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

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
    - this can be skimmed, see instead the paper
      Gabry et al. (2019). *Visualization in Bayesian workflow*
      https://doi.org/10.1111/rssa.12378
- 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

Simon Newcomb's light of speed experiment in 1882

Newcomb measured ($n = 66$) the time required for light to travel from his laboratory on the Potomac River to a mirror at the base of the Washington Monument and back, a total distance of 7422 meters.

Posterior predictive checking – example

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

# Posterior predictive checking – example

- Newcomb's speed of light measurements
  - model $y \sim \text{normal}(\mu, \sigma)$ with prior $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y^{rep}

Posterior predictive checking – example

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

Posterior predictive checking – example

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

Posterior predictive checking – example

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

Posterior predictive checking – example

- Newcomb's speed of light measurements
  - model $y \sim \text{normal}(\mu, \sigma)$ with prior $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate y^{rep}
  - draw $\mu^{(s)}, \sigma^{(s)}$ from the posterior $p(\mu, \sigma|y)$
  - draw $y^{\text{rep}\,(s)}$ from $\text{normal}(\mu^{(s)}, \sigma^{(s)})$
  - repeat n times to get y^{rep} with n replicates
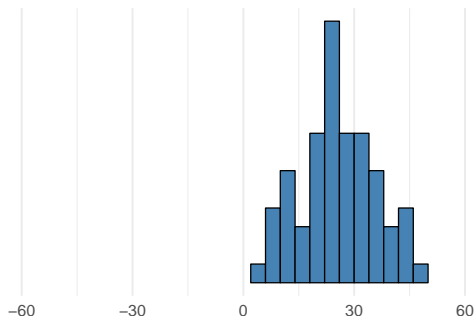
Replicates vs. future observation

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

Posterior predictive checking – example

- Generate several replicated datasets y^{rep}

Posterior predictive checking – example

- Generate several replicated datasets y^{rep}
- Compare to the original dataset

Posterior predictive checking – example

- Generate several replicated datasets y^{rep}
- Compare to the original dataset
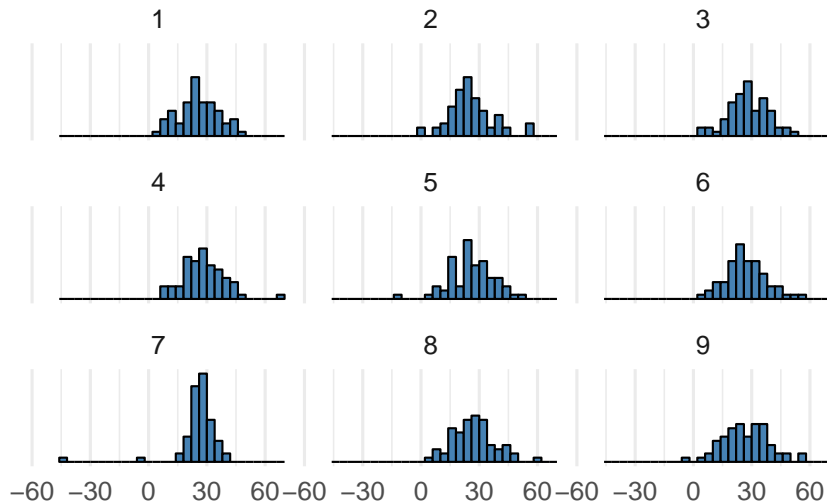
Posterior predictive checking – bayesplot

```
ppc_hist(y, yrep[1:8,])
```
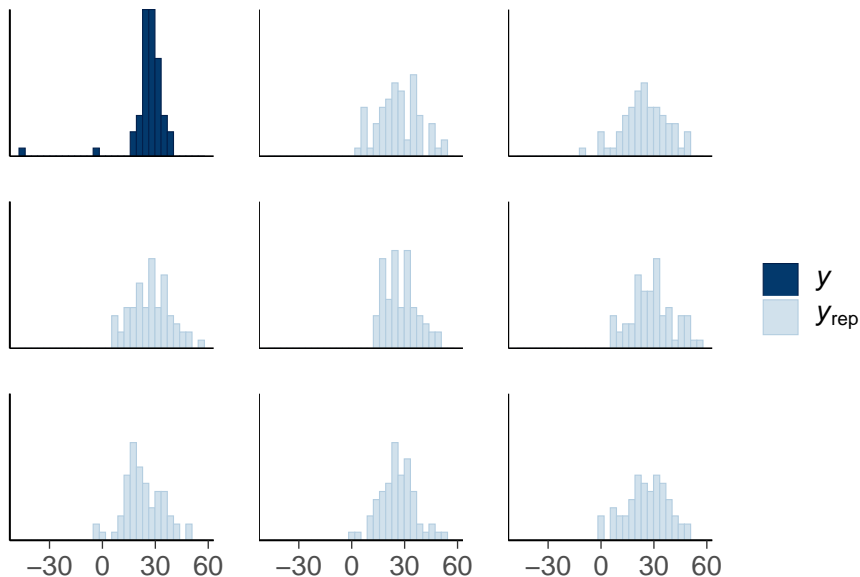
Posterior predictive checking – bayesplot

```
ppc_dens_overlay(y, yrep[1:100,])
```
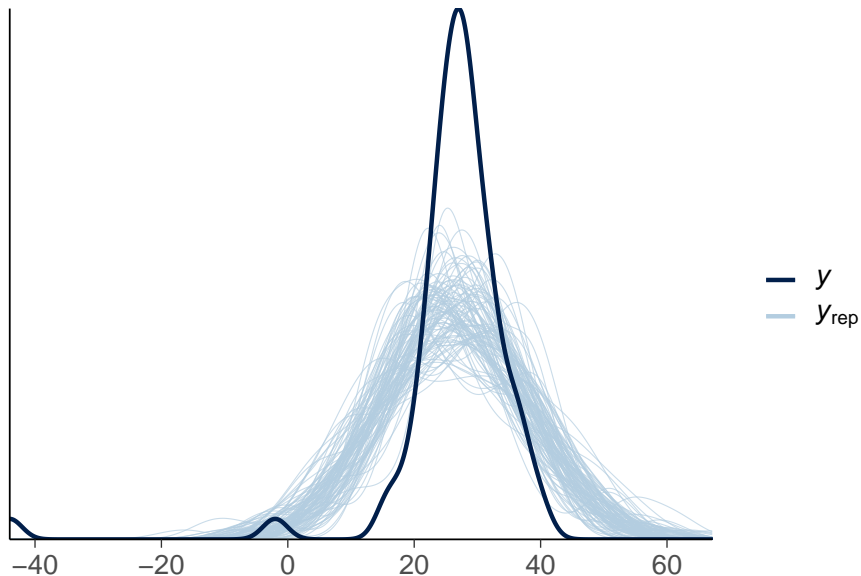
Posterior predictive checking – bayesplot

```
ppc_ecdf_overlay(y, yrep[1:100,])
```
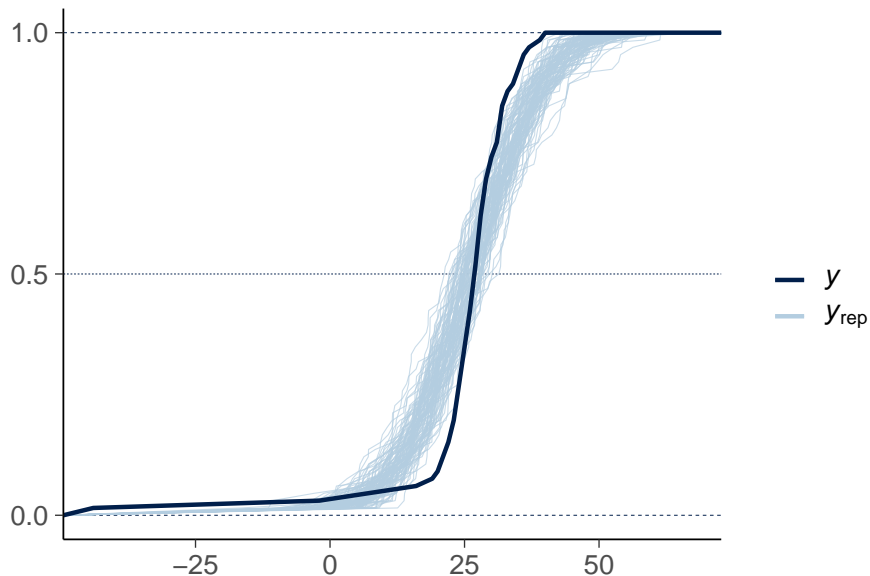
Posterior predictive checking – bayesplot

```
ppc_scatter(y, yrep[1:4,]) + geom_abline()
```
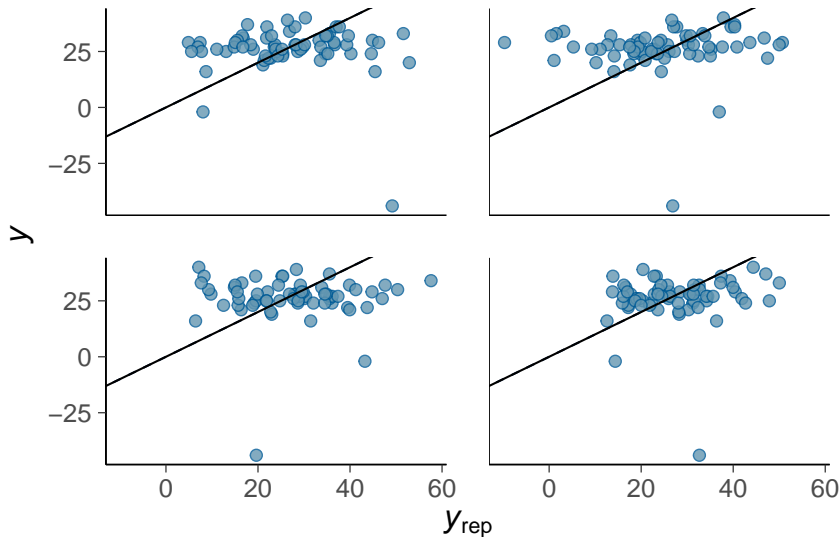
Posterior predictive checking with test statistic

- Replicated data sets y^{rep}
- 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 $T(y, \theta) = \min(y)$

Posterior predictive checking – example

- Compute test statistic for data $T(y, \theta) = \min(y)$
- Compute test statistic $\min(y^{\text{rep}})$ for many replicated datasets

Posterior predictive checking – example

- Compute test statistic for data $T(y, \theta) = \min(y)$
- Compute test statistic $\min(y^{\text{rep}})$ for many replicated datasets

Minimum of y and yrep
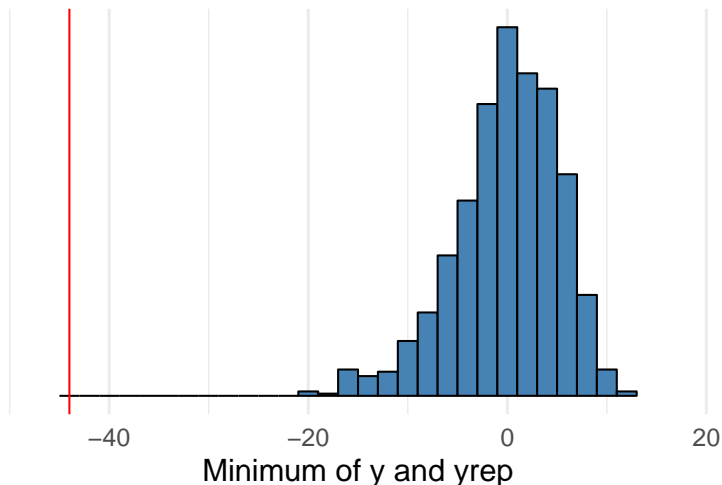
Posterior predictive checking – example

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

Posterior predictive checking – example

- Good test statistic is (almost) *ancillary* (fi: *aputunnusluku*)
  - 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 checking – example

- Good test statistic is (almost) *ancillary* (fi: *aputunnusluku*)
  - 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

Variance of y and yrep
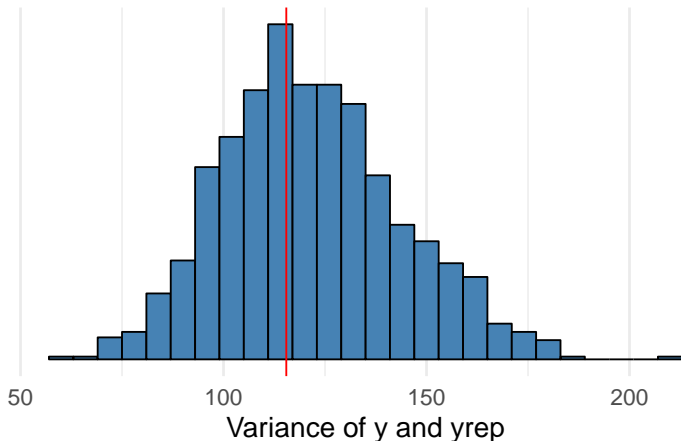
Posterior predictive checking

- *Posterior predictive p-value*

$$
\begin{aligned}
p &= \Pr(T(y^{\text{rep}}, \theta) \geq T(y, \theta)|y) \\
&= \int \int I_{T(y^{\text{rep}}, \theta) \geq T(y, \theta)} p(y^{\text{rep}}|\theta) p(\theta|y) dy^{\text{rep}} d\theta
\end{aligned}
$$

where I is an indicator function

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

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

- Posterior predictive p-value (ppp-value) estimates whether difference between the model and data could arise by chance
- Not commonly used, as
    - not calibrated in case of non-ancillary statistic
    - the distribution of test statistic has more information

Posterior predictive checking – bayesplot

`ppc_stat(y, yrep)`, the default statistic "mean" is usually bad

$T = \text{mean}$
$T(y_{\text{rep}})$

$T(y)$
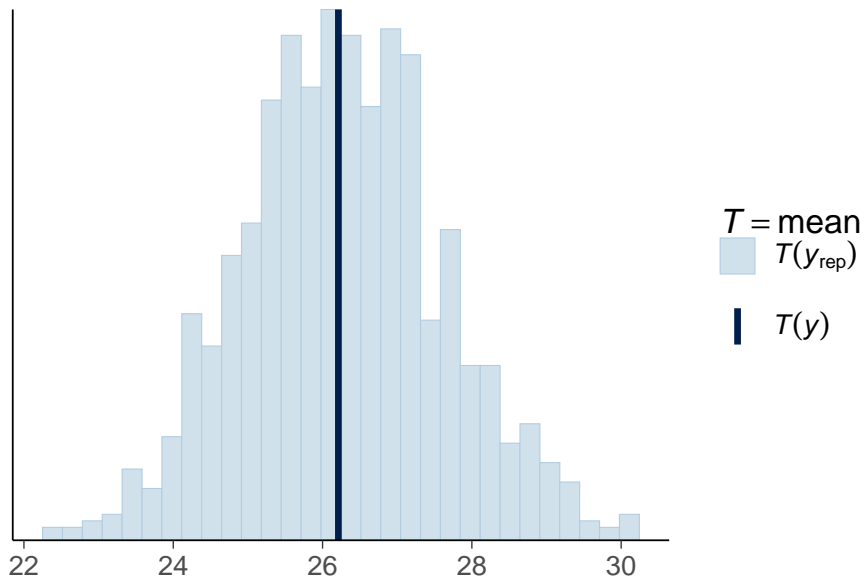
Posterior predictive checking – bayesplot

```
ppc_stat(y, yrep, stat="min")
```
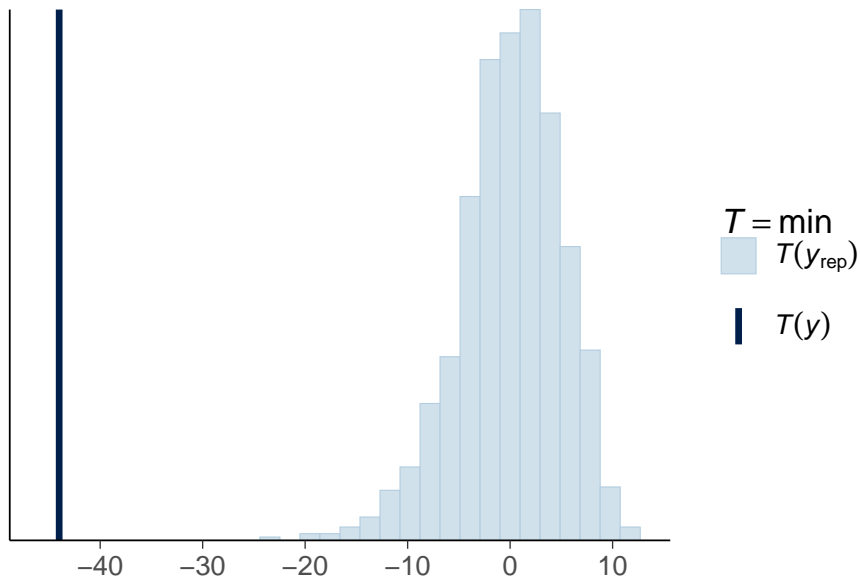
Posterior predictive checking – bayesplot

```
ppc_stat(y, yrep, stat="max")
```
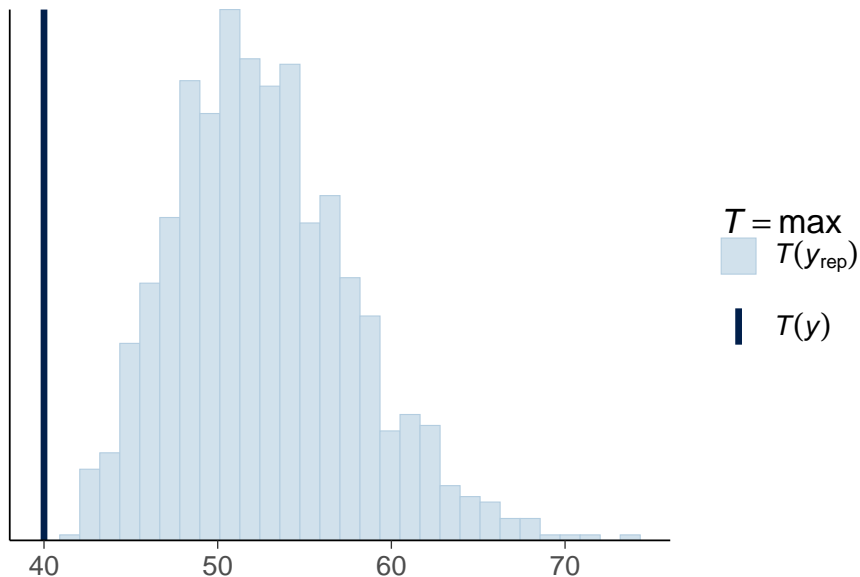
Posterior predictive checking – bayesplot

```
ppc_stat2d(y, yrep, stat=c("min","max"))
```
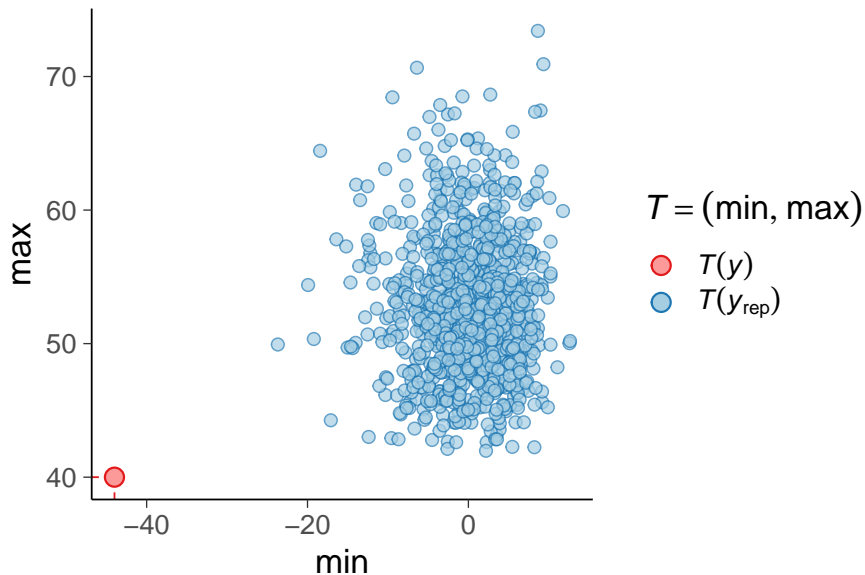
Example: Exposure to air pollution

- Example from Jonah Gabry, Daniel Simpson, Aki Vehtari, Michael Betancourt, and Andrew Gelman (2019). Visualization in Bayesian workflow. https://doi.org/10.1111/rssa.12378
- Estimation of human exposure to air pollution from particulate matter measuring less than 2.5 microns in diameter ($PM_{2.5}$)
  - Exposure to $PM_{2.5}$ is linked to a number of poor health outcomes and a recent report estimated that $PM_{2.5}$ is responsible for three million deaths worldwide each year (Shaddick et al., 2017)
  - In order to estimate the public health effect of ambient $PM_{2.5}$, we need a good estimate of the $PM_{2.5}$ 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

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

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

Example: Exposure to air pollution

Prior predictive checking

Prior predictive distribution with vague prior

log(PM2.5)

Example: Exposure to air pollution

Prior predictive checking

Prior predictive distribution with vague prior

Pallastunturi fells
Concrete
Neutron star

log(PM2.5)

Example: Exposure to air pollution

Prior predictive checking

Prior predictive distribution with weakly informative
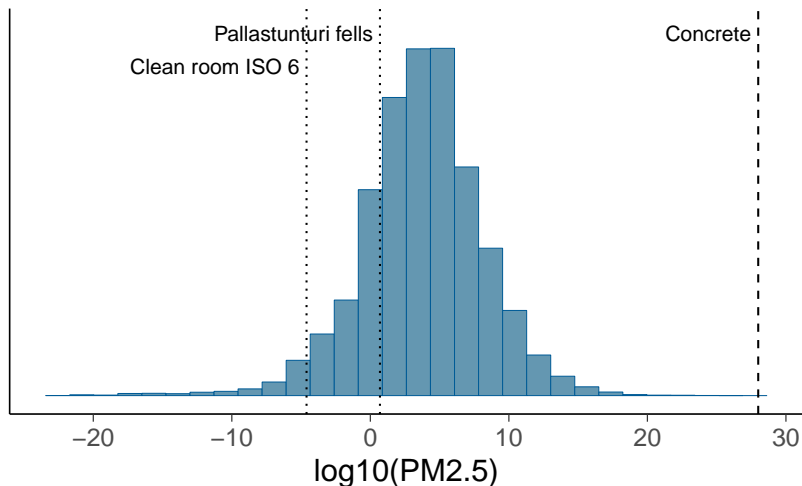
Example: Exposure to air pollution

Posterior predictive checking – marginal predictive distributions
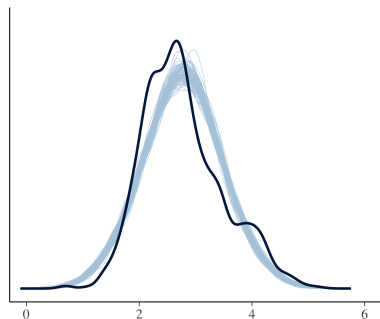
(a) Model 1
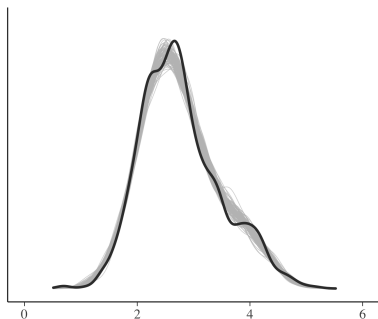
(b) Model 2

Example: Exposure to air pollution

Posterior predictive checking – test statistic (skewness)
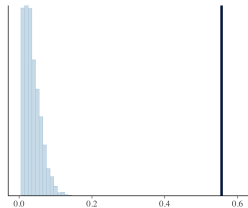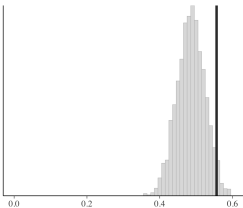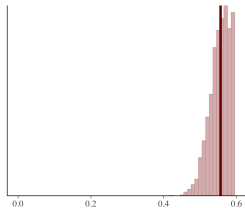
(a) Model 1   (b) Model 2   (c) Model 3

Example: Exposure to air pollution

Posterior predictive checking – test statistic (median for groups)
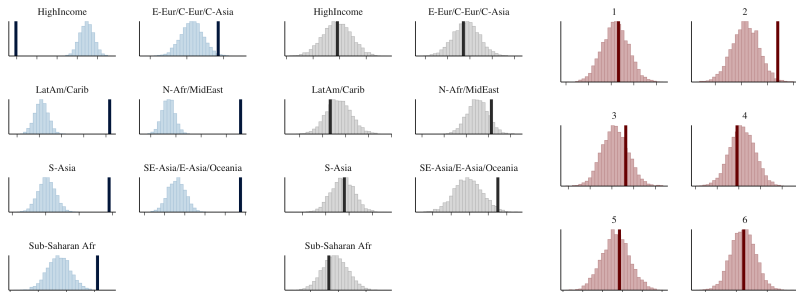
(a) Model 1

(b) Model 2

(c) Model 3

Positive target

Model for weight

Model for log(weight)
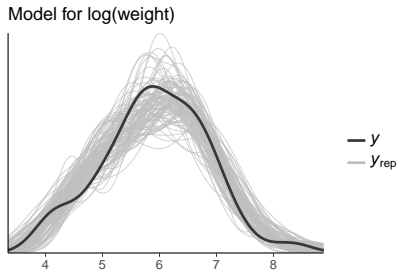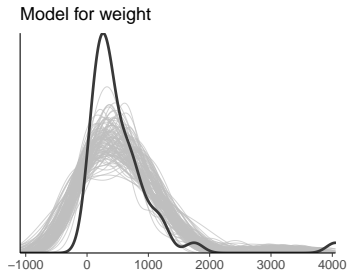
Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 11.

Student retention

Latent hierarchical linear + spline

```
nstudents | trials(nstudents1) ~ (assignment | year) +
  s(assignment, k=4), family=binomial()
```

Latent functions + posterior uncertainty

Student retention

Latent hierarchical linear + spline

```
nstudents | trials(nstudents1) ~ (assignment | year) +
  s(assignment, k=4), family=binomial()
```
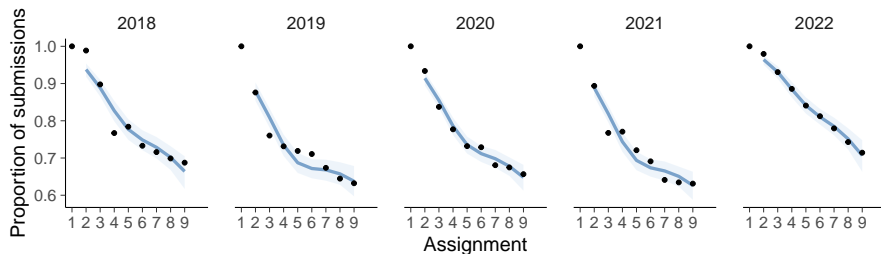
Latent functions + posterior uncertainty
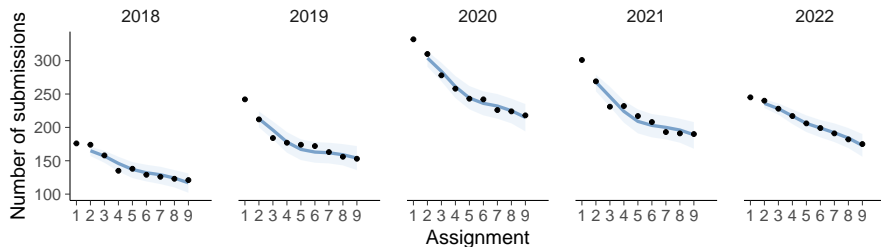
Student retention

1. Latent hierarchical linear model

```
nstudents | trials(nstudents1) ~ (assignment | year),
  family=binomial()
```

2. Latent hierarchical linear model + spline

```
nstudents | trials(nstudents1) ~ (assignment | year) +
  s(assignment, k=4), family=binomial()
```

Student retention – Posterior predictive distributions

with `tidybayes`
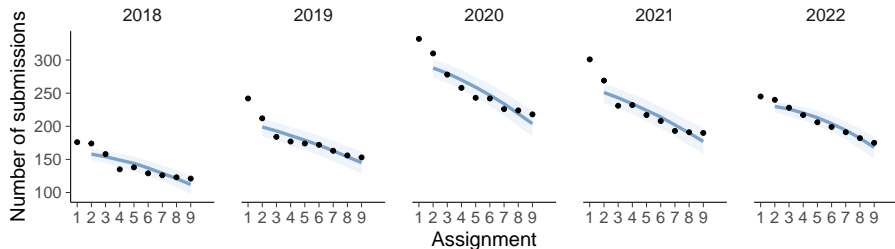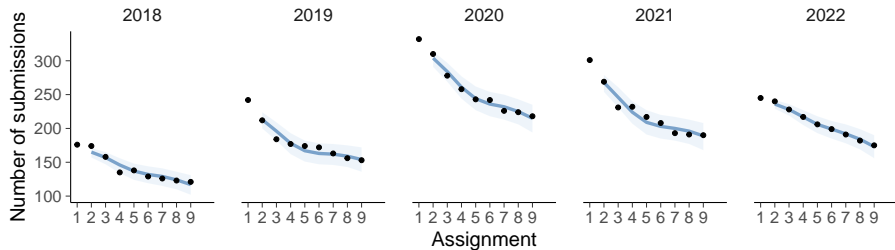
Student retention – Marginal PPC

`pp_check(fit, ndraws=100)`

Latent hierarchical linear model
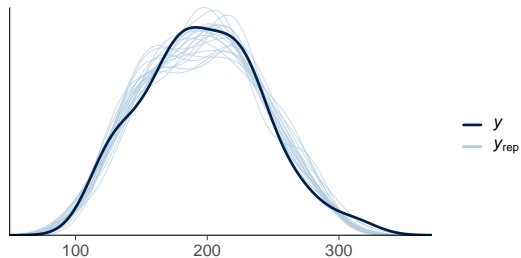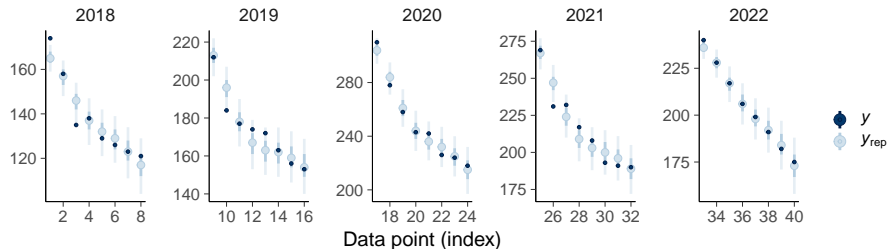

Latent hierarchical linear model + spline
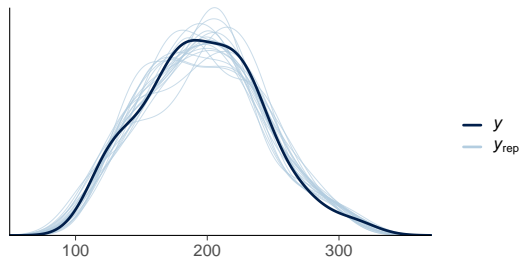
Student retention – Posterior predictive intervals

`pp_check(fit, type = "intervals_grouped", group="year")`
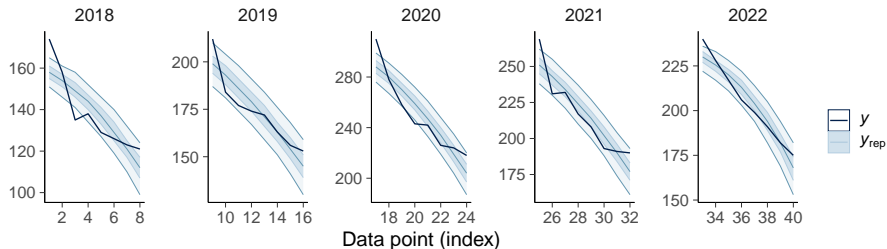
Latent hierarchical linear model
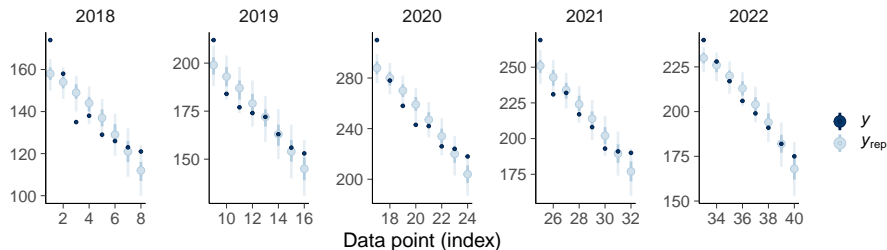
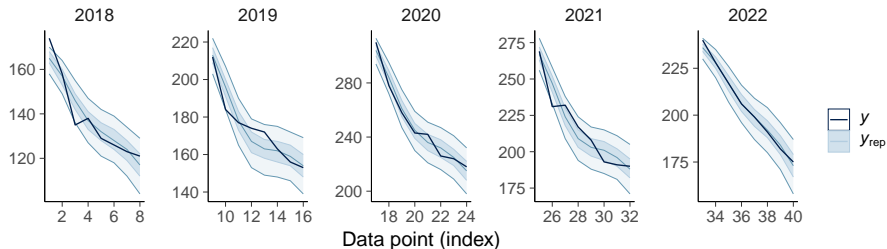Latent hierarchical linear model + spline

Student retention – Posterior predictive ribbon

```
pp_check(fit, type = "ribbon_grouped", group="year")
```
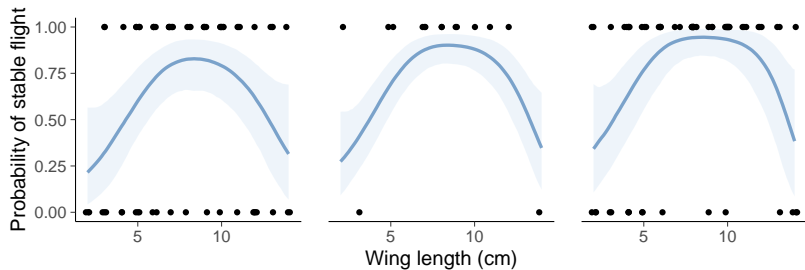
Latent hierarchical linear model
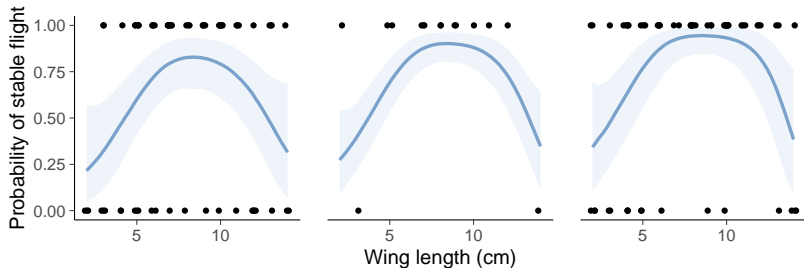

Latent hierarchical linear model + spline

PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```
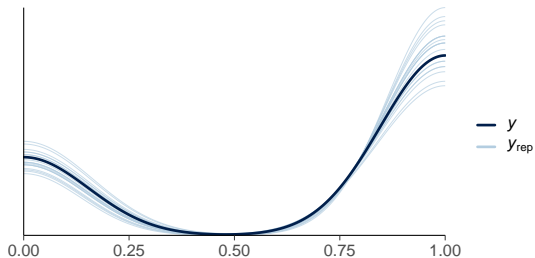
PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```
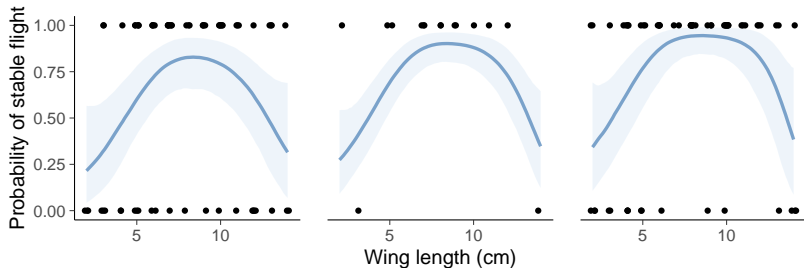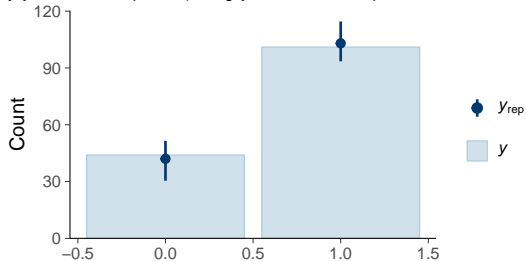


```
pp_check(fit, ndraws=20)
```

PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```
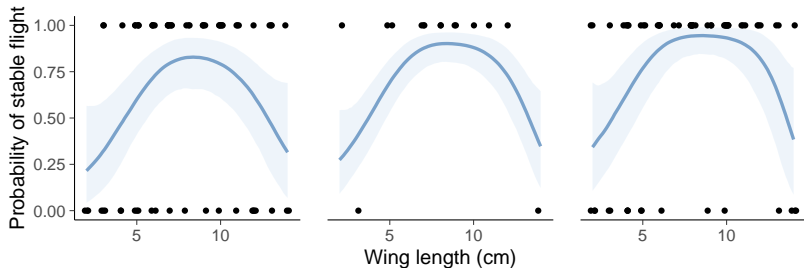


```
pp_check(fit, type="bars")
```
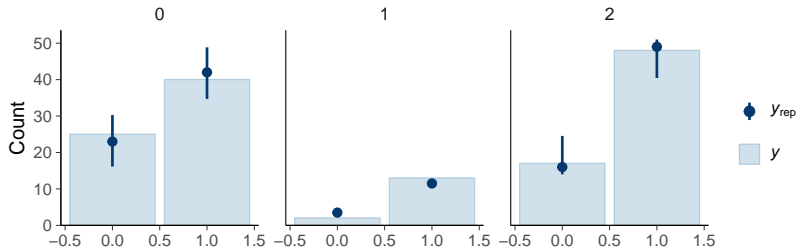
PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```
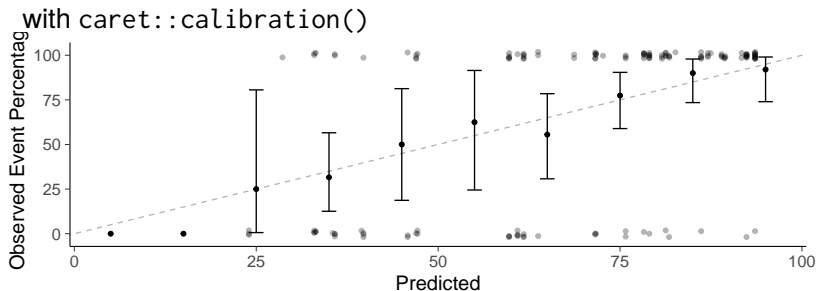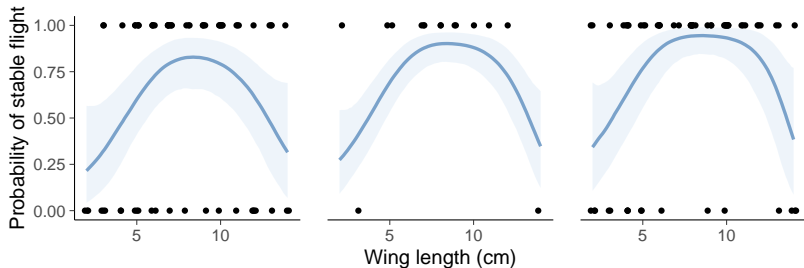


```
pp_check(fit, type="bars_grouped")
```

PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```
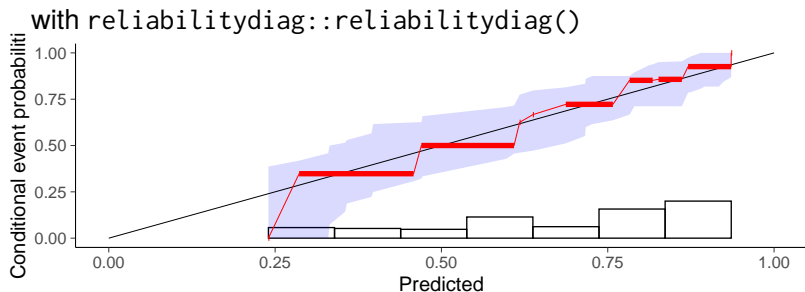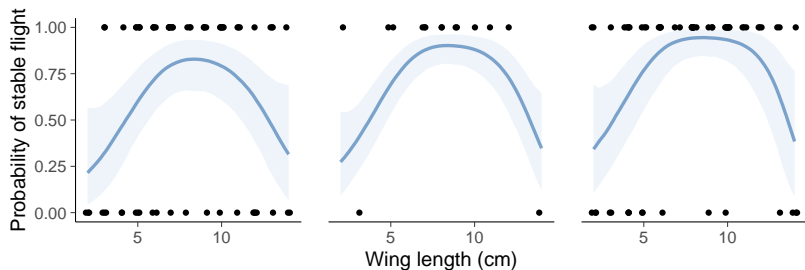

with `caret::calibration()`

PPC for binary target – Helicopters

```
stable_flight ~ s(wing_length) + s(wing_length, by = nclips),
family = bernoulli()
```


with `reliabilitydiag::reliabilitydiag()`

Posterior predictive checking – Stan code

- demo demos_rstan/ppc/poisson-ppc.Rmd

```stan
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);
    }
}
```

PPC for count data – Poisson model

```
ppc_dens_overlay(y, yrep[1:50,])
```
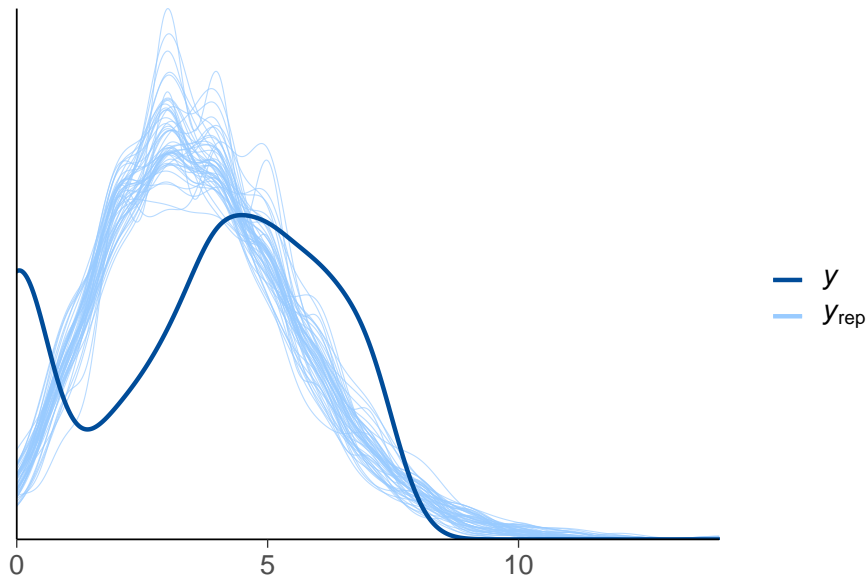
PPC for count data – Poisson model

```
ppc_rootogram(y, yrep)
```
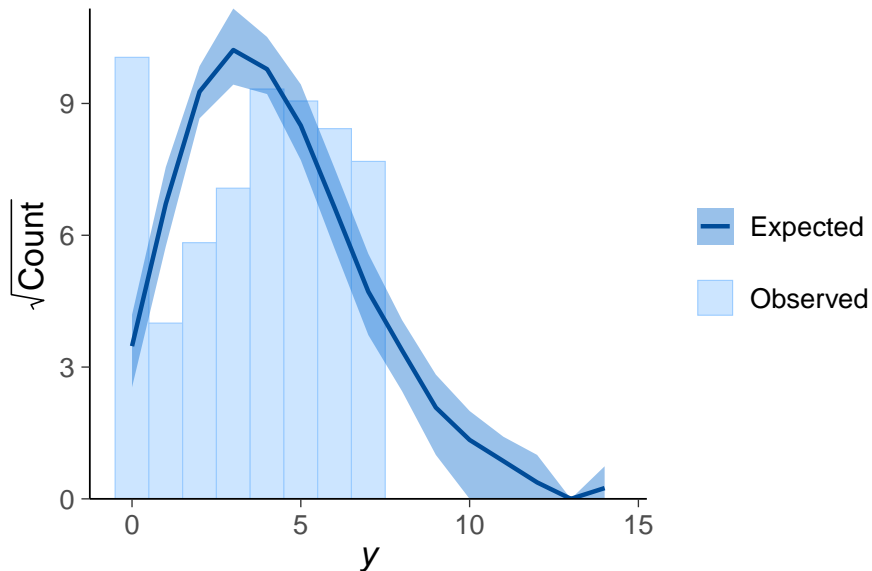
PPC for count data – Poisson model

```
prop_zero <- function(x) mean(x == 0)
ppc_stat(y, yrep, stat = "prop_zero")
```


$T = $ prop_zero
$T(y_{rep})$

$T(y)$
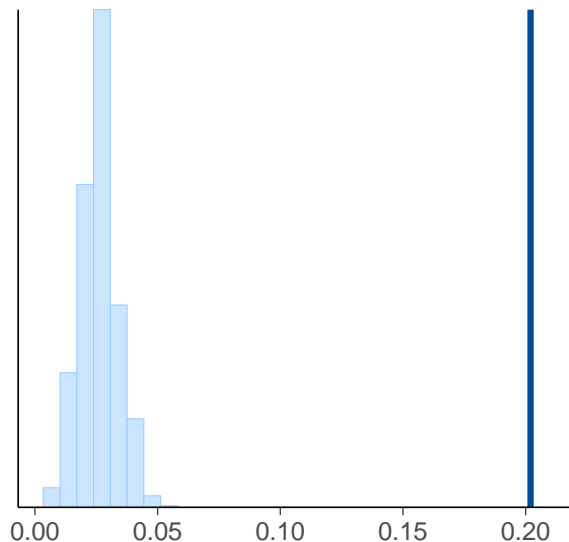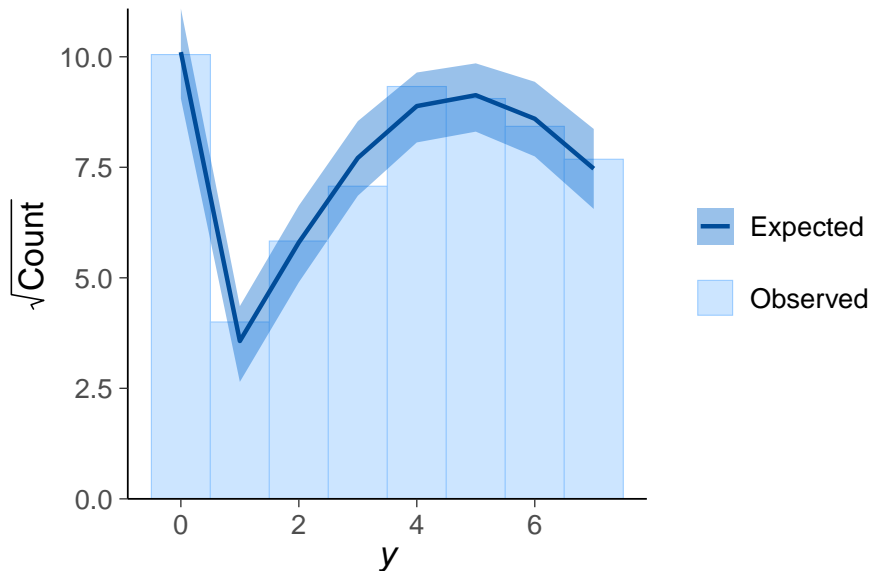
PPC for count data – hurdle truncated Poisson model

`ppc_rootogram(y, yrep2)`

PPC for count data – hurdle truncated Poisson model

```
prop_zero <- function(x) mean(x == 0)
ppc_stat(y, yrep2, stat = "prop_zero")
```


$T = \text{prop\_zero}$
$T(y_{\text{rep}})$

$T(y)$
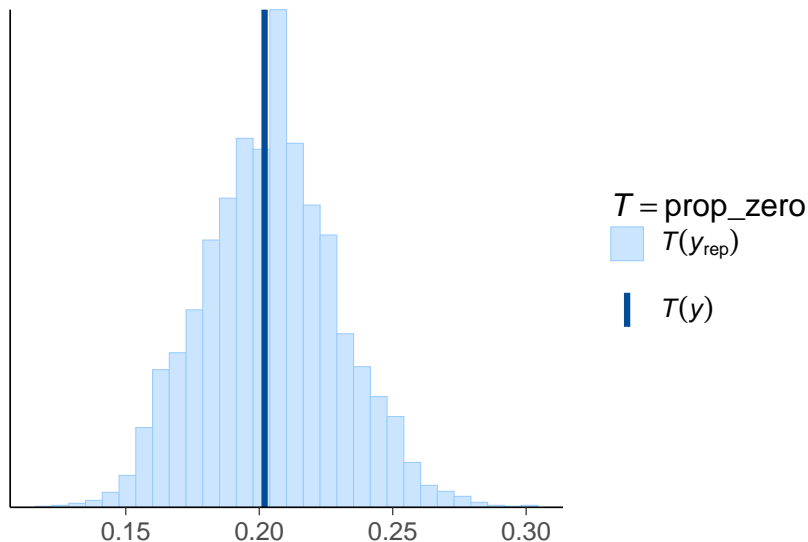
Further reading and examples

- Gabry, Simpson, Vehtari, Betancourt, and Gelman (2019). Visualization in Bayesian workflow. https://doi.org/10.1111/rssa.12378.

- 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

Sensitivity analysis

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

Sensitivity analysis

- How much different choices in model structure and priors affect the results
  - test different models and priors
    `priorsense` and `adjustr` packages use importance sampling for faster prior sensitivity analysis

Sensitivity analysis

- How much different choices in model structure and priors affect the results
  - test different models and priors
    priorsense and adjustr packages use importance sampling for faster prior sensitivity analysis
  - 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

Sensitivity analysis

- How much different choices in model structure and priors affect the results
  - test different models and priors
    priorsense and adjustr packages use importance sampling for faster prior sensitivity analysis
  - 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