Graphical posterior predictive checks using the bayesplot package

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Introduction

This vignette focuses on graphical posterior predictive checks (PPC). Plots of parameter estimates from MCMC draws are covered in the separate vignette *Plotting MCMC draws*, and MCMC diagnostics are covered in the *Visual MCMC diagnostics* vignette.

Graphical posterior predictive checks (PPCs)

The **bayesplot** package provides various plotting functions for *graphical posterior predictive checking*, that is, creating graphical displays comparing observed data to simulated data from the posterior predictive distribution (Gabry et al, 2019).

The idea behind posterior predictive checking is simple: if a model is a good fit then we should be able to use it to generate data that looks a lot like the data we observed. To generate the data used for posterior predictive checks (PPCs) we simulate from the *posterior predictive distribution*. This is the distribution of the outcome variable implied by a model after using the observed data y (a vector of N outcome values) to update our beliefs about unknown model parameters θ. The posterior predictive distribution for observation $\widetilde{y}$ can be written as

$$p(\widetilde{y} \,|\, y) = \int p(\widetilde{y} \,|\, \theta)\, p(\theta \,|\, y)\, d\theta.$$

Typically we will also condition on X (a matrix of predictor variables).

For each draw (simulation) $s = 1, \ldots, S$ of the parameters from the posterior distribution,

$\theta^{(s)} \sim p(\theta \mid y)$, we draw an entire vector of N outcomes $\widetilde{y}^{(s)}$ from the posterior predictive distribution by simulating from the data model conditional on parameters $\theta^{(s)}$. The result is an $S \times N$ matrix of draws $\widetilde{y}$.

When simulating from the posterior predictive distribution we can use either the same values of the predictors X that we used when fitting the model or new observations of those predictors. When we use the same values of X we denote the resulting simulations by y^{rep}, as they can be thought of as replications of the outcome y rather than predictions for future observations ($\widetilde{y}$ using predictors $\widetilde{X}$). This corresponds to the notation from Gelman et al. (2013) and is the notation used throughout the package documentation.

Using the replicated datasets drawn from the posterior predictive distribution, the functions in the **bayesplot** package create various graphical displays comparing the observed data y to the replications. The names of the **bayesplot** plotting functions for posterior predictive checking all have the prefix `ppc_`.

Setup

In addition to **bayesplot** we'll load the following packages:

- **ggplot2**, in case we want to customize the ggplot objects created by **bayesplot**
- **rstanarm**, for fitting the example models used throughout the vignette

```
library("bayesplot")
library("ggplot2")
library("rstanarm")
```

Example models

To demonstrate some of the various PPCs that can be created with the **bayesplot** package we'll use an example of comparing Poisson and Negative binomial regression models from one of the **rstanarm** package vignettes (Gabry and Goodrich, 2017).

> We want to make inferences about the efficacy of a certain pest management system at reducing the number of roaches in urban apartments. […] The regression predictors for the model are the pre-treatment number of roaches `roach1`, the treatment indicator `treatment`, and a variable `senior` indicating whether the apartment is in a building restricted to elderly residents. Because the number of days for which the roach traps were used is not the same for all apartments in the sample, we include it as an exposure […].

First we fit a Poisson regression model with outcome variable `y` representing the roach count in each apartment at the end of the experiment.

```
head(roaches) # see help("rstanarm-datasets")
```

```
    y roach1 treatment senior exposure2
1 153 308.00         1      0  0.800000
```

```
2 127 331.25         1      0  0.600000
3   7   1.67         1      0  1.000000
4   7   3.00         1      0  1.000000
5   0   2.00         1      0  1.142857
6   0   0.00         1      0  1.000000
```

```
roaches$roach100 <- roaches$roach1 / 100 # pre-treatment number of roaches (in 100s)
```

```
# using rstanarm's default priors. For details ee the section on default
# weakly informative priors at https://mc-stan.org/rstanarm/articles/priors.html
fit_poisson <- stan_glm(
  y ~ roach100 + treatment + senior,
  offset = log(exposure2),
  family = poisson(link = "log"),
  data = roaches,
  seed = 1111,
  refresh = 0 # suppresses all output as of v2.18.1 of rstan
)
```

```
print(fit_poisson)
```

```
stan_glm
 family:       poisson [log]
 formula:      y ~ roach100 + treatment + senior
 observations: 262
 predictors:   4
------
            Median MAD_SD
(Intercept)  3.1    0.0  
roach100     0.7    0.0  
treatment   -0.5    0.0  
senior      -0.4    0.0  

------
* For help interpreting the printed output see ?print.stanreg
* For info on the priors used see ?prior_summary.stanreg
```

We'll also fit the negative binomial model that we'll compare to the Poisson:

```
fit_nb <- update(fit_poisson, family = "neg_binomial_2")
```

```
print(fit_nb)
```

```
stan_glm
 family:       neg_binomial_2 [log]
 formula:      y ~ roach100 + treatment + senior
 observations: 262
 predictors:   4
------
            Median MAD_SD
(Intercept)  2.8    0.2
roach100     1.3    0.3
treatment   -0.8    0.3
senior      -0.3    0.3

Auxiliary parameter(s):
                      Median MAD_SD
reciprocal_dispersion 0.3    0.0

------
* For help interpreting the printed output see ?print.stanreg
* For info on the priors used see ?prior_summary.stanreg
```

Defining `y` and `yrep`

In order to use the PPC functions from the **bayesplot** package we need a vector `y` of outcome values,

```
y <- roaches$y
```

and a matrix `yrep` of draws from the posterior predictive distribution,

```
yrep_poisson <- posterior_predict(fit_poisson, draws = 500)
yrep_nb <- posterior_predict(fit_nb, draws = 500)
dim(yrep_poisson)
```

```
[1] 500 262
```

```
dim(yrep_nb)
```

```
[1] 500 262
```

Each row of the matrix is a draw from the posterior predictive distribution, i.e. a vector with one element for each of the data points in `y`.

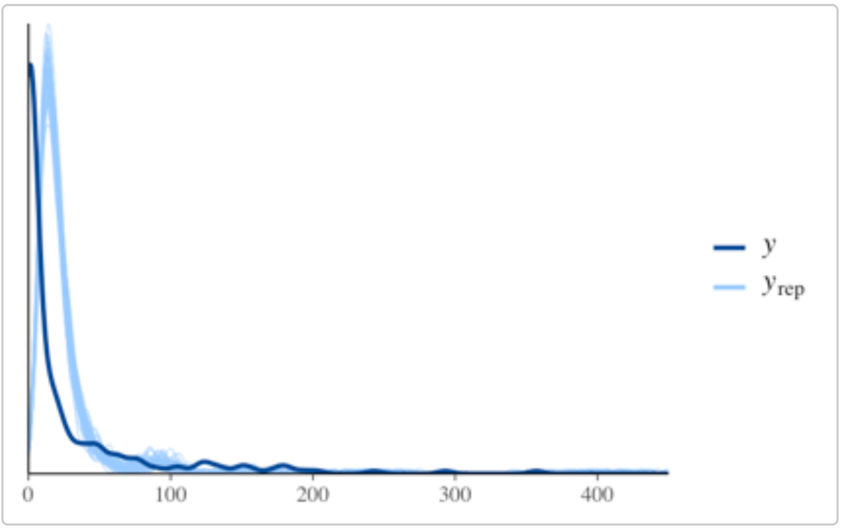
Since we fit the models using **rstanarm** we used its special `posterior_predict` function, but if we were using a model fit with the **rstan** package we could create `yrep` in the `generated quantities` block of the Stan program or by doing simulations in R after fitting the model. Draws from the posterior predictive distribution can be used with **bayesplot** regardless of whether or not the model was fit using an interface to Stan. **bayesplot** just requires a `yrep` matrix that has `number_of_draws` rows and `number_of_observations` columns.

Histograms and density estimates

ppc_dens_overlay

The first PPC we'll look at is a comparison of the distribution of `y` and the distributions of some of the simulated datasets (rows) in the `yrep` matrix.

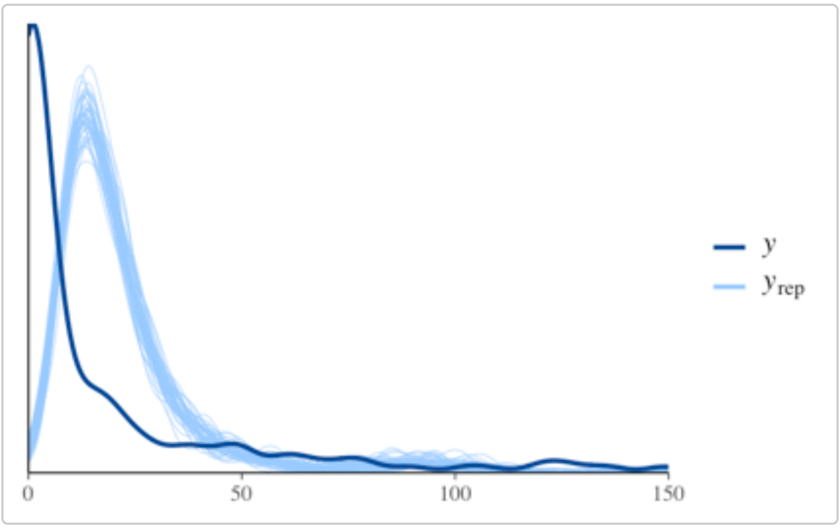
```
color_scheme_set("brightblue")
ppc_dens_overlay(y, yrep_poisson[1:50, ])
```



In the plot above, the dark line is the distribution of the observed outcomes `y` and each of the 50 lighter lines is the kernel density estimate of one of the replications of `y` from the posterior predictive distribution (i.e., one of the rows in `yrep`). This plot makes it easy to see that this model fails to account for the large proportion of zeros in `y`. That is, the model predicts fewer zeros than were actually observed.

To see the discrepancy at the lower values of more clearly we can use the `xlim` function from **ggplot2** to restrict the range of the x-axis:

```
ppc_dens_overlay(y, yrep_poisson[1:50, ]) + xlim(0, 150)
```

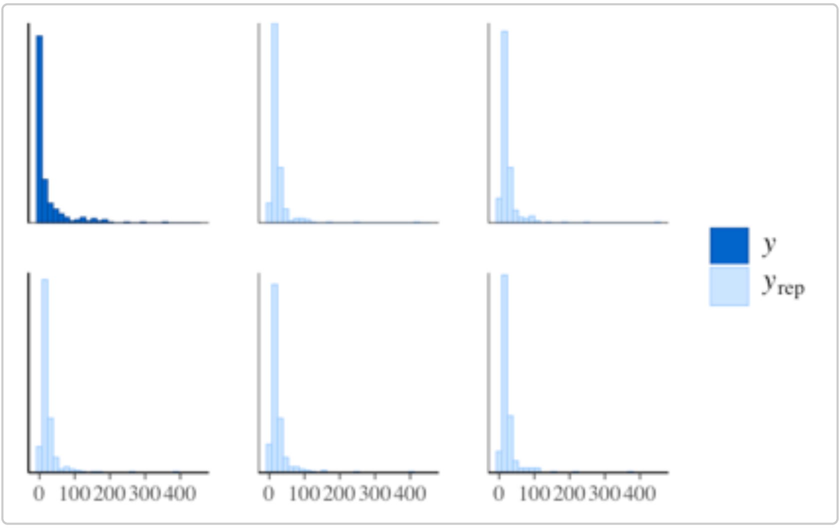


See Figure 6 in Gabry et al. (2019) for another example of using `ppc_dens_overlay`.

ppc_hist

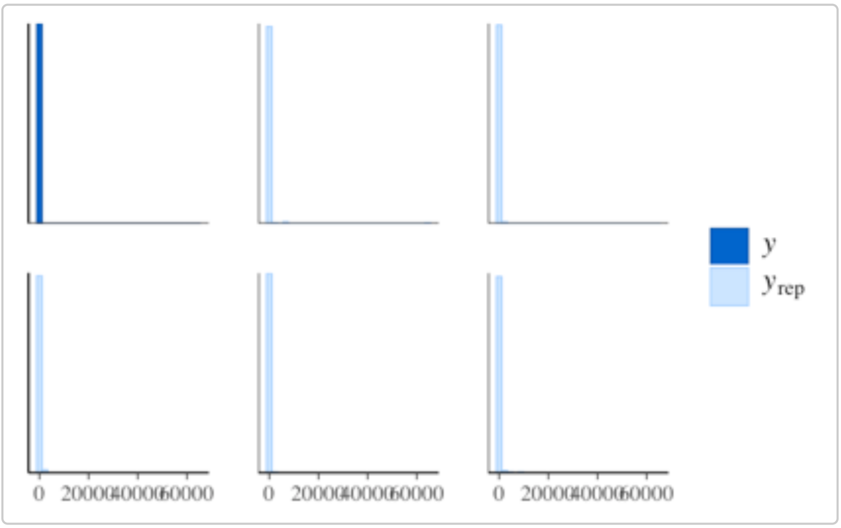
We could see the same thing from a different perspective by looking at separate histograms of `y` and some of the `yrep` datasets using the `ppc_hist` function:

```r
ppc_hist(y, yrep_poisson[1:5, ])
```



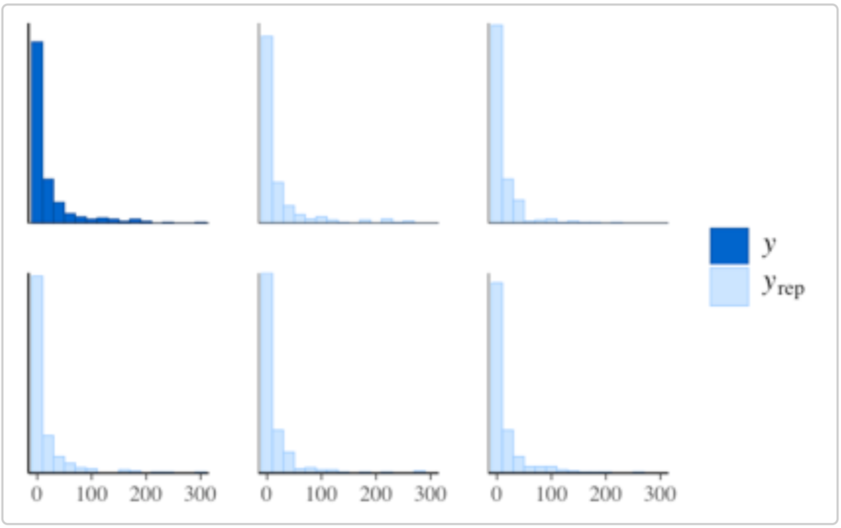
The same plot for the negative binomial model looks much different:

```r
ppc_hist(y, yrep_nb[1:5, ])
```



The negative binomial model does better handling the number of zeros in the data, but it occasionally predicts values that are way too large, which is why the x-axes extend to such high values in the plot and make it difficult to read. To see the predictions for the smaller values more clearly we can zoom in:

```r
ppc_hist(y, yrep_nb[1:5, ], binwidth = 20) +
  coord_cartesian(xlim = c(-1, 300))
```



Distributions of test statistics

Another way to see that the Poisson model predicts too few zeros is to look at the distribution of the proportion of zeros over the replicated datasets from the posterior predictive distribution in `yrep` and compare to the proportion of observed zeros in `y`.

ppc_stat

First we define a function that takes a vector as input and returns the proportion of zeros:

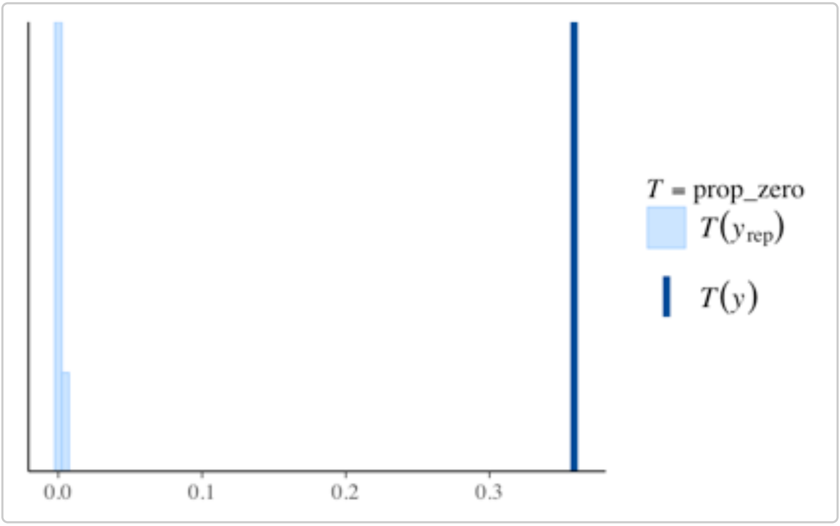
```r
prop_zero <- function(x) mean(x == 0)
```

```
prop_zero(y) # check proportion of zeros in y
```

```
[1] 0.3587786
```

The `stat` argument to `ppc_stat` accepts a function or the name of a function for computing a test statistic from a vector of data. In our case we can specify `stat = "prop_zero"` since we've already defined the `prop_zero` function, but we also could have used `stat = function(x) mean(x == 0)`.

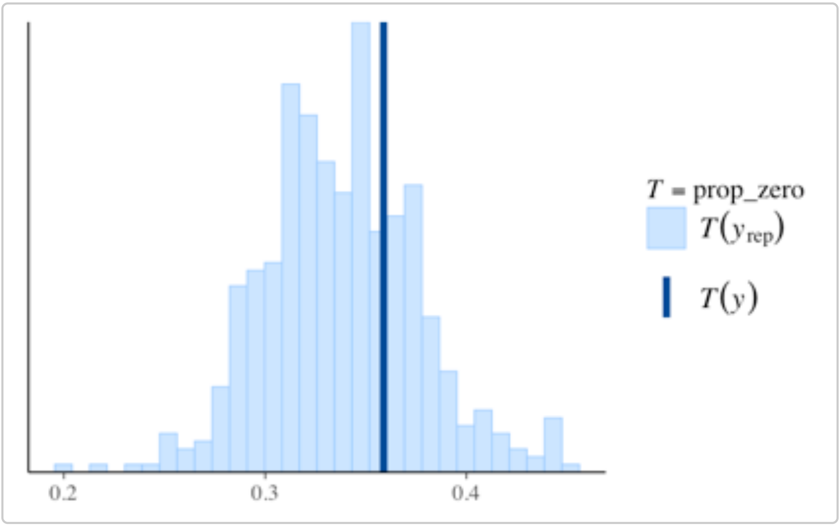
```
ppc_stat(y, yrep_poisson, stat = "prop_zero", binwidth = 0.005)
```



The dark line is at the value $T(y)$, i.e. the value of the test statistic computed from the observed y, in this case `prop_zero(y)`. The lighter area on the left is actually a histogram of the proportion of zeros in in the `yrep` simulations, but it can be hard to see because almost none of the simulated datasets in `yrep` have any zeros.

Here's the same plot for the negative binomial model:

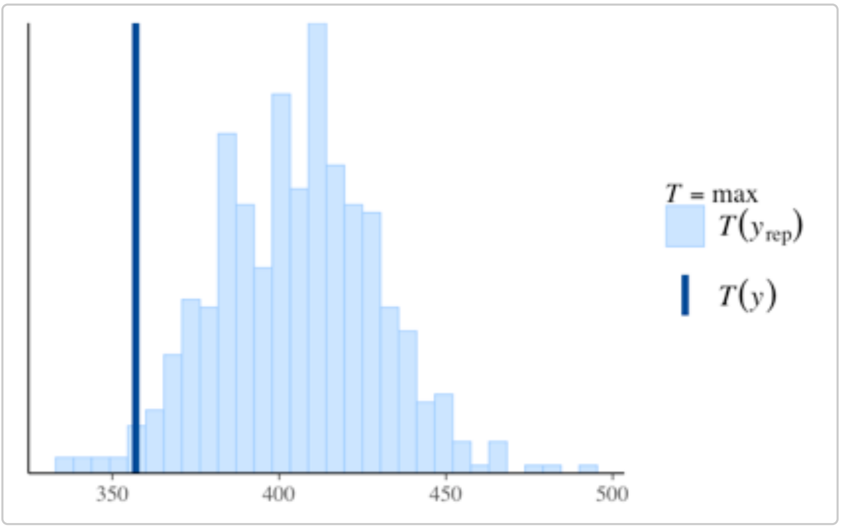
```
ppc_stat(y, yrep_nb, stat = "prop_zero")
```



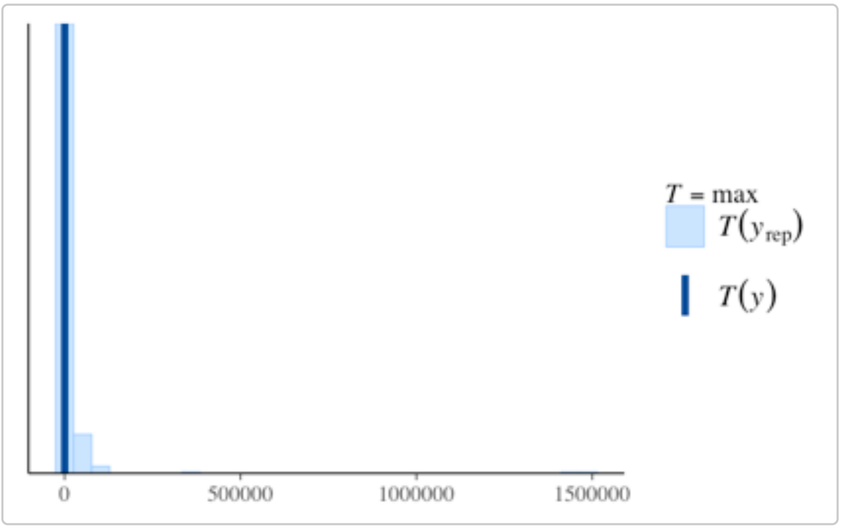
Again we see that the negative binomial model does a much better job predicting the proportion of observed zeros than the Poisson.

However, if we look instead at the distribution of the maximum value in the replications, we can see that the Poisson model makes more realistic predictions than the negative binomial:

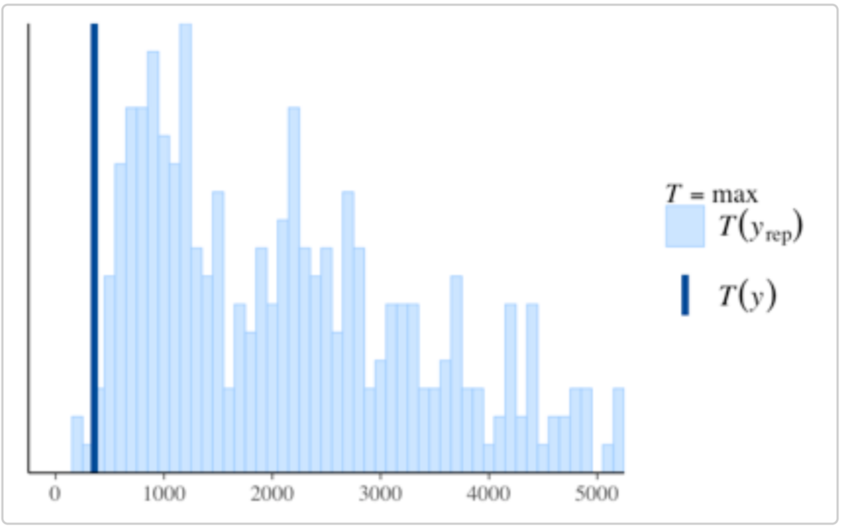
```
ppc_stat(y, yrep_poisson, stat = "max")
```



```
ppc_stat(y, yrep_nb, stat = "max")
```



```
ppc_stat(y, yrep_nb, stat = "max", binwidth = 100) +
  coord_cartesian(xlim = c(-1, 5000))
```



See Figure 7 in Gabry et al. (2019) for another example of using `ppc_stat`.

Other PPCs and PPCs by group

There are many additional PPCs available, including plots of predictive intervals, distributions of predictive errors, and more. For links to the documentation for all of the various PPC plots see `help("PPC-overview")` from R or the online documentation on the Stan website.

The `available_ppc` function can also be used to list the names of all PPC plotting functions:

```
available_ppc()
```

```
bayesplot PPC module:
  ppc_bars
  ppc_bars_grouped
  ppc_boxplot
  ppc_data
  ppc_dens
  ppc_dens_overlay
  ppc_ecdf_overlay
  ppc_error_binned
  ppc_error_hist
  ppc_error_hist_grouped
  ppc_error_scatter
  ppc_error_scatter_avg
  ppc_error_scatter_avg_vs_x
  ppc_freqpoly
  ppc_freqpoly_grouped
  ppc_hist
  ppc_intervals
  ppc_intervals_data
  ppc_intervals_grouped
  ppc_loo_intervals
  ppc_loo_pit
  ppc_loo_pit_overlay
  ppc_loo_pit_qq
  ppc_loo_ribbon
  ppc_ribbon
  ppc_ribbon_data
  ppc_ribbon_grouped
  ppc_rootogram
  ppc_scatter
  ppc_scatter_avg
  ppc_scatter_avg_grouped
  ppc_stat
  ppc_stat_2d
  ppc_stat_freqpoly_grouped
  ppc_stat_grouped
  ppc_violin_grouped
```

Many of the available PPCs can also be carried out within levels of a grouping variable. Any function for PPCs by group will have a name ending in `_grouped` and will accept an additional argument `group`. The full list of currently available `_grouped` functions is:

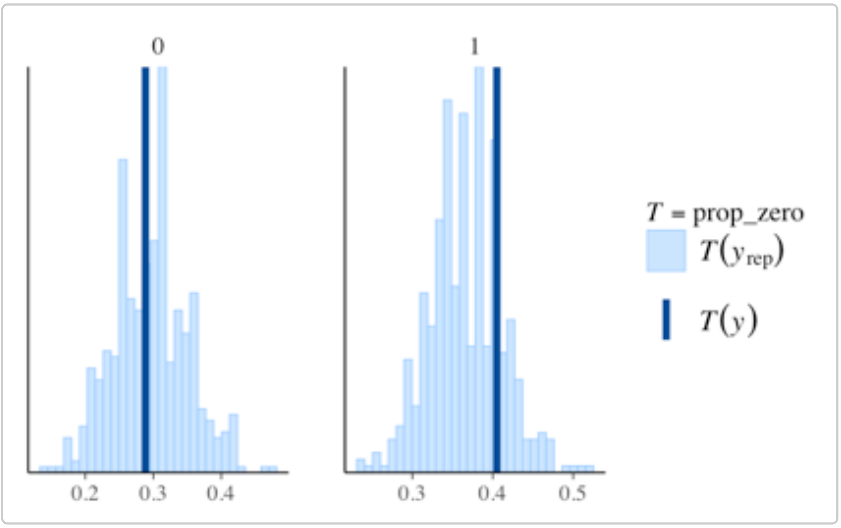
```
available_ppc(pattern = "_grouped")
```

```
bayesplot PPC module:
(matching pattern '_grouped')
  ppc_bars_grouped
  ppc_error_hist_grouped
  ppc_freqpoly_grouped
  ppc_intervals_grouped
  ppc_ribbon_grouped
  ppc_scatter_avg_grouped
  ppc_stat_freqpoly_grouped
  ppc_stat_grouped
  ppc_violin_grouped
```

ppc_stat_grouped

For example, `ppc_stat_grouped` is the same as `ppc_stat` except that the test statistic is computed within levels of the grouping variable and a separate plot is made for each level:

```
ppc_stat_grouped(y, yrep_nb, group = roaches$treatment, stat = "prop_zero")
```



See Figure 8 in Gabry et al. (2019) for another example of using `ppc_stat_grouped`.

Providing an interface to bayesplot PPCs from another package

The **bayesplot** package provides the S3 generic function `pp_check`. Authors of R packages for Bayesian inference are encouraged to define methods for the fitted model objects created by their packages. This will hopefully be convenient for both users and developers and contribute to the use of the same naming conventions across many of the R packages for Bayesian data analysis.

To provide an interface to **bayesplot** from your package, you can very easily define a `pp_check` method (or multiple `pp_check` methods) for the fitted model objects created by your package. All a `pp_check` method needs to do is provide the `y` vector and `yrep` matrix arguments to the various plotting functions included in **bayesplot**.

Defining a `pp_check` method

Here is an example for how to define a simple `pp_check` method in a package that creates fitted model objects of class `"foo"`. We will define a method `pp_check.foo` that extracts the data `y` and the draws from the posterior predictive distribution `yrep` from an object of class `"foo"` and then calls one of the plotting functions from **bayesplot**.

Suppose that objects of class `"foo"` are lists with named components, two of which are `y` and `yrep`. Here's a simple method `pp_check.foo` that offers the user the option of two different plots:

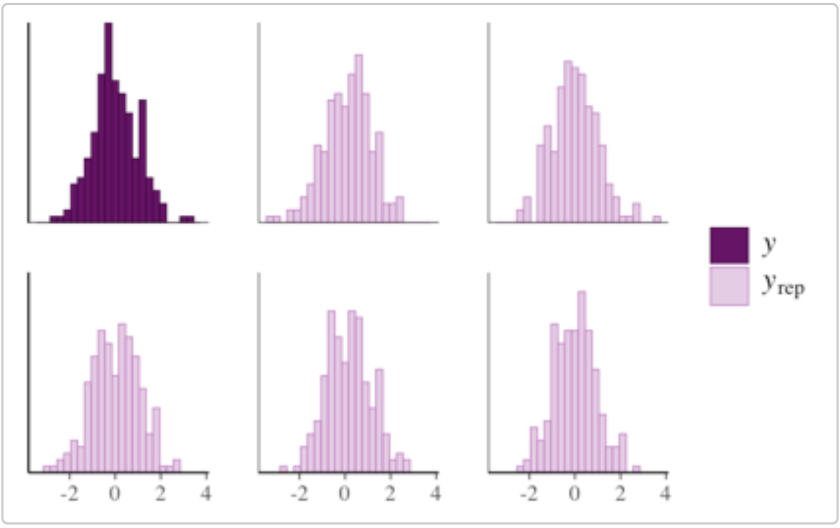
```
# @param object An object of class "foo".
# @param type The type of plot.
# @param ... Optional arguments passed on to the bayesplot plotting function.
pp_check.foo <- function(object, type = c("multiple", "overlaid"), ...) {
  type <- match.arg(type)
  y <- object[["y"]]
  yrep <- object[["yrep"]]
  stopifnot(nrow(yrep) >= 50)
  samp <- sample(nrow(yrep), size = ifelse(type == "overlaid", 50, 5))
  yrep <- yrep[samp, ]
```

```
    if (type == "overlaid") {
      ppc_dens_overlay(y, yrep, ...)
    } else {
      ppc_hist(y, yrep, ...)
    }
  }
```

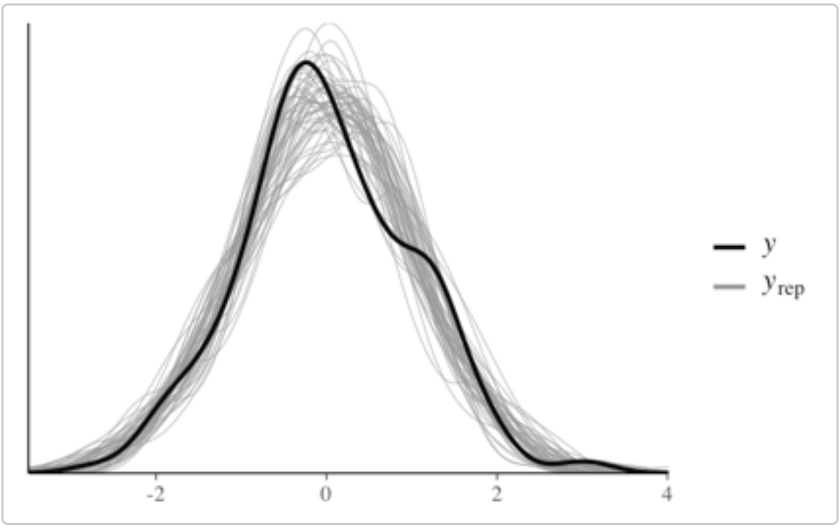
To try out `pp_check.foo` we can just make a list with `y` and `yrep` components and give it class `foo`:

```
x <- list(y = rnorm(200), yrep = matrix(rnorm(1e5), nrow = 500, ncol = 200))
class(x) <- "foo"
```

```
color_scheme_set("purple")
pp_check(x, type = "multiple", binwidth = 0.3)
```



```
color_scheme_set("darkgray")
pp_check(x, type = "overlaid")
```



Examples of `pp_check` methods in other packages

Several packages currently use this approach to provide an interface to **bayesplot**'s graphical posterior predictive checks. See, for example, the `pp_check` methods in the **rstanarm** and **brms** packages.

References

Buerkner, P. (2017). brms: Bayesian Regression Models using Stan. R package version 1.7.0. https://CRAN.R-project.org/package=brms

Gabry, J., and Goodrich, B. (2017). rstanarm: Bayesian Applied Regression Modeling via Stan. R package version 2.15.3. https://mc-stan.org/rstanarm, https://CRAN.R-project.org/package=rstanarm

Gabry, J. , Simpson, D. , Vehtari, A. , Betancourt, M. and Gelman, A. (2019), Visualization in Bayesian workflow. *J. R. Stat. Soc. A*, 182: 389-402. :10.1111/rssa.12378. (journal version, arXiv preprint, code on GitHub)

Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., and Rubin, D. B. (2013). *Bayesian Data Analysis*. Chapman & Hall/CRC Press, London, third edition.

Stan Development Team. *Stan Modeling Language Users Guide and Reference Manual*. https://mc-stan.org/users/documentation/