STAT 576 Bayesian Analysis

Lecture 6: Model Checking

Chencheng Cai

Washington State University

Model Checking Methods

Goal:

- Assess the fit of the model to the data.
- Assess the fit of the model to our substantive knowledge.
- Assess the adequacy/robusteness of the model.

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Methods:

- Sensitivity Analysis.
  - Check whether other models generate a similar posterior.
- External Validation.
  - Posterior predictive checking.
- Internal Validation.
  - Cross-validation predictive checking.

Sensitivity Analysis

- How the results are affected by different choices of the model structure?
  - different models (binomial v.s. Poisson, normal v.s. t)
  - different priors
  - different structures (hierarchical v.s. separate)
  - different distribution families (Gaussian v.s. mixed Gaussian)

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  - different models (binomial v.s. Poisson, normal v.s. t)
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  - different structures (hierarchical v.s. separate)
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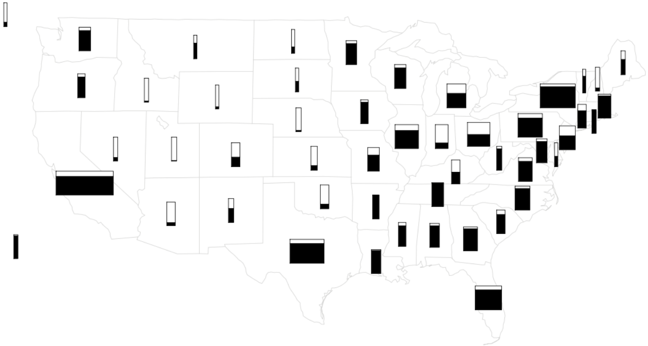
- Compare the sensitivity of essential inference quantities.
  - extreme quantities v.s. mean/median.
  - extrapolation v.s. interpolation.

Example: Election Prediction



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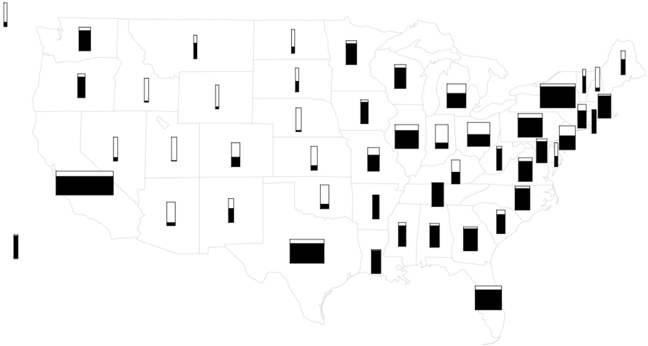

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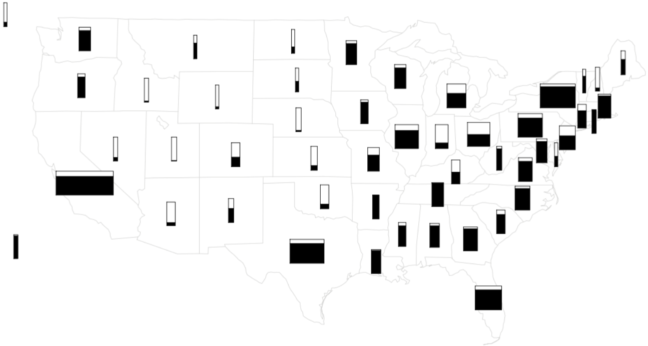

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- Hierarchical linear regression model.
- The model seems wrong at Texas and Florida.
- It is much easier to evaluate the performance afterwards.

Posterior Predictive Checking

- Idea: check the discrepancy between the predicted values and the observed values.

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- Procedure:
  - Generate simulated samples from the **joint posterior predictive distribution**
  - Compare the samples with the observed data.
  - Systematic differences imply the failings of the model.

Example: Light Speed Experiment

- Simon Newcomb set up an experiment in 1882 to measure the light speed.
- The travel time of light was recorded for the round-trip between
  - his lab on the Potomac river
  - a mirror at the base of the Washington Monument
- The total travel distance is 7422 meters.

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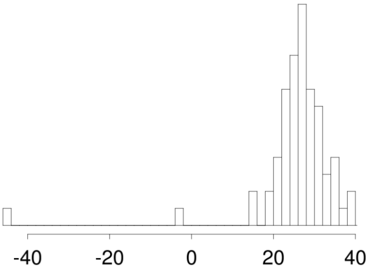
- The total travel distance is 7422 meters.
- The measurement was repeated $n = 66$ times.



Histogram for deviations from 24800 ns

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- A 95% credible interval is $[23.6, 28.8]$.
- We know the true value should be around 33.0.

Example: Light Speed Experiment

Generate posterior predictive replicates y^{rep}

- Draw $\mu^{(s)}, \sigma^{2(s)}$ from the joint posterior distribution $p(\mu, \sigma^2 \mid y)$.
- Draw $y^{rep(s)}$ from $\mathcal{N}(\mu^{(s)}, \sigma^{2(s)})$.
- Repeat the drawing to get n replicates of y^{rep}.

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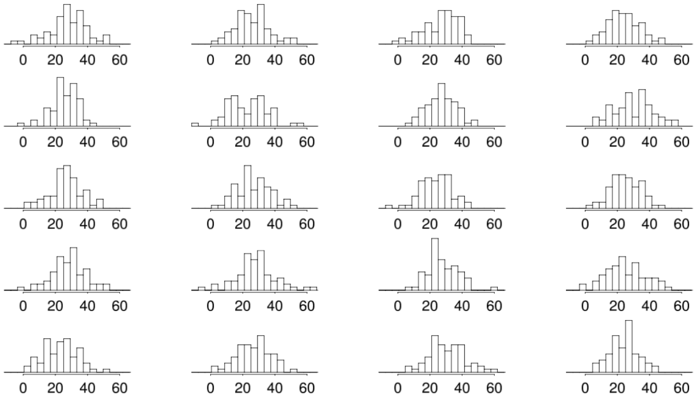

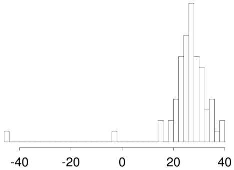

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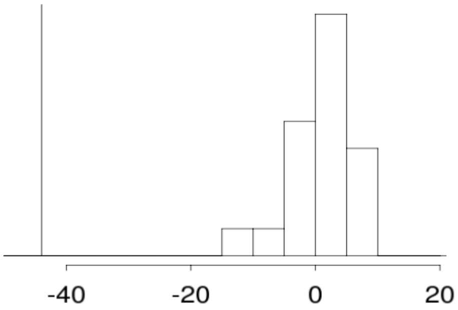
We get the histogram of the **smallest** travel time for all replicates.



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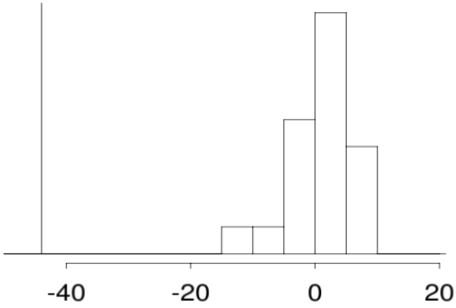

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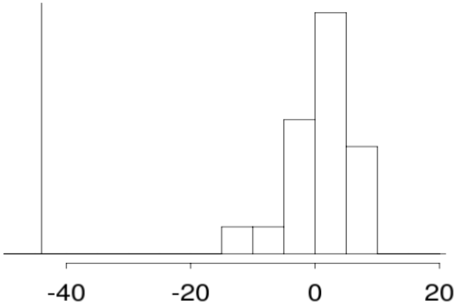

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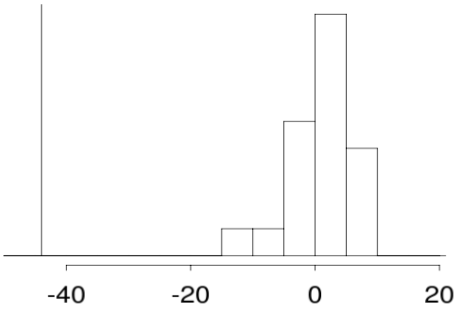

- Can hardly observe an occurrence that is less than -20.
- Decide: whether the **data** was wrong or the **model** was wrong?
- The model was wrong: should use heavy-tailed distribution or contaminated normal (mixed Gaussian).

Posterior Predictive Checking

- Replicated datasets:

$$p(y^{rep} \mid y) = \int \underbrace{p(y^{rep} \mid \theta)}_{obs.\ model} \underbrace{p(\theta \mid y)}_{posterior} d\mu(\theta)$$

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- In the light speed example, we choose $T(y, \theta) = \min(y)$ (also a test statistic).

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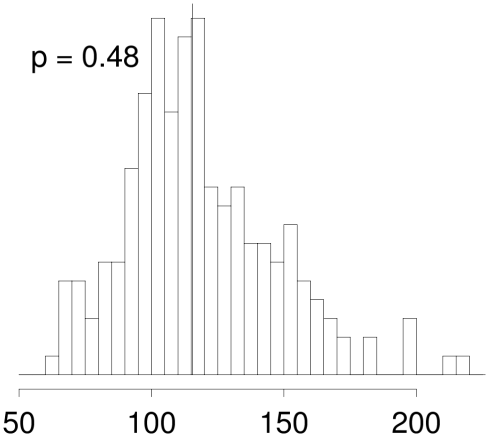
- The classical p-values measure how likely the data is coming from the null model.
- The posterior predictive p-values measure how likely the data is similar to the postetior predictive replicates.
- In Bayesian, θ is also random. p_B can be estimated by joint samples of (y^{rep}, θ).

$$\begin{aligned} p_B &= \iint \mathbb{I}\{T(y^{rep}, \theta) \geq T(y, \theta)\} p(y^{rep} \mid \theta) p(\theta \mid y) d\mu(\theta) d\mu(y^{rep}) \\ &\approx \frac{1}{S} \sum_{s=1}^{S} \mathbb{I}\{T(y^{rep(s)}, \theta^{(s)}) \geq T(y, \theta^{(s)})\} \end{aligned}$$

Example: Light Speed Experiment

If we use the sample variance as the test quantity:



Cannot tell the discrepancy — because the sample variance is a sufficient statistics.

Posterior Predictive Checking

- A **good** test statistic is ancilliary
  - ancilliary: depends on the observed data but independent of the parameters.
- A **bad** test statsistic is highly dependent of the parameters.
  - i.e. sufficient statistics.

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- If we have multiple test statistics, we do not conduct p-value justification.
  - See the smoking example in the textbook.

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- If we have multiple test statistics, we do not conduct p-value justification.
  - See the smoking example in the textbook.
- An extreme p-value often suggests the weakness of the current model. The next step is to revise the model.

Example: Educational Testing

Data: the effects of coaching programs for the SAT-V scores for students in 8 schools.

School	Estimated treatment effect, y_j	Standard error of effect estimate, σ_j
A	28	15
B	8	10
C	−3	16
D	7	11
E	−1	9
F	1	11
G	18	10
H	12	18

Example: Educational Testing

Separate estimation:

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- Most schools have small effects (0-12).
- Two have negative effects.
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Hierarchical model:

- $\theta_1, \ldots, \theta_8 \sim \mathcal{N}(\mu, \tau^2)$ i.i.d.
- $y_j \mid \theta_j \sim (\theta_j, \sigma_j^2)$ independent.
- choose flat prior $p(\mu, \tau) \propto 1$.

Example: Educational Testing

Hierarchical model:

- By drawing posterior samples:
  - draw $\mu^{(s)}, \tau^{(s)}$ from $p(\mu, \tau \mid y)$
  - draw $\theta_1^{(s)}, \ldots, \theta_8^{(s)}$ from $p(\theta_1, \ldots, \theta_8 \mid \mu^{(s)}, \tau^{(s)}, y)$

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- we have the posterior quantiles for each school:

School	Posterior quantiles				
	2.5%	25%	median	75%	97.5%
A	-2	7	10	16	31
B	-5	3	8	12	23
C	-11	2	7	11	19
D	-7	4	8	11	21
E	-9	1	5	10	18
F	-7	2	6	10	28
G	-1	7	10	15	26
H	-6	3	8	13	33

Example: Educational Testing — Model Checking

- Assumptions:
  - normality of y_j.
  - exchangeability of the priors for θ_j's.
  - normality of prior of θ_j.
  - flat hyperprior.

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- Assumptions:
  - normality of y_j.
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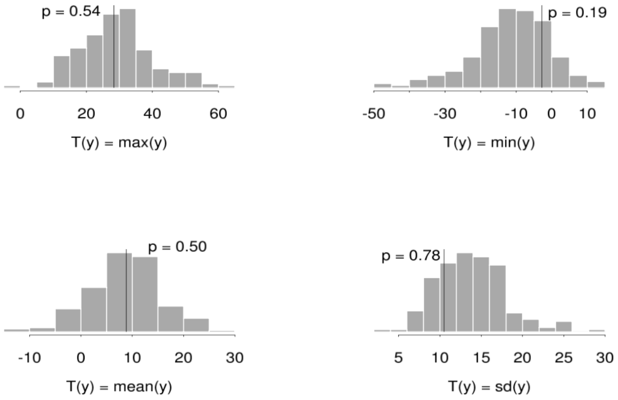
  - flat hyperprior.
- Comparing posterior inferences to substantive knowledge:
  - Individual effects between 5 and 10 seems reasonable.
  - Some lower bounds go to negative.

Example: Educational Testing — Model Checking

- Posterior predictive checking.
  - $y^{rep} = (y_1^{rep}, \ldots, y_8^{rep})$
  - Test statistics: max, min, mean, s.d.



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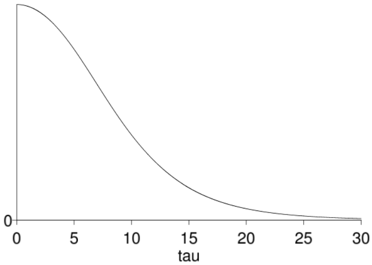
Sensitivity Analysis:

- Uniform prior for τ: the marginal posterior for τ
  — no significant change if we multiply it by another prior



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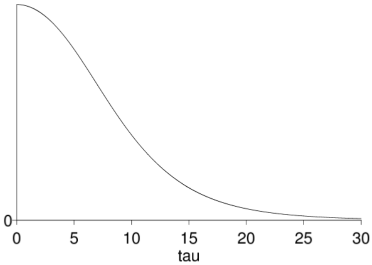

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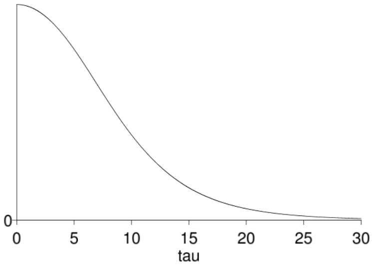

- normality of $y_j \mid \theta_j, \sigma_j$: ensured by experimental designa and CLT.
- normality of the prior for θ_j's:
  One may consider other heavy-tailed distributions. But needs advanced sampling techniques.

Model Evaluation

- We need certain criterion in evaluating a model.
- — provide a "perfomance measure" of the model
- — provide a standard for comparing models
- A very intuitive way is to compare the predicted values with the true values.

Prediction Accuracy

Compare y_i (observation) with prediction:

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- if the prediction is a **point prediction** $\hat{y}_i$:
  - mean squared error: $n^{-1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$
  - mean absolute error: $n^{-1} \sum_{i=1}^{n} |y_i - \hat{y}_i|$

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Justification

If we have the true distribution F (with density f) such that $y_1, \ldots, y_n \sim F,\ i.i.d.$.
Then

$$\text{lpd} = \frac{1}{n} \sum_{i=1}^{n} \log p(y_i \mid \theta) \xrightarrow{a.s.} \mathbb{E}_F[\log p(y_i \mid \theta)] = \int f(y) \log p(y \mid \theta) d\mu(y)$$

$$= \underbrace{\int f(y) \log f(y) d\mu(y)}_{\text{neg. entropy of } F} - \underbrace{\int f(y) \log \frac{f(y)}{p(y \mid \theta)} d\mu(y)}_{\text{Kullback-Leibler divergence } \mathrm{KL}(f || p_\theta)}$$

Prediction Accuracy — Log-Predictive Density

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- $\mathbb{E}_{\text{post}}$ is the expectation is taken for θ w.r.t. the posterior.
- $p_{\text{post}}(\tilde{y}_i)$ is the predictive density for $\tilde{y}_i$ induced from the posterior $p_{\text{post}}(\theta)$.

The **expected predictive density** for $\tilde{y}_i$ is

$$\text{elpd} = \mathbb{E}_F[\log p_{\text{post}}(\tilde{y}_i)] = \int f(\tilde{y}_i) \log p_{\text{post}}(\tilde{y}_i) d\mu(\tilde{y}_i)$$

Prediction Accuracy — Log-Predictive Density

Bayesian version: the expected predictive density:

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Frequentist version: the expected predictve density given $\hat{\theta}$:

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The connection is given by

$$p(\tilde{y}_i \mid y) = \int p(\tilde{y}_i \mid \theta) p(\theta \mid y) d\mu(\theta)$$

Prediction Accuracy — Evaluation

- In practice, we do not know $\theta \longrightarrow$ we cannot calculate $\log p(y_i \mid \theta)$.
- Instead, we work with an averaged version w.r.t. $\theta \sim p(\theta \mid y)$ (the posterior).

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- We summarize the predictive accuracy of the fitted model to data by the **log pointwise predictive density**:

$$\mathrm{lppd} = \log \prod_{i=1}^{n} p_{\text{post}}(y_i) = \sum_{i=1}^{n} \log \int p(y_i \mid \theta) p_{\text{post}}(\theta) d\mu(\theta)$$

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- It is called "pointwise" because we ignore any dependence structure between the observations and only compute the marginal.
- If we don't have a closed-form for the integral, we can draw $\theta^{(1)}, \ldots, \theta^{(S)} \sim p_{\text{post}}(\theta)$ i.i.d., and

$$\widehat{\text{lppd}} = \sum_{i=1}^{n} \log \left(\frac{1}{S} \sum_{s=1}^{S} p(y_i \mid \theta^{(s)}) \right)$$

Prediction Accuracy — Estimation

- We want to estimat the expected predictive accuracy using **out-of-sample** data.

Prediction Accuracy — Estimation

- We want to estimat the expected predictive accuracy using **out-of-sample** data.
- Several methods can be used to estimate the out-of-sample predictive accuracy by the existing data.
  - **Within-sample predictive accuracy**: use the log predicitive density on the training data.
  - **Adjusted within-sample predictive accuracy**: adjust the within-sample predictive accuracy by the expected overestimation. Also known as **information criterion**.
  - **Cross-validation**: split training and testing data and estimate the predictive accuracy on the testing data.

Akaike Information Criterion (AIC)

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Why $-k$ in estimated epld (or $2k$ in AIC)?

- Overestimation from using in-sample data

$$\log p(y \mid \hat{\theta}_{\mathsf{mle}}) - \frac{k}{2} \approx \mathbb{E}_F[\log p(\tilde{y} \mid \theta_0)] \approx \mathbb{E}_F[\log p(\tilde{y} \mid \hat{\theta}_{\mathsf{mle}})] + \frac{k}{2}$$

Deviance Information Criterion (DIC)

DIC is a Bayesian version of AIC:

$$\widehat{\text{elpd}}_{\text{DIC}} = \log p(y \mid \hat{\theta}_{\text{Bayes}}) - p_{\text{DIC}}$$

where p_{DIC} is the effective number of parameters:

$$p_{\text{DIC}} = 2\left(\log p(y \mid \hat{\theta}_{\text{Bayes}}) - \mathbb{E}_{\text{post}}[\log p(y \mid \theta)]\right)$$

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WAIC revises DIC in two ways:

- replace $\hat{\theta}_{\text{Bayes}}$ by an average over $p_{\text{post}}(\theta)$.
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$$p_{\text{WAIC}} = 2\sum_{i=1}^{n}\left(\log \mathbb{E}_{\text{post}}[p(y_i \mid \theta)] - \mathbb{E}_{\text{post}}[\log p(y_i \mid \theta)]\right)$$

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Similarly, we define WAIC by

$$\text{WAIC} = -2\text{lppd} + 2p_{\text{WAIC}}$$

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- All estimators are equivelent asymptotically.
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- Only WAIC is fully Bayesian.

- Bayesian information criterion (BIC) has a different goal and therefore is not discussed here.

Leave-One-Out Cross Validation (LOO-CV)

The Bayesian LOO-CV estimate of out-of-sample predictive fit is

$$\text{lppd}_{\text{loo-cv}} = \sum_{i=1}^{n} \log p_{\text{post}(-i)}(y_i) = \sum_{i=1}^{n} \log \int p(y_i \mid \theta) \underbrace{p(\theta \mid y \setminus \{y_i\})}_{\text{posterior with all obs. except } y_i} d\mu(\theta)$$

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- In practice, the above integral can be replaced by Monte Carlo sample mean.
- $\text{lppd}_{\text{loo-cv}}$ underestimates the predictive accuracy because it uses $n-1$ observations instead of n.
- The bias can be estimated by

$$b = \text{lppd} - \overline{\text{lppd}}_{-i}$$

where

$$\overline{\text{lppd}}_{-i} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \log p_{\text{post}(-i)}(y_j)$$

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If we compare the formula to other methods, we can the effective numbers of parameters are

$$p_{\text{loo-cv}} = \mathrm{lppd} - \mathrm{lppd}_{\text{loo-cv}}$$
$$p_{\text{cloo-cv}} = \overline{\mathrm{lppd}}_{-i} - \mathrm{lppd}_{\text{loo-cv}}$$

Example: SAT-V Score

		No pooling ($\tau = \infty$)	Complete pooling ($\tau = 0$)	Hierarchical model (τ estimated)
AIC	$-2\,\text{lpd} = -2\log p(y\vert\hat{\theta}_{\text{mle}})$	54.6	59.4	
	k	8.0	1.0	
	$\text{AIC} = -2\,\widehat{\text{elpd}}_{\text{AIC}}$	70.6	61.4	
DIC	$-2\,\text{lpd} = -2\log p(y\vert\hat{\theta}_{\text{Bayes}})$	54.6	59.4	57.4
	p_{DIC}	8.0	1.0	2.8
	$\text{DIC} = -2\,\widehat{\text{elpd}}_{\text{DIC}}$	70.6	61.4	63.0
WAIC	$-2\,\text{lppd} = -2\sum_i \log p_{\text{post}}(y_i)$	60.2	59.8	59.2
	$p_{\text{WAIC}\,1}$	2.5	0.6	1.0
	$p_{\text{WAIC}\,2}$	4.0	0.7	1.3
	$\text{WAIC} = -2\,\widehat{\text{elppd}}_{\text{WAIC}\,2}$	68.2	61.2	61.8
LOO-CV	$-2\,\text{lppd}$		59.8	59.2
	$p_{\text{loo-cv}}$		0.5	1.8
	$-2\,\text{lppd}_{\text{loo-cv}}$		60.8	62.8

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- Likelihood: $p(y \mid H_1)$ and $p(y \mid H_2)$
- Posterior:

$$p(H_i \mid y) = \frac{p(H_i)p(y \mid H_i)}{p(H_1)p(y \mid H_1) + p(H_2)p(y \mid H_2)}, \quad i = 1, 2$$

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- To decide, we look at the posterior ratio:

$$\frac{p(H_2 \mid y)}{p(H_1 \mid y)} = \frac{p(H_2)}{p(H_1)} \times \underbrace{\frac{p(y \mid H_2)}{p(y \mid H_1)}}_{\text{Bayes Factor}(H_2;H_1)}$$

  The decision depends on the magnitude of the Bayes Factor of the two models.

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Common decisions based on the Bayes Factor:

Bayes factor	1 to 3.2	3.2 to 10	10 to 100	> 100
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- Bayes factor works better for discrete models than continuous models.