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- Introduction

Bayesian Statistics and Data Analysis
Lecture 8a

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Thanks to Aki Vehtari, Aalto University

Section 1

Introduction

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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

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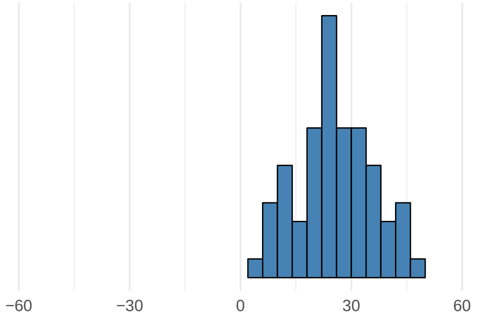
Posterior predictive checking – example

- Newcomb's speed of light measurements
  - model $y \sim \mathcal{N}(\mu, \sigma)$ 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 $\mathcal{N}(\mu^{(s)}, \sigma^{(s)})$
  - repeat n times to get y^{rep} with n replicates



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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.

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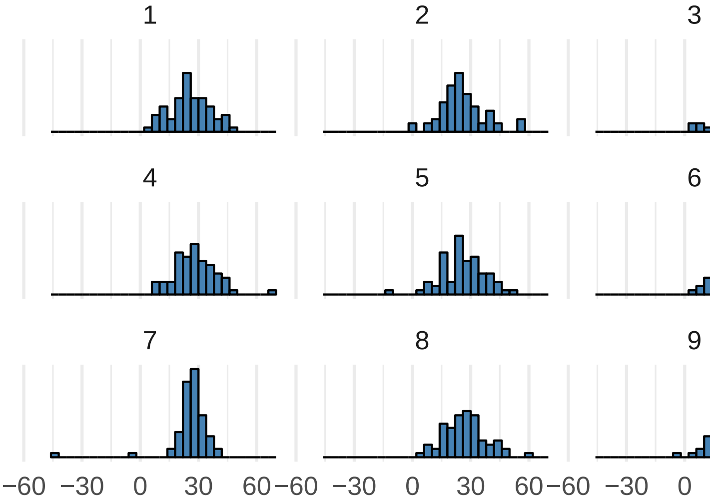
Posterior predictive checking – example

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



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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 $T(y^{\mathrm{rep}}, \theta)$
  - can be easier to compare summary quantities than data sets

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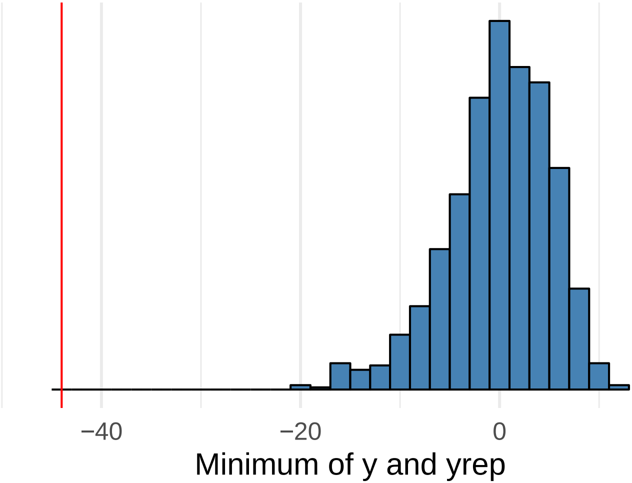
Posterior predictive checking – example

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



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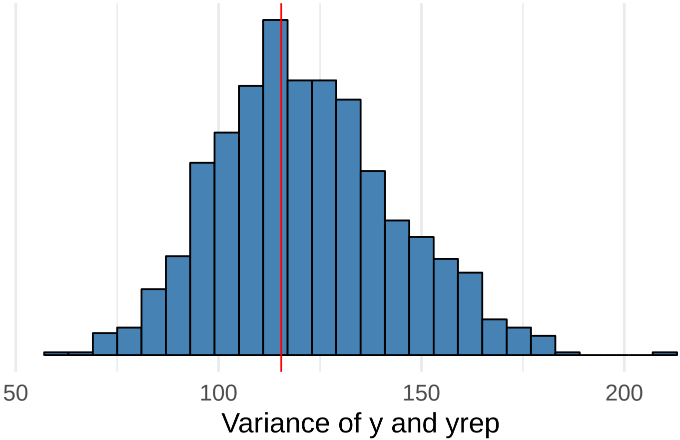
Posterior predictive checking – example

- 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



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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

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

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

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Marginal and CV predictive checking

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

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

if $T(y_i) = y_i$

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

- 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)

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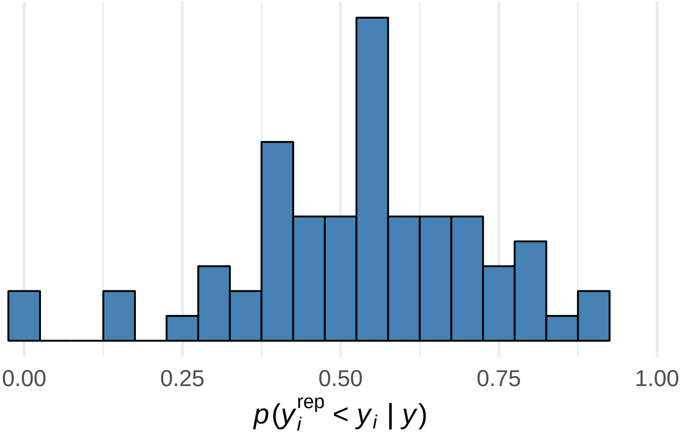
Marginal predictive checking - Example

- Marginal tail area or Probability integral transform (PIT)

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

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



Sensitivity analysis

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- 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 (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 ($\mathrm{PM}_{2.5}$)
  - Exposure to $\mathrm{PM}_{2.5}$ is linked to a number of poor health outcomes and a recent report estimated that $\mathrm{PM}_{2.5}$ is responsible for three million deaths worldwide each year (Shaddick et al., 2017)
  - In order to estimate the public health effect of ambient $\mathrm{PM}_{2.5}$, we need a good estimate of the $\mathrm{PM}_{2.5}$ concentration at the same spatial resolution as our population estimates.

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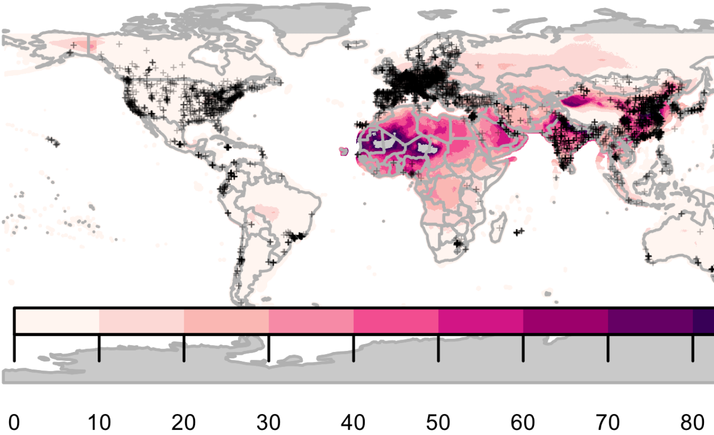
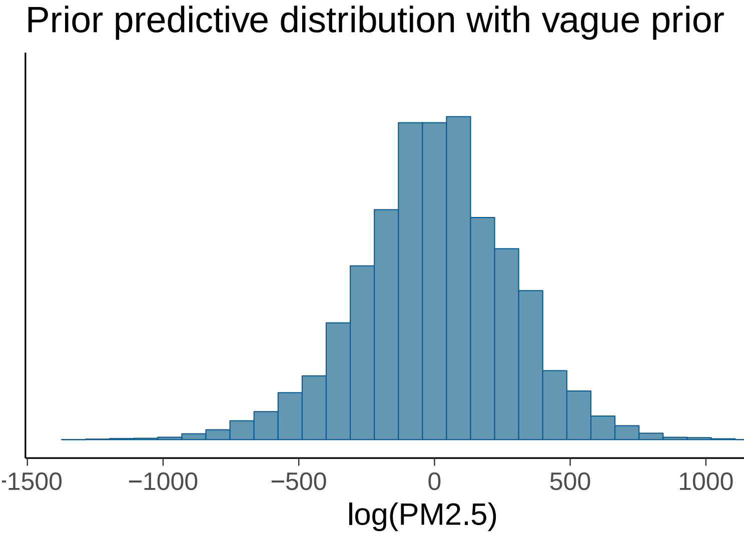
Example: Exposure to air pollution

- 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



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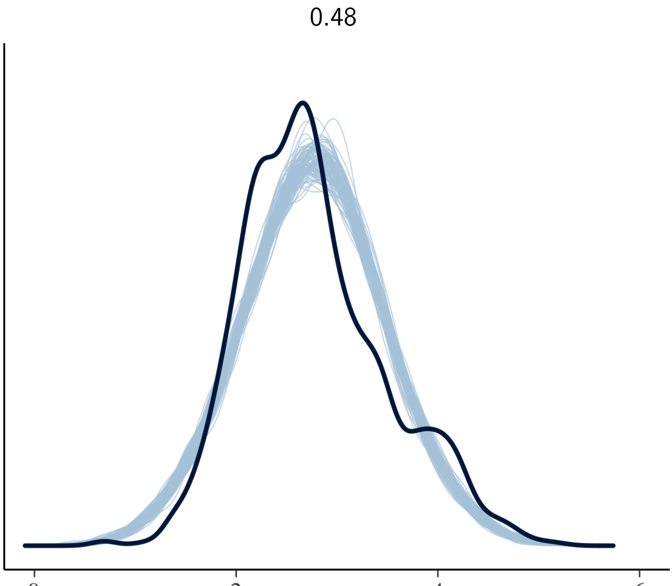
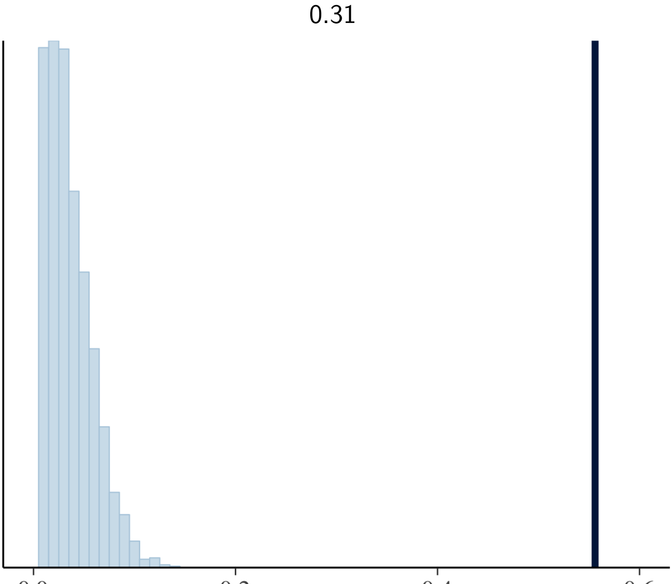
Example: Exposure to air pollution

Posterior predictive checking – marginal predictive distributions



Example: Exposure to air pollution

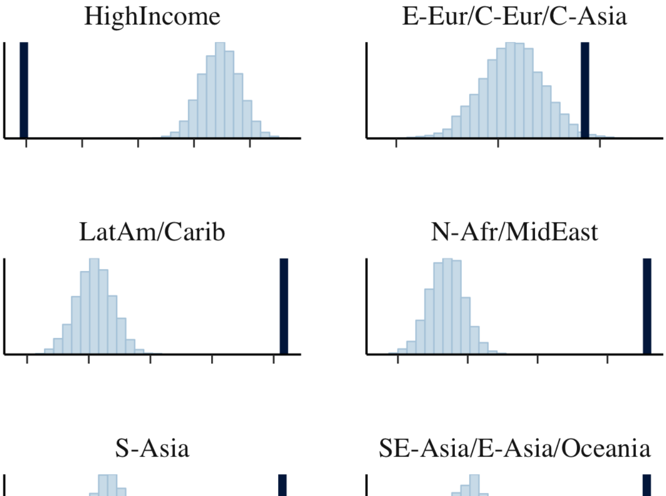
Posterior predictive checking – test statistic (skewness)



Example: Exposure to air pollution

Posterior predictive checking – test statistic (median for groups)

.31



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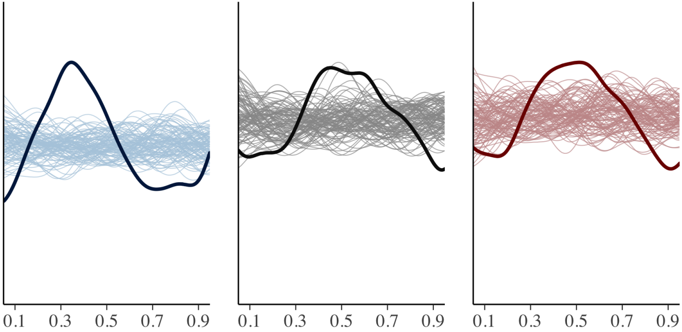
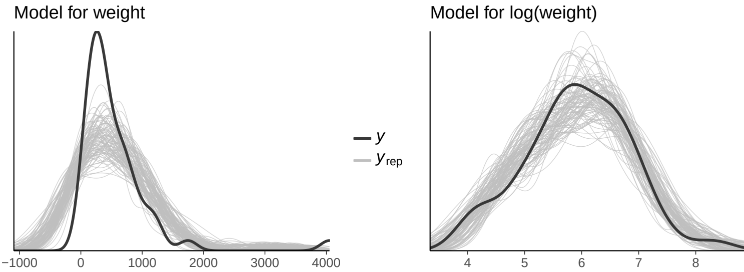
Example: Exposure to air pollution

LOO predictive checking – LOO-PIT



EDIT 2020: These plots use boundary corrected KDE which is a better choice than the non-boundary corrected KDE used in the plots in the paper.

Example of posterior predictive checking



Predicting the yields of mesquite bushes.

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

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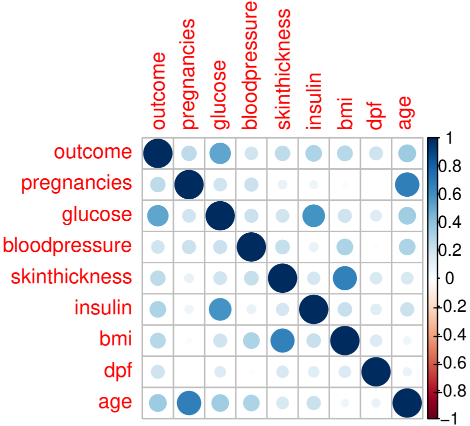
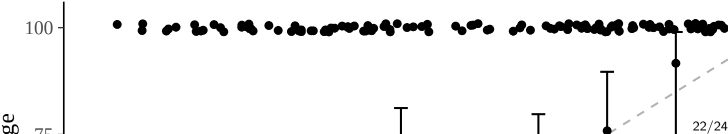
Example of posterior predictive checking

Diabetes prediction with logistic regression - diabetes demo



PPC

with binning 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 (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
- 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