What do we need from a PPL to support Bayesian workflow?

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What is Bayesian workflow?

- Bayesian workflow involves
  - **designing/porting** models,
  - **fitting** models to data,
  - **validating** computation,
  - **evaluating** models,
  - **modifying** models,
  - addressing **computational issues**,
  - **comparing** models, and
  - **using** models.

Textbook form of workflow

1. Set up a **full probability model**: a joint distribution for observables and unobservables consistent with knowledge about the scientific problem and data collection.

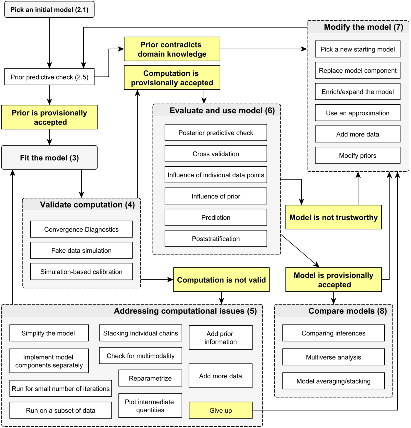
2. **Condition on observed data**: calculate and interpret the posterior distribution.

3. **Evaluate**: does it fit data, are conclusions reasonable, is it sensitive to assumptions?

4. **Iterate**: If model fails evaluation, go back to (1).

   - Gelman et al. 2013. *Bayesian Data Analysis, 3rd Edition.* Chapman & Hall.

Our actual workflow



Bayesian model

- y is **observed data**, θ are **unknown parameters**
  - suppress unmodeled predictors/features x
- **prior** $p(\theta)$
- **sampling** $p(y \mid \theta)$
  - likelihood $\mathcal{L}(\theta) = p(y \mid \theta)$ for fixed y
- **joint** $p(y, \theta)$
- **posterior** $p(\theta \mid y)$

Bayesian inference is expectation

- **parameter estimate** $\hat{\theta} = \mathbb{E}[\theta \mid y]$
- **event probability** $\Pr[C] = \mathbb{E}[I_C(\theta) \mid y]$
- **posterior predictive** $p(\tilde{y} \mid y) = \mathbb{E}[p(\tilde{y} \mid \theta) \mid y]$

Expectations via Monte Carlo

- calculate **asymptotically exact** expectations by averaging

$$\begin{aligned}\mathbb{E}[f(\theta) \mid y] &= \int_{\Theta} f(\theta) \cdot p(\theta \mid y)\,\mathrm{d}\theta \\ &= \lim_{M\to\infty} \tfrac{1}{M} \sum_{m=1}^{M} f(\theta^{(m)}) \\ &\approx \tfrac{1}{M} \sum_{m=1}^{M} (\theta^{(m)}),\end{aligned}$$

- MCMC **central limit theorem** says that if draws

$$\theta^{(1)}, \ldots, \theta^{(M)} \sim p(\theta \mid y)$$

have **effective sample size** M_{eff}, then

$$\text{standard error (of estimate)} = \frac{\text{posterior standard deviation}}{\sqrt{M_{\text{eff}}}}$$

Probabilistic programs typically. . .

- code Bayesian joint densities
- support sampling from the posterior to compute expectations
  - often with approximate variational posteriors
  - sometimes with acceleration like control variates
- but it turns out that we
  need more than posterior sampling for workflow

Prior predictive checks

- prior predictive checks simulate data from the marginal

$$y^{\mathrm{sim}} \sim p(y)$$

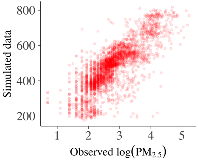
- often by generating from prior and sampling distributions

$$\theta^{\mathrm{sim}} \sim p(\theta) \qquad y^{\mathrm{sim}} \sim p(y \mid \theta^{\mathrm{sim}})$$

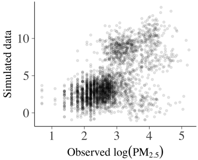
- then we compare simulated data y^{sim} to observed y

• Gabry, Simpson, Vehtari, Betancourt, Gelman. 2019. Visualization in Bayesian workflow. *JRSS A*.

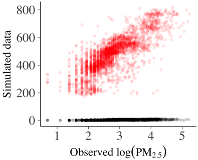
Prior predictive example



(a) Vague priors



(b) Weakly informative priors



(c) Comparison

- **particulate matter pollution** model with prior on $\log(\mathrm{PM}_{2.5})$
- **vague prior** generates values as dense as neutron star
- **weakly informative** prior controls scale
- subtle with priors on **interacting parameters**
  - why we need a PPL!

How does Stan fare?

- Stan model for **posterior inference**

```
data { int<lower=0> N; int<lower=0, upper=1> y[N]; }
parameters { real<lower=0, upper=1> theta; }
model { theta ~ beta(2, 10);  y ~ binomial(theta); }
```

- Simulate $\theta^{\text{sim}} \sim p(\theta)$ with $N = 0$, but can't simulate y
- Stan model for **prior predictive checks**

```
data { int N; }
parameters { real<lower=0, upper=1> theta; }
model { theta ~ beta(2, 10); }
generated quantities {
  int y_sim[N] = bernoulli_rng(N, theta);
}
```

How do other PPLs fare?

- **PyMC3** also declares data with **`observed=`**

```
y_obs = pm.Normal("y_obs", mu=X @ weights,
                  sigma=noise, observed=y)
```

- **ADMB** declares data in a **`DATA_SECTION`**
- **Pyro** uses effect handler **`condition()`** for data, e.g.,

```
poutine.condition(model, data={"z": 1.0})
```

- **Turing.jl** assigns data variables before just-in-time compilation; values may be specified **`missing`**
- **BUGS** sets data at run time w.r.t. its neutral graphical model

```
theta ~ dbeta(2, 10); for (n in 1:N) y[n] ~ dbern(theta);
```

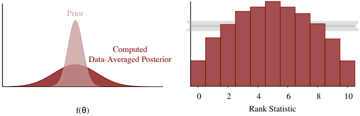
Simulation-based Calibration

- to **validate inference** w.r.t. well-specified data
  - approximate inference like VI will fail
- draw $\theta^{\text{sim}} \sim p(\theta)$ from the prior
- draw $y^{\text{sim}} \sim p(y \mid \theta^{\text{sim}})$ from the sampling distribution
- draw $\theta^{(1)}, \ldots, \theta^{(M)} \sim p(\theta \mid y^{\text{sim}})$ from algorithm to test
- because $(y^{\text{sim}}, \theta^{\text{sim}}) \sim p(y, \theta)$ and $(y^{\text{sim}}, \theta^{(m)}) \sim p(y, \theta)$, θ^{sim} should have uniform rank among the $\theta^{(m)}$

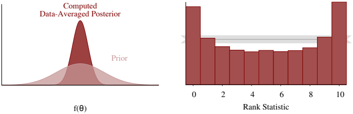
- Cook, Gelman, Rubin. 2006. Validation of software for Bayesian models using posterior quantiles. *JCGS*.
- Talts, Betancourt, Simpson, Vehtari, Gelman. 2018. Validating Bayesian inference algorithms with simulation-based calibration. *arXiv*

SBC diagnoses

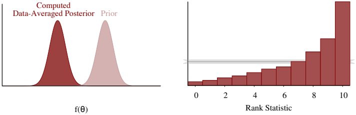
- **over-dispersed**:



- **under-dispersed**:



- **skewed**:



How do PPLs fare on SBC?

- simulation-based calibration requires simulating from prior and sampling distribution
- presents same problem with data specification as prior predictive checks

Posterior predictive checks

- Simulate new data from posterior for draws $m \in 1{:}M$,

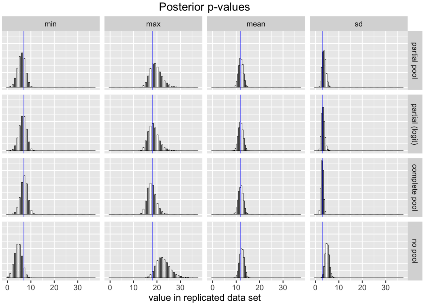
$$\begin{aligned} \theta^{(m)} &\sim p(\theta \mid y) \\ y^{\text{sim}(m)} &\sim p(y \mid \theta^{(m)}) \end{aligned}$$

- Compare statistics $s(y)$ on observed data to those of posterior simulations $s(y^{\text{sim}(m)})$, e.g.,
  - $s()$ can be anything, e.g., mean, max, sd, quantiles, ranks, skew, etc.

- Plot, or compute two-sided posterior p-values to automate,

$$\begin{aligned} p\text{-value} = \min(\ & \Pr[s(y) < s(y^{\text{sim}})], \\ & 1 - \Pr[s(y) < s(y^{\text{sim}})]\ ) \end{aligned}$$

Posterior predictive example



- model of repeated binary trials (baseball batting avg.)
  - vertical line is $s(y)$, histogram is $s(y^{\text{sim}(m)})$
  - max() and sd() statistics “reject” the no-pooling model

PPL support for PPCs

- requires extracting posterior draws and simulating data from them
- still the same problem of flexibly specifying data vs. parameters (i.e., knowns vs. unknowns)

Cross-validation

- divide data into train/test split (say y and $\tilde{y}$)
- fit model on training set
- evaluate predictive log density on test set,

$$\begin{aligned}\log p(\tilde{y} \mid y) &\approx \log \frac{1}{M} \sum_{m=1}^{M} p(\tilde{y} \mid \theta^{\mathrm{sim}(m)}) \\ &= \text{log-sum-exp}_{m=1}^{M} \log p(\tilde{y} \mid \theta^{\mathrm{sim}(m)}) - \log(M)\end{aligned}$$

PPL support for X-val

- fit with one data set y and evaluate with another $\tilde{y}$
- **BUGS** almost succeeds

```
for (n in 1:N) y[n] ~ dnorm(alpha + x[n] * beta, tau)
tau ~ gamma(1, 1);  alpha ~ normal(0, 2);  beta ~ normal(0, 2)
```

  by letting $y = y^{\text{train}}, y^{\text{test}}$ be partially missing

  - but doesn't let you retrieve the log density values for y^{test}
  - this also seamlessly handles missing data (that's modeled)

- **Turing.jl** allows the same thing (values?)
- other PPLs require additional sampling statements for the test data

Stan for X-val

- Stan codes **leave-one-out X-val** by specifying test point

```
data {
  int N; int[N] y;  int nt;
}
parameters {
  real mu; real<lower=0> sigma;
}
model {
  append_row(y[:nt-1], y[nt+1:]) ~ normal(mu, sigma);
  mu ~ normal(0, 1);  sigma ~ lognormal(0, 1);
}
generated quantities {
  real lp = normal_lpdf(y[nt] | mu, sigma);
}
```

- but it's a **totally different model**

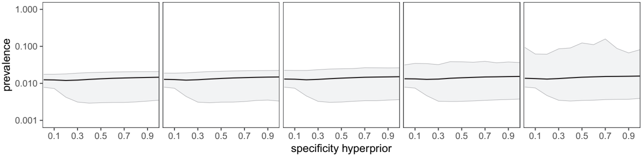
Sensitivity analysis

- we'd like to understand how **changes in our model affect posterior inference**
- e.g., vary priors and see how posterior expectations changes
- all PPLs let you evaluate alternative constants easily
- **derivative-based sensitivity** w.r.t. const. c is trickier

$$\frac{\partial}{\partial c}\mathbb{E}[f(\theta) \mid y, c]$$

Ryan Giordano modified Stan's C++ to compute this for his (Berkeley) Ph.D. thesis, but it's not exposed

Sensitivity example



- Estimated Covid seroprevalence (y axis) as a function of
  - the hyperprior for specificity (x-axis)
  - the hyperprior for sensitivity (facets with values from left-to-right 0.01, 0.25, 0.5, 0.75, 1.0)

- Gelman, Carpenter. 2020. Bayesian analysis of tests with unknown specificity and sensitivity. *JRSS C.*

Workflow goes beyond inference

- **clamp/pin parameters** to fixed values?
  - Stan requires moving the variable from the parameter to the data block
- working with **multiple (related) models**?
  - model comparison
  - model reparameterization
  - model averaging/mixing/stacking
- **autogenerating** concurrent or GPU code?
  - Stan requires using parallel map functions in the program

‘

Naming and persistence is hard

- how to **name and store multiple model variants**?
  - `uk-covid-icar`, `uk-covid-rw1`, `uk-covid-rw2`, `uk-covid-rw2-icar`, `uk-covid-rw2-bym2`, `uk-covid-rw2-bym2pc`, `uk-covid-rw2-bym2pc-no-socio`, *ad infinitum* . . .
  - plus multiple versions of the same model (over time)
- how to **name and store output**?
- how to work with **distributed teams**?
  - e.g., how to **share results** given that samples can be large?
  - or that they run on clusters in pieces

Other workflow issues

- data may be tied up with **privacy** and/or **intellectual property** concerns
  - e.g., medical records, search logs, street views, etc.
- end application may require **deployment in production**
  - bundle with Docker, or otherwise deploy
  - robustness is a key issue
  - update as new data comes in

- **What are we missing?**

Democratization of modeling

- **expression-based iterfaces** use PPLs under the hood, but give users simpler specification sublanguages
  - **brms**: expression interface in R
  - a Poisson GLM with log link is a one-liner

```
y ~ age + base * treatment + (1 | patient)
```

- **fully encapsulated interfaces** use PPLs under the hood but give users a menu of model choices
  - **Prophet** (time-series with trends and cycles)
  - **Torsten** (PK/PD compartment models)
- these systems involve **lots of defaults**
  - **evaluation crosses application boundaries**

Elephant in the room: Modularity

- how to **modularize model components** like hierarchical priors or GP priors?
- Stan lets users define **functions**
  - e.g., a random-walk or ICAR prior's density function
- but they **can't cross block boundaries**, e.g., data, parameter, model, generated quantities
- what about other PPLs?
- a residual problem: **density is modular, behavior isn't**
  - a prior can only be understood in the context of a likelihood and a data set

References

- **workflow paper**
  - Gelman, Vehtari, Simpson, Margossian, Carpenter, Yao, Kennedy, Gabry, Bürkner, Modrák. 2020. Bayesian workflow. *arXiv*.
- open-access **workflow book**
  - Above authors++. 2022? *Bayesian Workflow*. Chapman & Hall/CRC.
  - GitHub repo: https://github.com/jgabry/bayes-workflow-book