

- Model Checking and Assessment
- Posterior predictive checking
  - Marginal Predictive Checking
  - Sensitivity analysis
  - Example

#### Bayesian Statistics and Data Analysis Lecture 8a

Måns Magnusson Department of Statistics, Uppsala University Thanks to Aki Vehtari, Aalto University



- Model Checking and Assessment
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• Priors are part of model. Describe them only there.



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- R and computational details not the main interest.
   Describe the general results (that you can trust the computations) and refer to the appendix first details



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- Remember look at the instructions. I have failed people with 4.5 pages. Or just 3 pages. Why do I care about this?
- For posteriordb students: (1) Please describe the data (or how you similate data) under data. Use the exact models that are in the papers. (2) Ignore prior recommendations see it as replication study



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#### Section 1

Model Checking and Assessment





#### Model Checking and Assessment

- Posterior predictive checking
  - Marginal Predictive Checking
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# The Box process: Probabilistic modeling

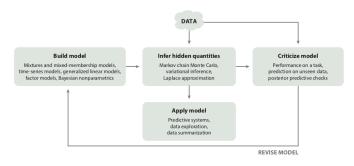


Figure: The Box approach (Box, 1976, Blei, 2014)



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#### Model assessment

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



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  - compare predictions to completely new observations



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#### Model assessment

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



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#### Section 2

Posterior predictive checking



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- Newcombs speed of light measurements
  - model  $y \sim \mathcal{N}(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$



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- ullet Posterior predictive replicate  $y^{\mathrm{rep}}$



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  - model  $y \sim \mathcal{N}(\mu, \sigma)$  with prior  $(\mu, \log \sigma) \propto 1$
- Posterior predictive replicate  $y^{\text{rep}}$ 
  - draw  $\mu^{(s)}, \sigma^{(s)}$  from the posterior  $p(\mu, \sigma|y)$



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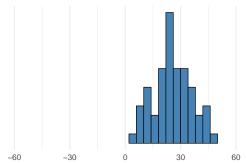
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  - repeat n times to get  $y^{rep}$  with n replicates



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  - example y<sup>rep</sup>:





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# Replicates vs. predictive distributions

 Predictive ỹ is the next not yet observed possible observation.



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# Replicates vs. predictive distributions

- Predictive ỹ is the next not yet observed possible observation.
- y<sup>rep</sup> refers to replicating the whole experiment (potentially with same values of x)
   i.e. obtaining as many replicated observations as in the original data.



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• Generate replicated datasets  $y^{\text{rep}}$ 



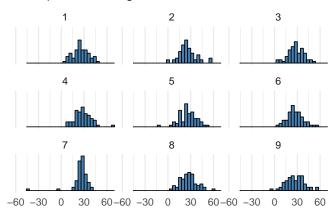
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- Generate replicated datasets  $y^{\text{rep}}$
- Compare to the original dataset



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- Generate replicated datasets  $y^{\text{rep}}$
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# Posterior predictive checking with test statistic

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



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



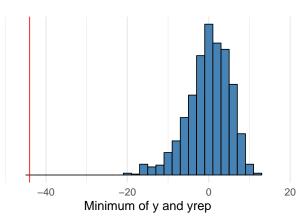
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#### Posterior predictive checking – example

- Good test statistic is ancillary (or almost)
  - a statistic T(X) that does not depend on the parameters of the model are ancillary
     e.g. in a normal model with known σ²,

$$s^2 = \sum_{i}^{n} \frac{(x_i - \bar{x})^2}{n-1},$$

is ancillary ( $\mu$  cancel out).

• So is the (interquantile) range



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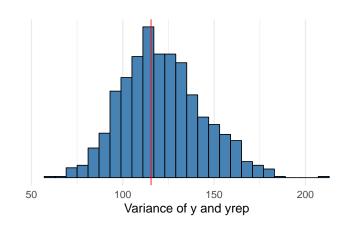
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- Connections:
  - Sufficient statistic: contains all the information about  $\theta$
  - Ancillary statistic: contains no information about  $\theta$



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• Posterior predictive p-value

$$egin{array}{lcl} p & = & \mathsf{Pr}(T(y^{\mathrm{rep}}, heta) \geq T(y, heta) | y) \ & = & \int \int I_{T(y^{\mathrm{rep}}, heta) \geq T(y, heta)} p(y^{\mathrm{rep}} | heta) p( heta | y) dy^{\mathrm{rep}} d heta \end{array}$$

where I is an indicator function



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 having (y<sup>rep (s)</sup>, θ<sup>(s)</sup>) from the posterior predictive distribution (Monte Carlo):

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



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



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- Posterior predictive p-value (ppp-value): could difference between the model and data arise by chance
- Not commonly used, since the distribution of test statistic  $T(y,\theta)$  has more information



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#### Subsection 1

Marginal Predictive Checking



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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

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



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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  $T(y_i) = y_i$ 

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

- 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:
     Pr(ỹ<sub>i</sub>|y<sub>-i</sub>) (cross-validation)



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# Marginal predictive checking - Example

Marginal tail area or Probability integral transform (PIT)

$$p_i = p(y_i^{\rm rep} \le y_i|y)$$

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



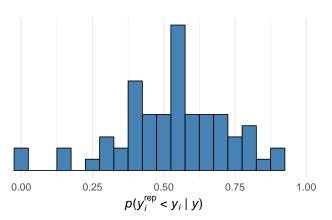
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### Marginal predictive checking - Example

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#### Subsection 2



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



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



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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



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    - 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



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#### Subsection 3

Example





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 Example from Jonah Gabry, Daniel Simpson, Aki Vehtari, Michael Betancourt, and Andrew Gelman (2019).
 Visualization in Bayesian workflow.

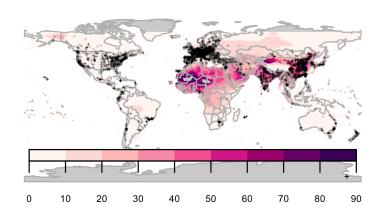
https://doi.org/10.1111/rssa.12378

- 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.



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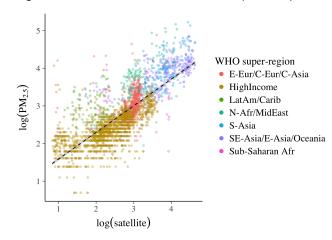
- Direct measurements of PM 2.5 from ground monitors at 2980 locations
- High-resolution satellite data of aerosol optical depth





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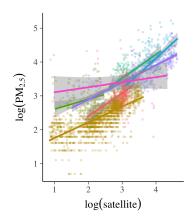
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- Three models:
  - 1. Linear regression

$$y_{ij} \sim N(\beta_0 + \beta_1 x_{ij}, \sigma^2)$$

- 2. Hiearchical linear regression (WHO super regions)
- 3. Hiearchical linear regression (clustered super regions)

$$y_{ij} \sim N(\beta_0 \beta_{0j} + (\beta_1 + \beta_{1j}) x_{ij}, \sigma^2)$$

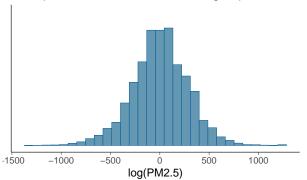
where  $y_{ij}$  is the log of PM<sub>2.5</sub> concentration and  $x_{ij}$  is the satellite estimate, and  $j \in \{1, ..., J\}$  is the super-region indicator.



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## Example: Prior predictive checking

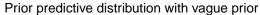


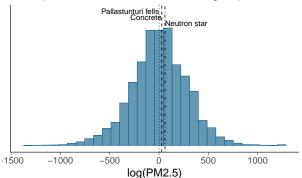




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## Example: Prior predictive checking



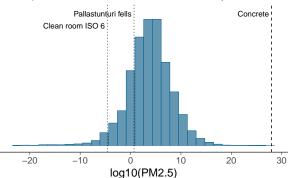




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### Example: Prior predictive checking







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### Example: Marginal predictive distributions

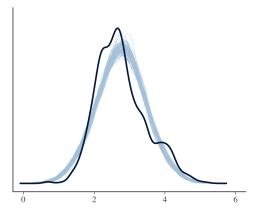


Figure: Model 1

Kernel density estimate of the observed dataset y (dark curve), with density estimates for 100 simulated datasets  $y^{(rep)}$  drawn from the posterior predictive distribution (thin, lighter lines)



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### Example: Marginal predictive distributions

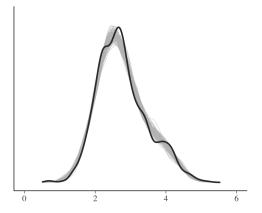


Figure: Model 2

Kernel density estimate of the observed dataset y (dark curve), with density estimates for 100 simulated datasets  $y^{\text{(rep)}}$  drawn from the posterior predictive distribution (thin, lighter lines)



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### Example: Marginal predictive distributions

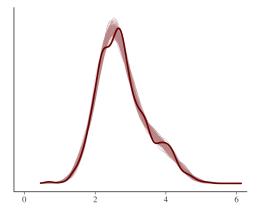


Figure: Model 3

Kernel density estimate of the observed dataset y (dark curve), with density estimates for 100 simulated datasets  $y^{(rep)}$  drawn from the posterior predictive distribution (thin, lighter lines)



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# Example: Test statistic (skewness)

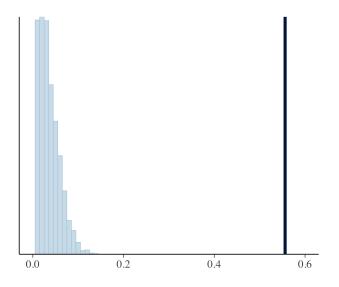


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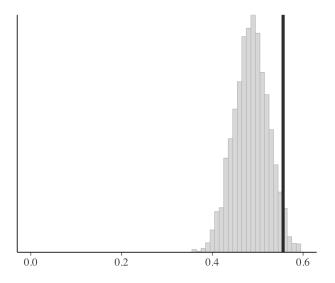


Figure: Model 2



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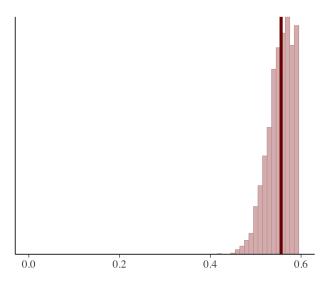


Figure: Model 3