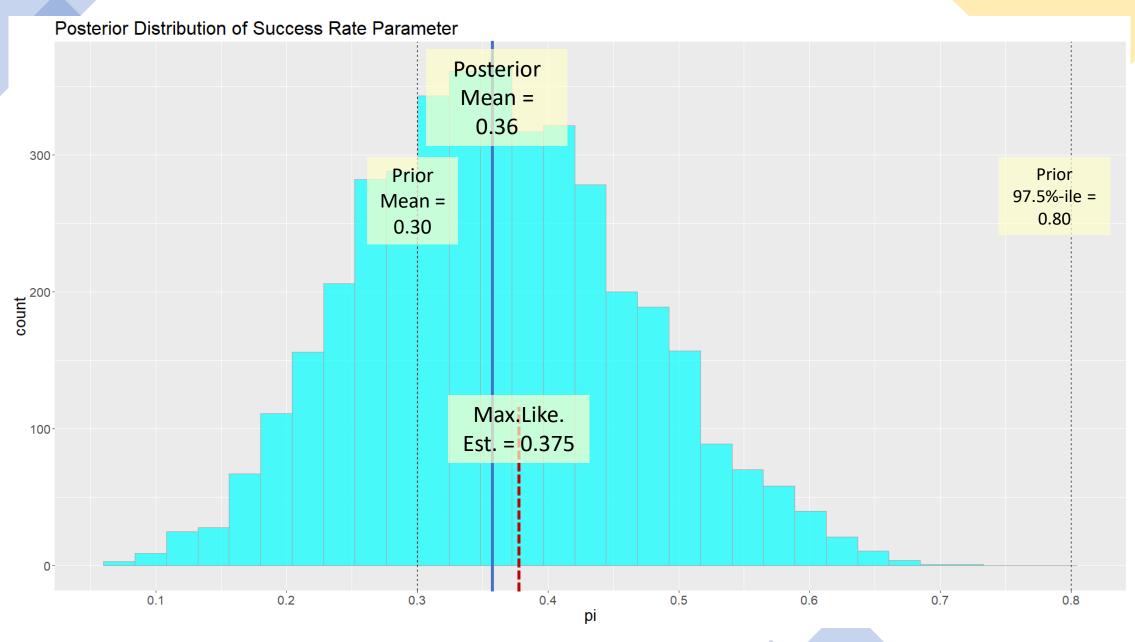


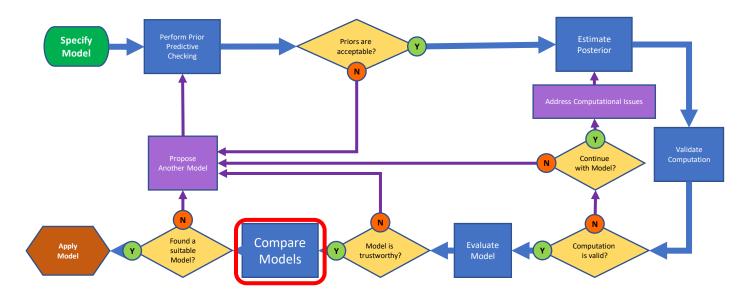


Bayesian Workflow 5. Evaluate Model

- Posterior Predictive Checking
 - Analogous to assessing the plausibility of simulated data from the prior distributions during Prior Predictive Checking, we do a similar check, now explicitly using the data to assess the quality of the posterior predicted responses.
- Leave-One-Out (LOO) Validation
 - Much recent work has been done on assessing the out-of-sample predictive ability of models using the posterior distribution. The "loo" calculation of the expected value of the log-posterior (elpd) is an efficient way of evaluating models.







Bayesian Workflow

6. Compare

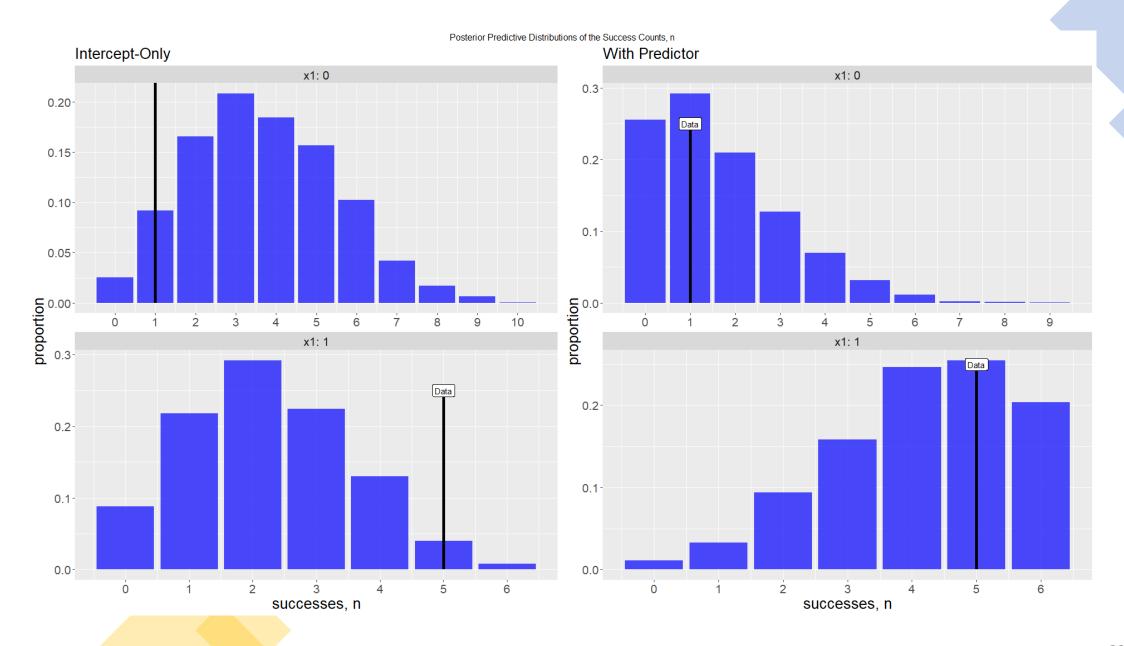
Models

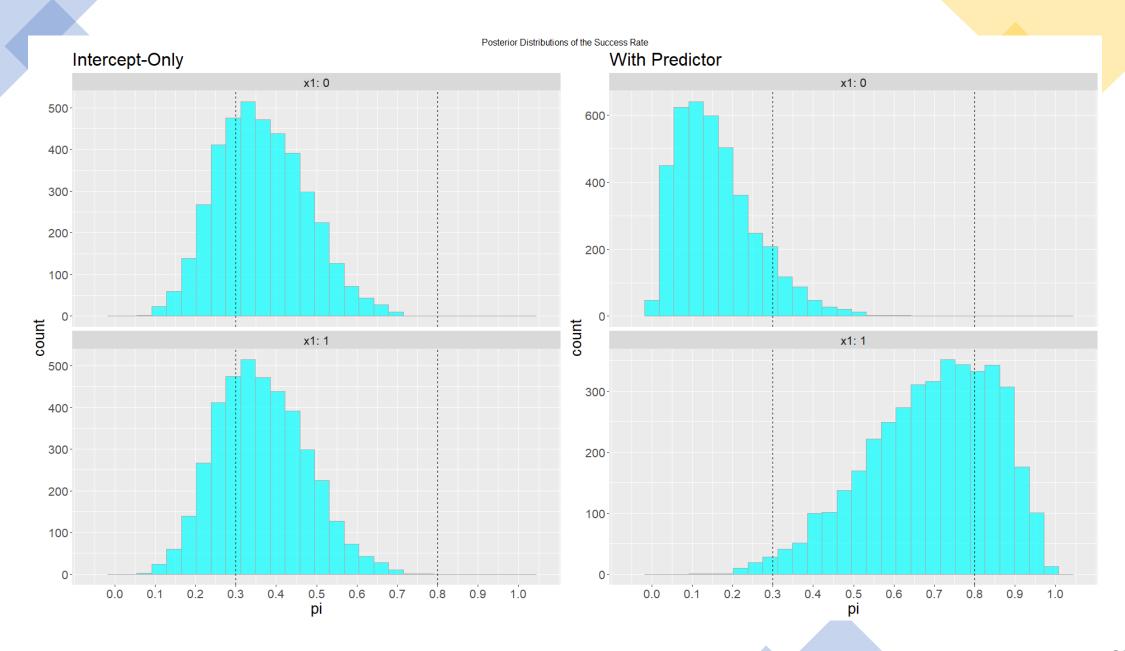
- Loo and Pointwise Comparison
 - The model with a significantly better loo-computed elpd is typically preferred. For models with comparable elpd, we usually pick the simpler of the model or the model that agrees most closely with our domain knowledge i.e. simplicity and expertise break the ties.
 - This tiny example can't show the value of loo & pointwise metrics. So, illustrate this below with data including a covariate x1 and building two models, one without the covariate as predictor (i.e., intercept only) and the other with it.

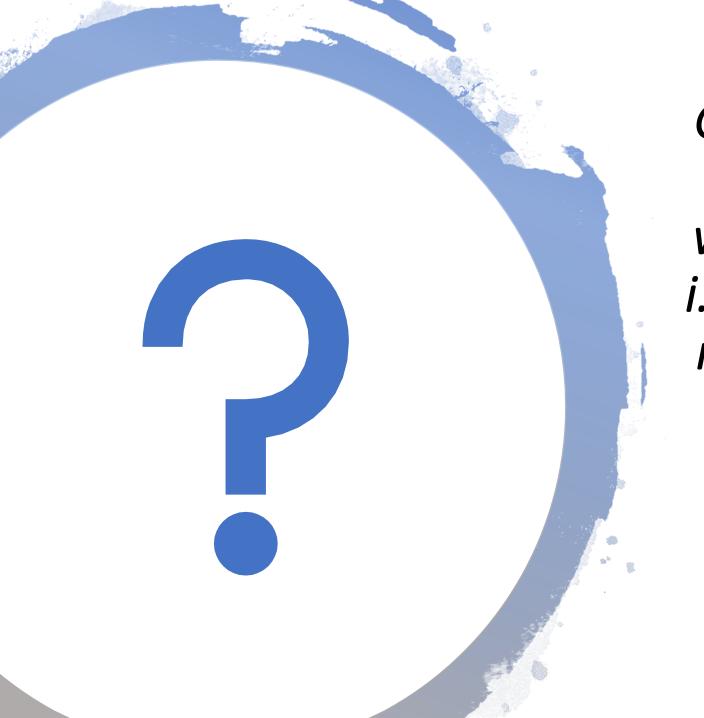
Model Comparison

```
> # Data w/covariate & two binomial-logit models.
> df2 <- tibble(n=c(5,1), N=c(6,10), x1=c(1,0))
> sim2 int <- brm(</pre>
    formula = n \mid trials(N) \sim 1,
    family = binomial(link="logit"),
    data = df2
    prior = set prior( prior = "normal(-1,1.5)",
           class="Intercept"),
    sample prior = "only"
> sim2 wx1 <- brm(
    formula = n \mid trials(N) \sim 1 + x1,
    family=binomial(link="logit"),
    data = df2
    prior = c(
        set prior( prior = "normal(-1,1.5)",
           class="Intercept"),
        set prior( prior = "normal(0,2)", class = "b")
    sample prior = "only"
> mod2 int <- update(
    sim2 int,
    sample prior = "no",
    save pars = save pars(all=TRUE)
> mod2 wx1 <- update(</pre>
    sim2 wx1,
    sample prior = "no",
    save pars = save pars(all=TRUE)
```

```
# Add the LOO criterion to both of them,
   then compare the models
> mod2 int <- add criterion(
    mod2 int,
    criterion = "loo",
    moment match = TRUE
> mod2 wx1 <- add criterion(</pre>
    mod2 wx1,
    criterion = "loo",
    moment match = TRUE
> loo compare(
    mod2 int,
    mod2 wx1,
    model names = c("intercept only", "with predictor")
               elpd diff se diff
with predictor 0.0
                          0.0
intercept only -5.8
                           0.2
```







Question for You: Given the complexity of Bayesian Analysis, when is it a good value, i.e. when does it provide results so valuable that they outweigh the additional complexity?

Use of Bayesian Analysis is Compelled by...

... These Issues

Uncertainty Quantification (UQ)

- Sparsity & Missing Data
- Risk & Decision Analysis; Post-Inference App: Explanations; Confirmations

Domain Knowledge (DK) Inclusion

 Expertise; Causality/Structural/State Space/Mechanism Representation

Heterogeneity

 Multi-level Behavior (context-specific; individualspecific)

Latent Structure

Factor Analysis; Conceptual Embeddings; Underlying Cognitive Constructs

Multiple Responses

Information Fusion;
 Multimodal Data Streams

Adaptation

 Autonomous & Active Learning Systems; Adaptive Questionnaires; Adaptive Experiments

Example: Predicting Success Rates

Base Model: $n \sim \text{Binomial}(N, \pi)$; prior $p(\pi)$

- **UQ:** posterior captures uncertainty $p(\pi | \{N,n\}_{Data})$; prior p(x), e.g. "error-in-variables"
- **DK Inclusion**: leverage expertise; interventions on x; $u(x) = f(x;\theta)$; captures mechanism (possibly nonlinear) $\pi = g^{-1}(u(x))$ (logit link function, g(.))
- **Heterogeneity:** hyper-personalization context- and individual-specific parameters $u(x_{ij}) = f(x_{ij}; \theta_{ij}); \ \theta_{ij} \sim Normal(\theta_i); \ \theta_j \sim Normal(\bar{\theta})$
- **Latent Structure:** cognitive constructs manifest as observed behavior; e.g. customer preferences $u(x,z) = f(x,z;\theta)$; z = h(x) captures theory of behavior
- Multiple Responses: universal latent constructs z driving behaviors measured by different modalities e.g. text reviews, videos, photos, survey responses. Augment trial-success data $y = \{N, n\}_{\text{Data}}$ with other data & add measurement models (likelihood modules)
- **Adaptation:** leverage UQ to compute learning objectives to generate new *x*; e.g. optimal product design; adaptive recommenders

More on Bayesian Analysis....

- Rasmus Baath "Bayesian Analysis (What, Why, How)" Tutorial
 - YouTube Videos (2017) (each ~30 min.)
- Michael Thompson's Flipboard e-zine mashup: <u>"Bayesian"</u>
- Prof. Andrew Gelman's blog:
 <u>"Statistical Modeling, Causal Inference, and Social Science"</u>
 - **Note:** Your obligations as a professional include being aware of the big issues faced by your profession. Read key Influencers.
- BANA 8090 Special Topics: Bayesian Analysis, instructor: M.L. Thompson
 - Spring 2021 (1st half)

Readings

- Statistics
 - Gelman et al. "<u>Bayesian Workflow</u>"
 - Gabry et al. "<u>Visualization in Bayesian Workflow</u>"
 - Gelman et al. "The Prior Can Often Only Be Understood in the Context of the Likelihood"
 - Richard McElreath "<u>Statistical Rethinking</u>"
- AI/ML
 - Chris Bishop (Microsoft Research) "Model-Based Machine Learning"
 - Daphne Koller & Nir Friedman "Probabilistic Graphical Models" (excerpt)
 - Norman Fenton & Martin Neil "<u>Risk Assessment & Decision Analysis with Bayesian Networks</u>" (<u>sample chapters</u>)

About the Presenter



Dr. Michael L. Thompson is retired from the Procter & Gamble Company, where he led Bayesian Analysis R&D in consumer & market modeling. His degrees are in Chemical Engineering: B.S., Northwestern University, '82; M.S., MIT, '84; and Ph.D., MIT, '96, with minor in Statistics and Artificial Intelligence. Michael has extensive experience in the process industry, having worked for Dow, Alcoa, Amoco, and Mitsubishi Chemical (Japan). At P&G for 21 years, Michael applied his expertise in Bayesian Analysis, especially Bayesian belief networks (BBN), to deliver results in the consumer-

packaged goods (CPG) industry. His contributions spanned business functions including R&D, Engineering, Manufacturing, Marketing, and Business Analytics. He has authored journal articles ranging from fluidized bed reactors to hybrid probabilistic and first-principles biochemical models to optimal consumer product design. Currently, Michael is a Term Adjunct in the Lindner College of Business at the University of Cincinnati, where he teaches Bayesian Analysis to candidates for the Master of Science in Business Analytics. He also serves on the Advisory Board for the Retail AI Lab of the Northwestern University Retail Analytics Council.