#### Chapter 6

- 6.1 The place of model checking in applied Bayesian statistics
- 6.2 Do the inferences from the model make sense?
- 6.3 Posterior predictive checking
- 6.4 Graphical posterior predictive checks (can be skipped)
- 6.5 Model checking for the educational testing example

#### Model checking

- demo6\_1: Posterior predictive checking light speed
- demo6\_2: Posterior predictive checking sequential dependence
- demo6\_3: Posterior predictive checking poor test statistic
- demo6\_4: Posterior predictive checking marginal predictive p-value

#### Model checking – overview

- Sensibility with respect to additional information not used in modeling
  - e.g., if posterior would claim that hazardous chemical decreases probability of death

### Model checking – overview

- Sensibility with respect to additional information not used in modeling
  - e.g., if posterior would claim that hazardous chemical decreases probability of death
- External validation
  - compare predictions to completely new observations
  - cf. relativity theory predictions

### Model checking – overview

- Sensibility with respect to additional information not used in modeling
  - e.g., if posterior would claim that hazardous chemical decreases probability of death
- External validation
  - compare predictions to completely new observations
  - cf. relativity theory predictions
- Internal validation
  - posterior predictive checking
  - cross-validation predictive checking

- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$

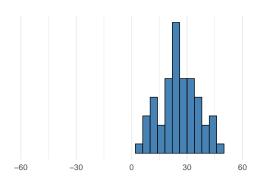
- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y<sup>rep</sup>

- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y<sup>rep</sup>
  - draw  $\mu^{(s)}, \sigma^{(s)}$  from the posterior  $p(\mu, \sigma | y)$

- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y<sup>rep</sup>
  - draw  $\mu^{(s)}, \sigma^{(s)}$  from the posterior  $p(\mu, \sigma | y)$
  - draw  $y^{\text{rep}(s)}$  from  $N(\mu^{(s)}, \sigma^{(s)})$

- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y<sup>rep</sup>
  - draw  $\mu^{(s)}, \sigma^{(s)}$  from the posterior  $p(\mu, \sigma | y)$
  - draw  $y^{\text{rep}(s)}$  from  $N(\mu^{(s)}, \sigma^{(s)})$
  - repat n times to get y<sup>rep</sup> with n replicates

- Newcomb's speed of light measurements
  - model  $y \sim N(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y<sup>rep</sup>
  - draw  $\mu^{(s)}, \sigma^{(s)}$  from the posterior  $p(\mu, \sigma | y)$
  - draw  $y^{\text{rep}(s)}$  from  $N(\mu^{(s)}, \sigma^{(s)})$
  - repat n times to get y<sup>rep</sup> with n replicates



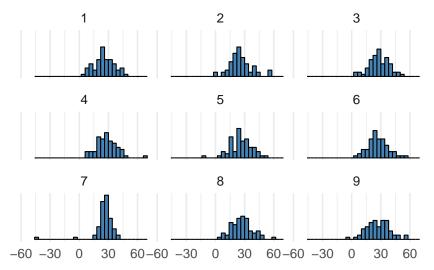
### Replicates vs. future observation

• Predictive  $\tilde{y}$  is the next not yet observed possible observation.  $y^{\text{rep}}$  refers to replicating the whole experiment (potentially with same values of x) and obtaining as many replicated observations as in the original data.

Generate several replicated datasets y<sup>rep</sup>

- Generate several replicated datasets y<sup>rep</sup>
- Compare to the original dataset

- Generate several replicated datasets y<sup>rep</sup>
- Compare to the original dataset



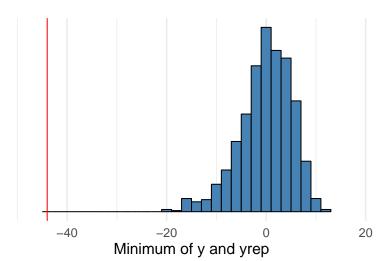
# Posterior predictive checking with test statistic

- Replicated data sets y<sup>rep</sup>
- Test quantity (or discrepancy measure)  $T(y, \theta)$ 
  - summary quantity for the observed data  $T(y, \theta)$
  - summary quantity for a replicated data  $T(y^{\text{rep}}, \theta)$
  - can be easier to compare summary quantities than data sets

• Compute test statistic for data  $T(y, \theta) = \min(y)$ 

- Compute test statistic for data  $T(y, \theta) = \min(y)$
- Compute test statistic min(y<sup>rep</sup>) for many replicated datasets

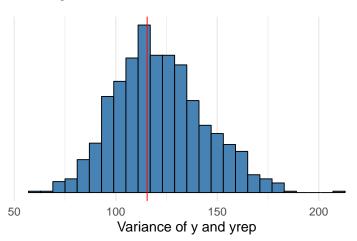
- Compute test statistic for data  $T(y, \theta) = \min(y)$
- Compute test statistic min(y<sup>rep</sup>) for many replicated datasets



- Good test statistic is ancillary (or almost)
  - ancillary if it depends only on observed data and if its distribution is independent of the parameters of the model

- Good test statistic is ancillary (or almost)
  - ancillary if it depends only on observed data and if its distribution is independent of the parameters of the model
- Bad test statistic is highly dependent of the parameters
  - e.g. variance for normal model

- Good test statistic is ancillary (or almost)
  - ancillary if it depends only on observed data and if its distribution is independent of the parameters of the model
- Bad test statistic is highly dependent of the parameters
  - . e.g. variance for normal model



Posterior predictive p-value

$$\rho = \Pr(T(y^{\text{rep}}, \theta) \ge T(y, \theta)|y) 
= \int \int I_{T(y^{\text{rep}}, \theta) \ge T(y, \theta)} p(y^{\text{rep}}|\theta) p(\theta|y) dy^{\text{rep}} d\theta$$

where I is an indicator function

Posterior predictive p-value

$$\rho = \Pr(T(y^{\text{rep}}, \theta) \ge T(y, \theta)|y) 
= \int \int I_{T(y^{\text{rep}}, \theta) \ge T(y, \theta)} p(y^{\text{rep}}|\theta) p(\theta|y) dy^{\text{rep}} d\theta$$

where I is an indicator function

• having  $(y^{\text{rep}(s)}, \theta^{(s)})$  from the posterior predictive distribution, easy to compute

$$T(y^{\text{rep}(s)}, \theta^{(s)}) \ge T(y, \theta^{(s)}), \quad s = 1, \dots, S$$

Posterior predictive p-value

$$\rho = \Pr(T(y^{\text{rep}}, \theta) \ge T(y, \theta)|y) 
= \int \int I_{T(y^{\text{rep}}, \theta) \ge T(y, \theta)} p(y^{\text{rep}}|\theta) p(\theta|y) dy^{\text{rep}} d\theta$$

where I is an indicator function

• having  $(y^{\text{rep}(s)}, \theta^{(s)})$  from the posterior predictive distribution, easy to compute

$$T(y^{\text{rep}(s)}, \theta^{(s)}) \ge T(y, \theta^{(s)}), \quad s = 1, \dots, S$$

 Posterior predictive p-value (ppp-value) estimated whether difference between the model and data could arise by chance

Posterior predictive p-value

$$p = \Pr(T(y^{\text{rep}}, \theta) \ge T(y, \theta)|y)$$
$$= \int \int I_{T(y^{\text{rep}}, \theta) \ge T(y, \theta)} p(y^{\text{rep}}|\theta) p(\theta|y) dy^{\text{rep}} d\theta$$

where I is an indicator function

• having  $(y^{\text{rep}(s)}, \theta^{(s)})$  from the posterior predictive distribution, easy to compute

$$T(y^{\text{rep}(s)}, \theta^{(s)}) \ge T(y, \theta^{(s)}), \quad s = 1, \dots, S$$

- Posterior predictive p-value (ppp-value) estimated whether difference between the model and data could arise by chance
- Not commonly used as the distribution of test statistic often more information

# Marginal and CV predictive checking

- Consider marginal predictive distributions  $p(\tilde{y}_i|y)$  and each observation separately
  - marginal posterior p-values

$$p_i = \Pr(T(y_i^{ ext{rep}}) \leq T(y_i)|y)$$
 if  $T(y_i) = y_i$   $p_i = \Pr(y_i^{ ext{rep}} \leq y_i|y)$ 

# Marginal and CV predictive checking

- Consider marginal predictive distributions  $p(\tilde{y}_i|y)$  and each observation separately
  - marginal posterior p-values

$$p_i = \mathsf{Pr}(T(y_i^{\mathrm{rep}}) \leq T(y_i)|y)$$
 if  $T(y_i) = y_i$   $p_i = \mathsf{Pr}(y_i^{\mathrm{rep}} \leq y_i|y)$ 

- if  $Pr(\tilde{y}_i|y)$  well calibrated, distribution of  $p_i$  would be uniform between 0 and 1
  - holds better for cross-validation predictive tests (cross-validation Ch 7)

### Marginal predictive checking - Example

Marginal tail area or Probability integral transform (PIT)

$$p_i = p(y_i^{\text{rep}} \leq y_i|y)$$

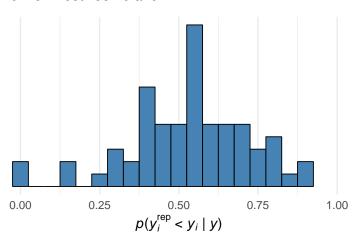
• if  $p(\tilde{y}_i|y)$  is well calibrated, distribution of  $p_i$ 's would be uniform between 0 and 1

#### Marginal predictive checking - Example

Marginal tail area or Probability integral transform (PIT)

$$p_i = p(y_i^{\text{rep}} \leq y_i|y)$$

• if  $p(\tilde{y}_i|y)$  is well calibrated, distribution of  $p_i$ 's would be uniform between 0 and 1



 How much different choices in model structure and priors affect the results

- How much different choices in model structure and priors affect the results
  - test different models and priors

- How much different choices in model structure and priors affect the results
  - test different models and priors
  - alternatively combine different models to one model
    - e.g. hierarchical model instead of separate and pooled
    - e.g. t distribution contains Gaussian as a special case
  - robust models are good for testing sensitivity to "outliers"
    - e.g. t instead of Gaussian

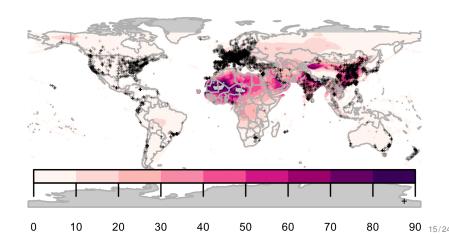
- How much different choices in model structure and priors affect the results
  - test different models and priors
  - alternatively combine different models to one model
    - e.g. hierarchical model instead of separate and pooled
    - e.g. *t* distribution contains Gaussian as a special case
  - robust models are good for testing sensitivity to "outliers"
    - e.g. t instead of Gaussian
- Compare sensitivity of essential inference quantities
  - extreme quantiles are more sensitive than means and medians
  - extrapolation is more sensitive than interpolation

#### Example: Exposure to air pollution

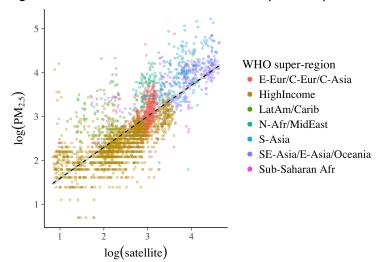
- Example from Jonah Gabry, Daniel Simpson, Aki Vehtari, Michael Betancourt, and Andrew Gelman (2017).
   Visualization in Bayesian workflow. https://arxiv.org/abs/1709.01449
- Estimation of human exposure to air pollution from particulate matter measuring less than 2.5 microns in diameter (PM<sub>2.5</sub>)
  - Exposure to PM<sub>2.5</sub> is linked to a number of poor health outcomes and a recent report estimated that PM<sub>2.5</sub> is responsible for three million deaths worldwide each year (Shaddick et al., 2017)
  - In order to estimate the public health effect of ambient PM<sub>2.5</sub>, we need a good estimate of the PM<sub>2.5</sub> concentration at the same spatial resolution as our population estimates.

#### Example: Exposure to air pollution

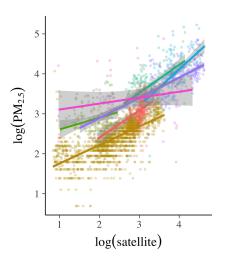
- Direct measurements of PM 2.5 from ground monitors at 2980 locations
- High-resolution satellite data of aerosol optical depth



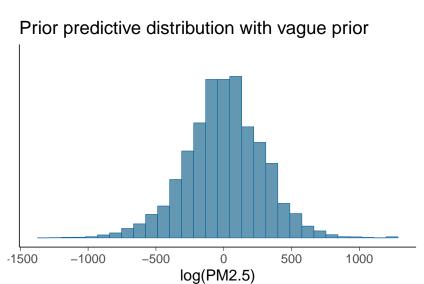
- Direct measurements of PM 2.5 from ground monitors at 2980 locations
- High-resolution satellite data of aerosol optical depth



- Direct measurements of PM 2.5 from ground monitors at 2980 locations
- High-resolution satellite data of aerosol optical depth

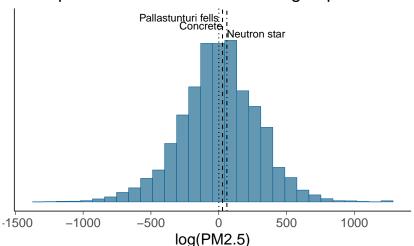


Prior predictive checking



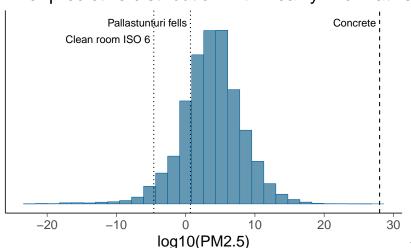
Prior predictive checking



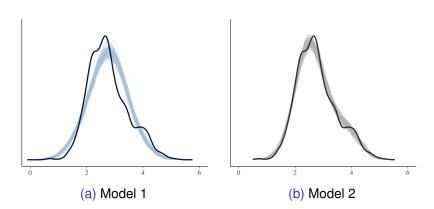


Prior predictive checking

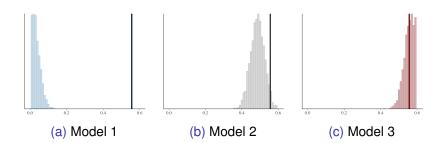




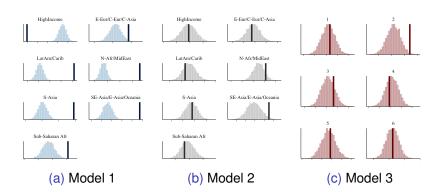
Posterior predictive checking – marginal predictive distributions



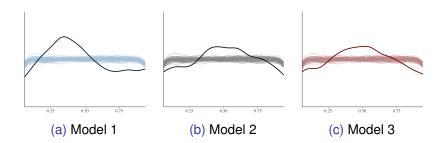
Posterior predictive checking – test statistic (skewness)

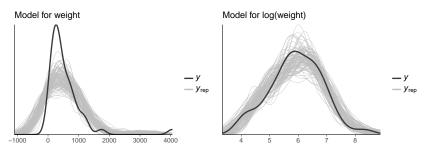


Posterior predictive checking – test statistic (median for groups)



LOO predictive checking - LOO-PIT

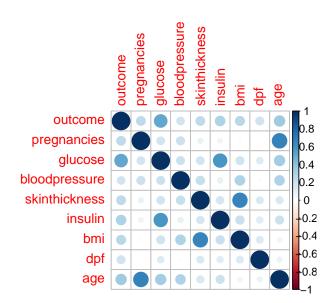




Predicting the yields of mesquite bushes.

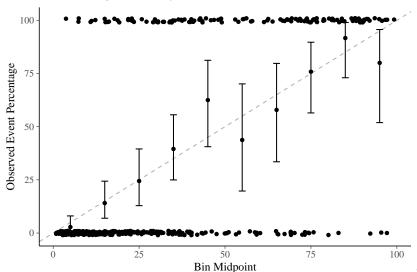
Gelman, Hill & Vehtari (2019): Regression and Other Stories, Chapter 11.

Diabetes prediction with logistic regression - diabetes demo

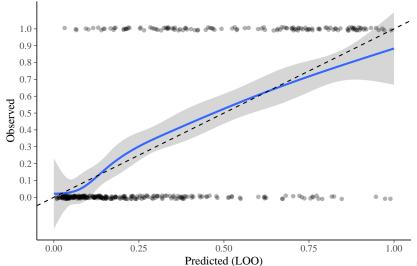


Diabetes prediction with logistic regression - diabetes demo

PPC with binning for binary data



Diabetes prediction with logistic regression - diabetes demo PPC with non-linear regression for binary data



## Posterior predictive checking

demo demos\_rstan/ppc/poisson-ppc.Rmd

```
data |
  int < lower = 1 > N:
  int <lower=0> y[N];
parameters {
  real < lower = 0 > lambda:
model {
  lambda ~ exponential(0.2);
  y ~ poisson(lambda);
generated quantities {
  real log lik[N];
  int y rep[N];
  for (n in 1:N) {
    y rep[n] = poisson rng(lambda);
    log lik[n] = poisson lpmf(y[n] | lambda);
```

## Further reading and examples

- Jonah Gabry, Daniel Simpson, Aki Vehtari, Michael Betancourt, and Andrew Gelman (2018). Visualization in Bayesian workflow. Journal of the Royal Statistical Society Series A, accepted for publication as discussion paper. arXiv preprint arXiv:1709.01449.
- Graphical posterior predictive checks using the bayesplot package http://mc-stan.org/bayesplot/articles/graphical-ppcs.html
- Another demo demos\_rstan/ppc/poisson-ppc.Rmd
- Michael Betancourt's workflow case study with prior and posterior predictive checking
  - for RStan https://betanalpha.github.io/assets/case\_studies/ principled bayesian workflow.html
  - for PyStan https://github.com/betanalpha/jupyter\_case\_ studies/blob/master/principled\_bayesian\_workflow/ principled\_bayesian\_workflow.ipynb