STA2201H Methods of Applied Statistics II

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Week 6: Model checking and visualizing the Bayesian workflow

Announcemnets

Outlook

- Model checking, comparison
- Multilevel models
- Splines, temporal models etc in a Bayesian multilevel framework
- Measurement error

Other

- A1 grades soon
- A2 out this week
- Also need to start thinking about research proposal

Overview

- Prior predictive checks
- Posterior predictive checks
- PSIS estimate of LOO-CV
- (brief) Information criteria
- (brief) Actually training and testing

Reading

- BDA chapter 6
- This lecture inspired by Gabry et al, 2019, "Visualization in the Bayesian Workflow"
- A newer paper extending these ideas by Gelman et al 2020: https://arxiv.org/abs/2011.01808
- Extra reading on PSIS: Vehtari, A., Gelman, A., and Gabry, J. 2017. "Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC".
- Betancourt, "Towards A Principled Bayesian Workflow"

Phases of the (Bayesian) statistical workflow

1) EDA
2) Model checks based on simulated data and the prior predictive distribution
3) Run the model, computational checks (trace plots etc)
4) Posterior predictive checks, cross-validation checks, other checks of data v predictions

Steps of building a Bayesian model

Model choice: need to decide on

- Likelihood
- Functional form of model for conditional expectation $E(Y|X)$
- Priors for parameters

Prior predictive distributions

- If we specify proper priors for all parameters in the model, our model is **generative**
- Yields a joint prior distribution on the parameters and data, and hence a prior marginal distribution for the data

Prior predictive distribution for new $\tilde{y}$

$$p(\tilde{y}) = \int_{\Theta} p(\tilde{y}, \theta) d\theta = \int_{\Theta} p(\tilde{y}|\theta) p(\theta) d\theta$$

In practice (in R) we can simulate values of θ from the prior distribution(s), and then simulate from the likelihood to generate values of $\tilde{y}$, and then look at the resulting distribution.

Prior predictive distributions

Why would we do this? We should be setting our priors so they make sense anyway.

Prior predictive distributions

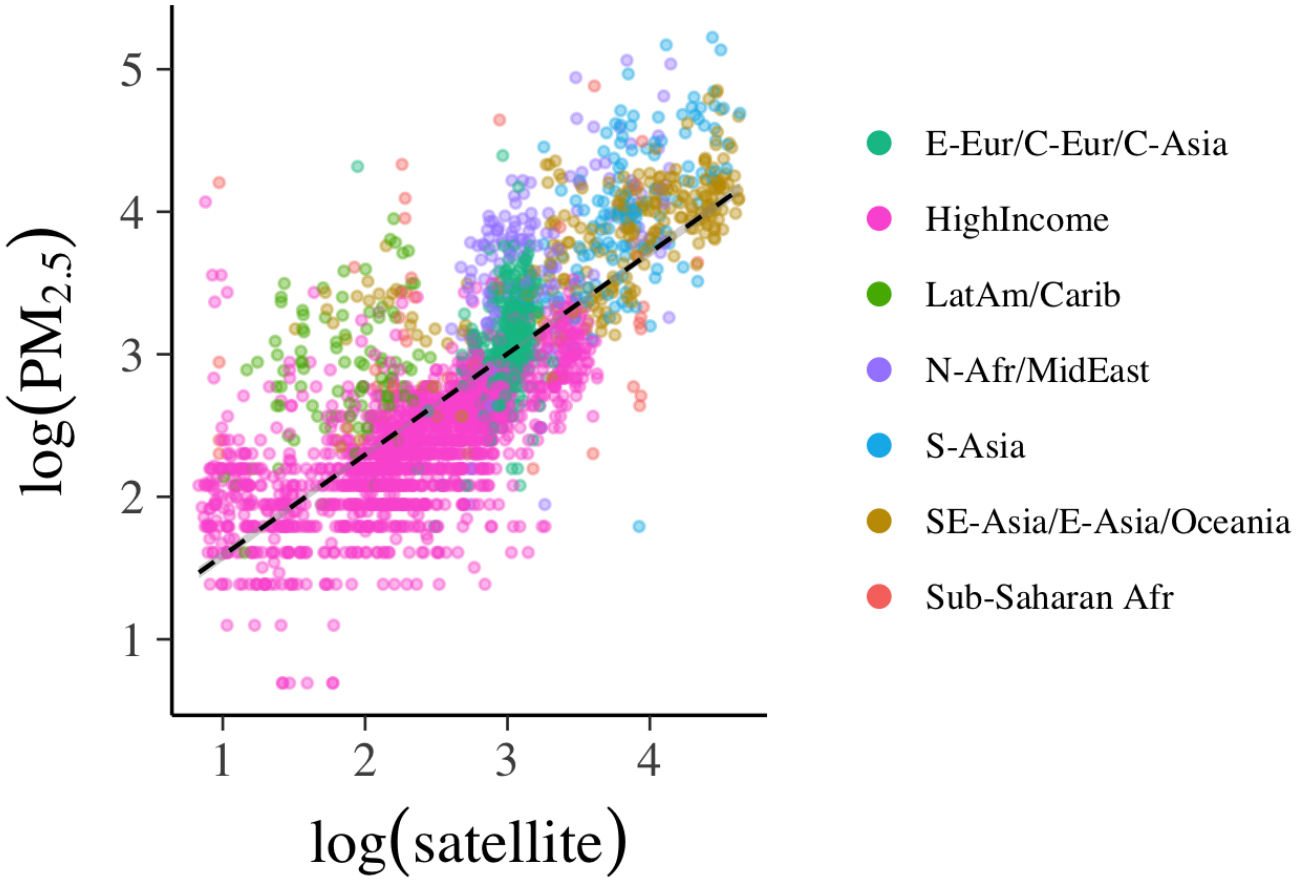
- Allows you to assess the interplay between the prior and the likelihood
- Assess whether the priors make sense for a particular problem

We want our priors to be set such that the prior data-generating distribution $p(y)$ could represent any data set that could plausibly be observed.

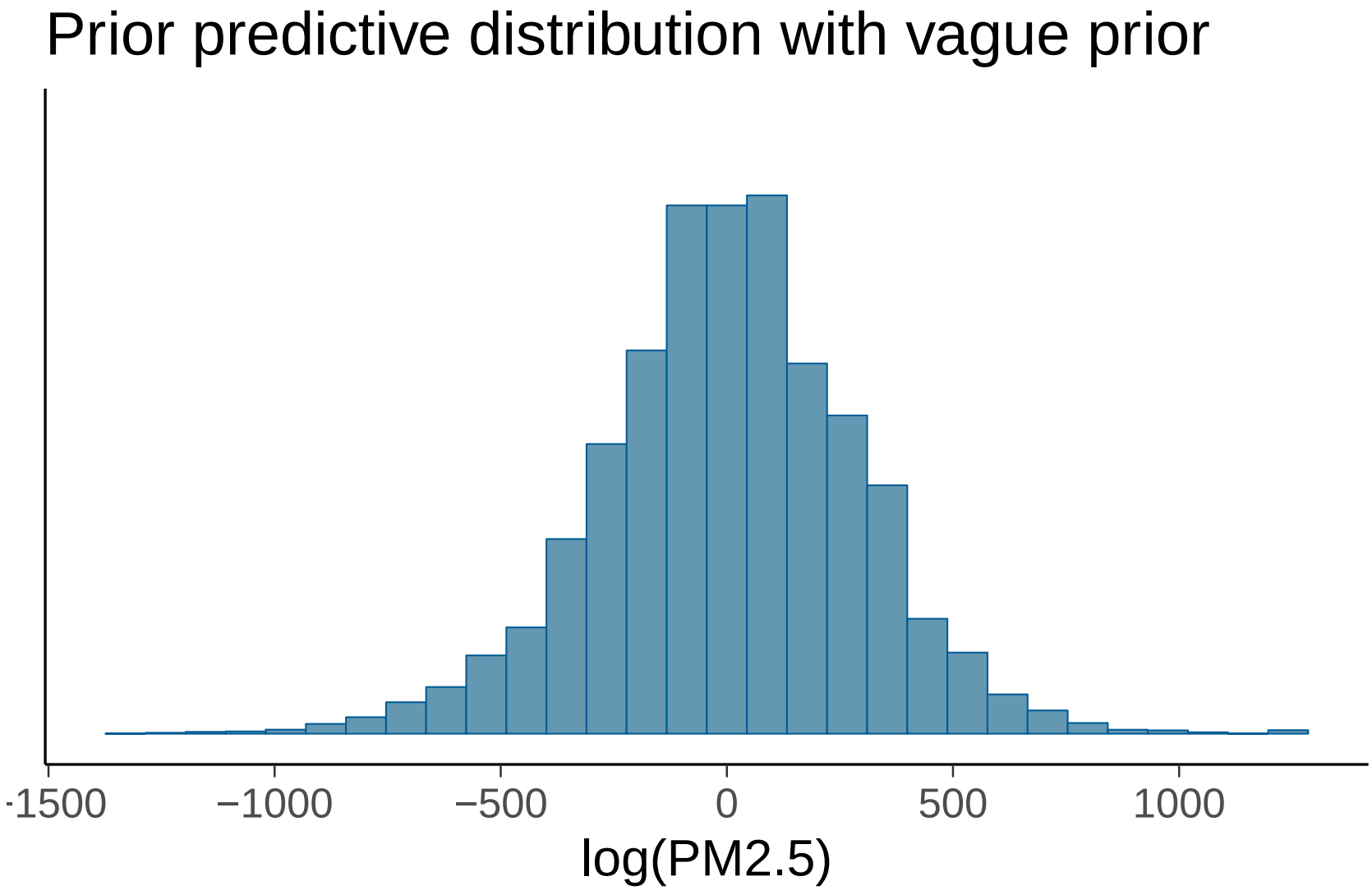
A *weakly informative joint prior data generating process* has at least some mass around extreme but plausible data sets, but no mass on completely implausible data sets.

Example: air pollution

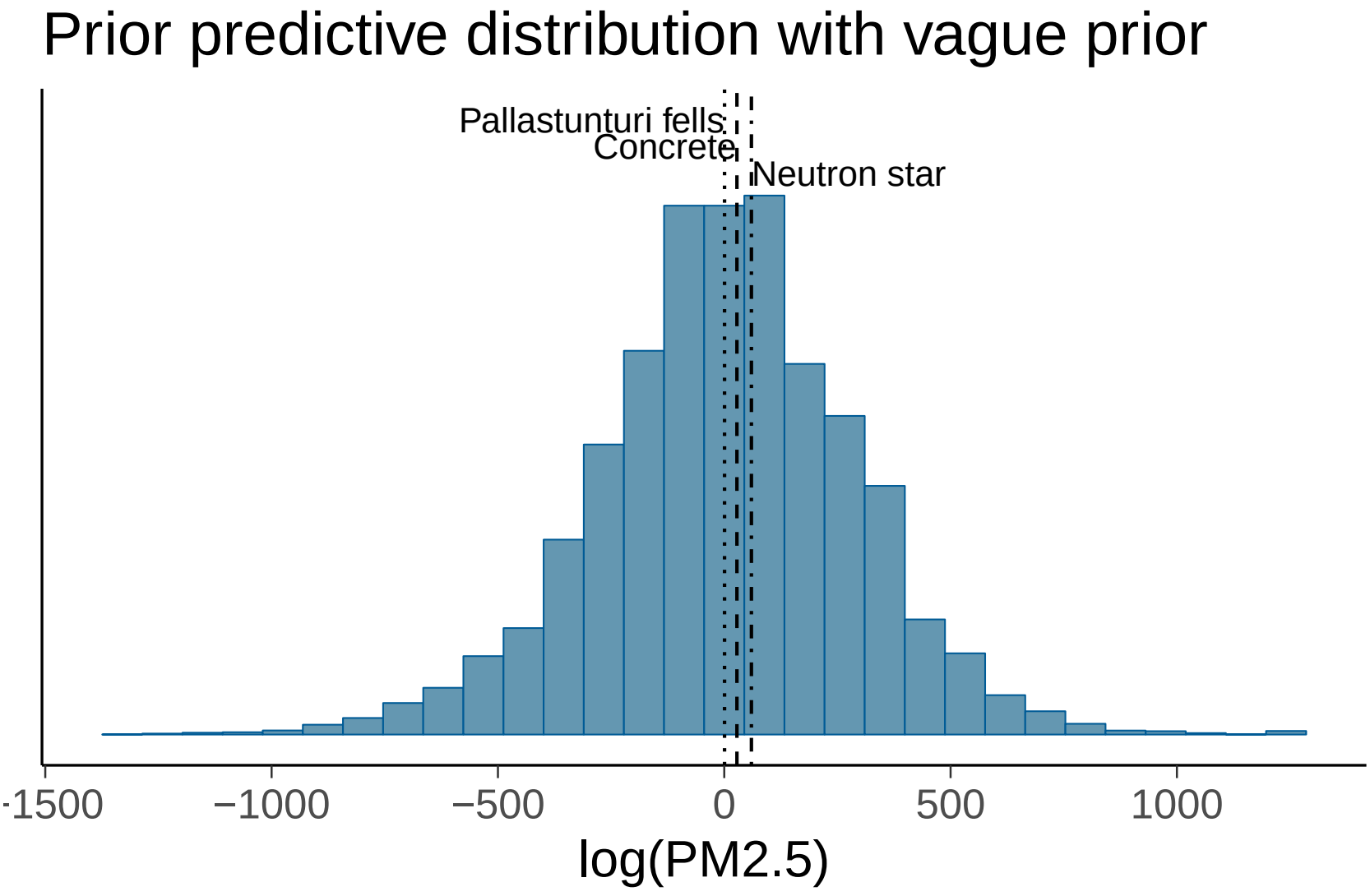
- Example in Gabry et al paper
- Goal: estimate exposure to $PM_{2.5}$
- Model relationship between ground measures and satellite data



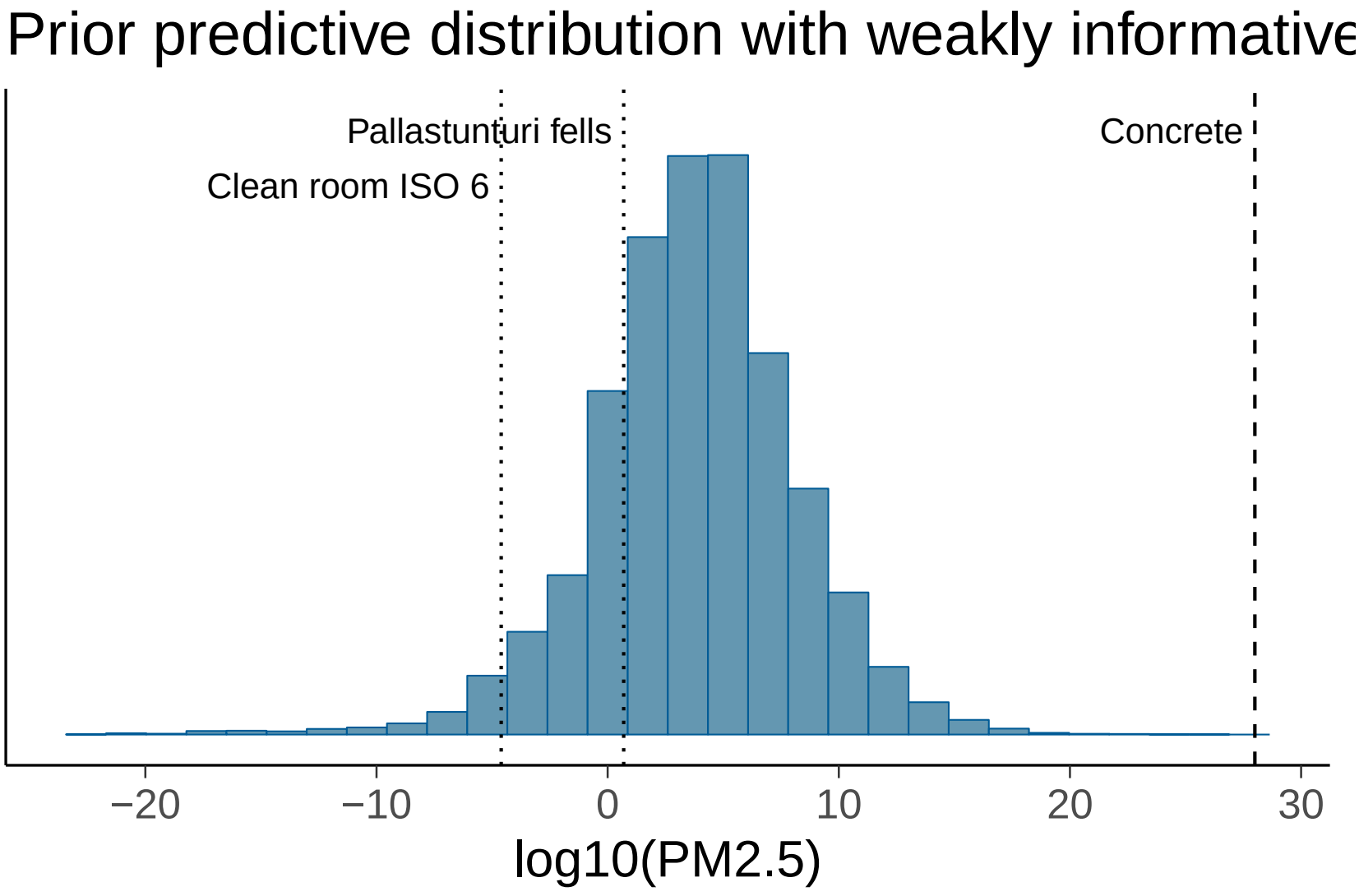
Example: air pollution



Example: air pollution



Example: air pollution

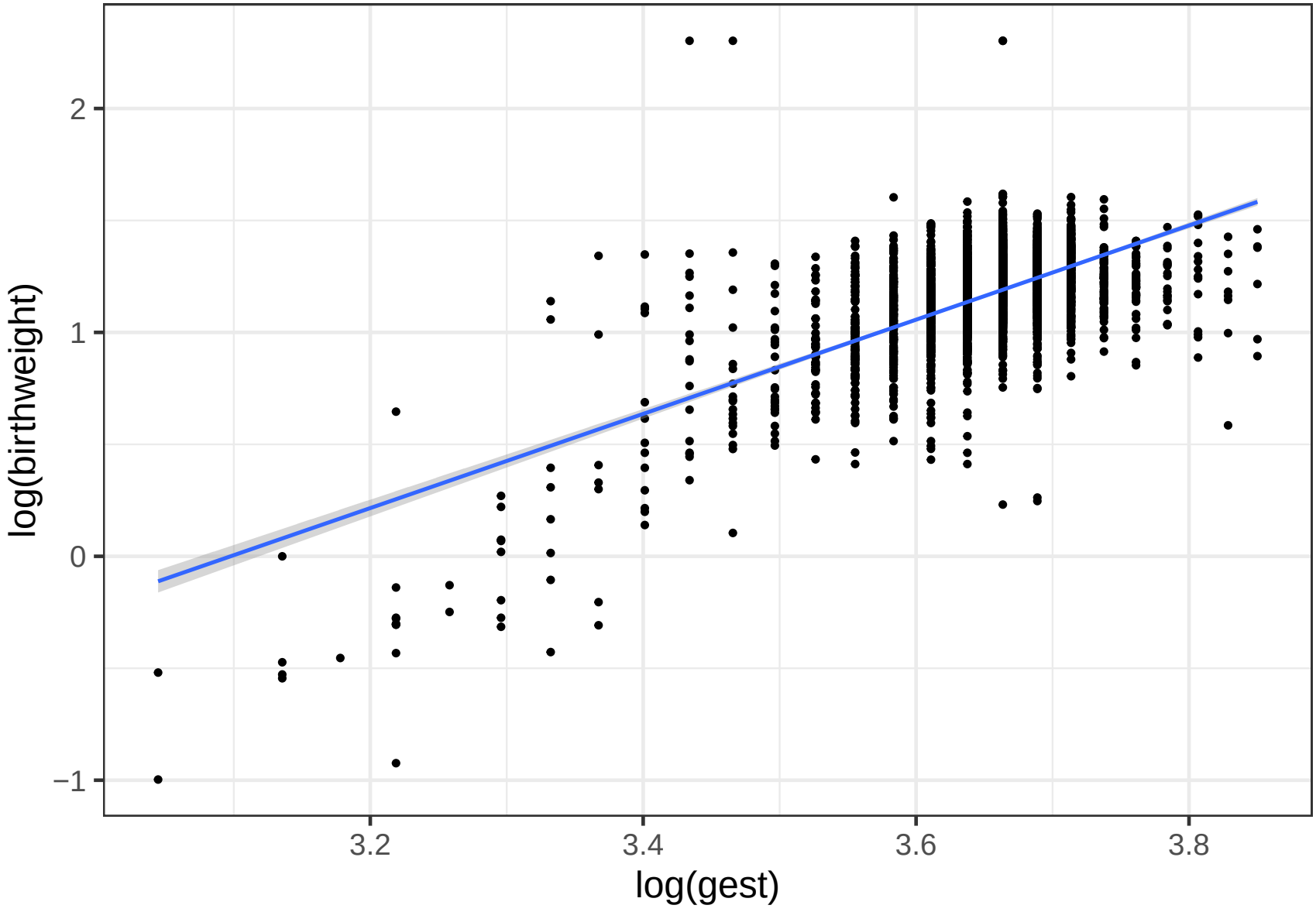


Example: births

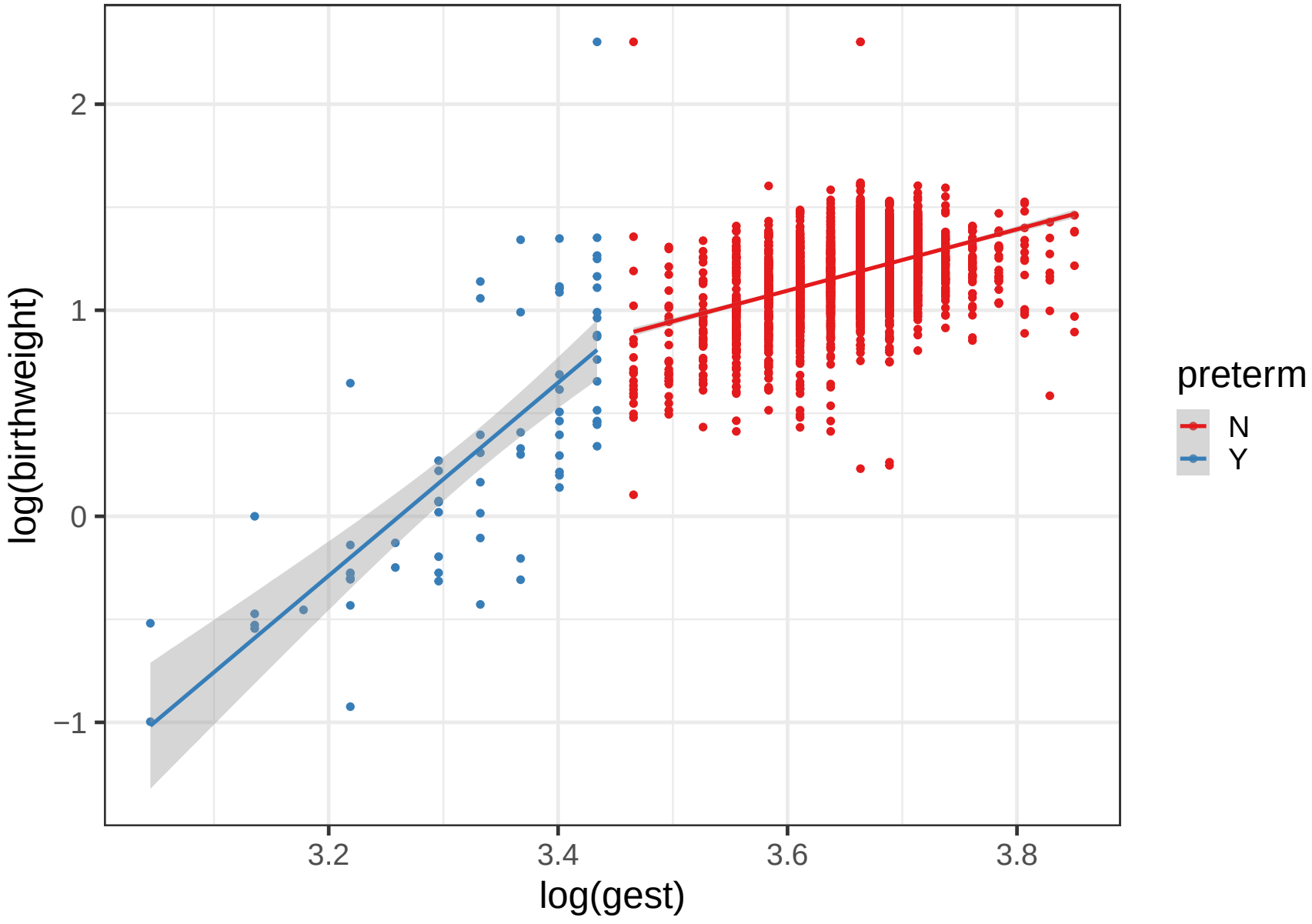
Example: births data

- Looking at all births in 2017 in US
- Interested in investigating patterns in birth weight
- Just using .1% sample for now

Weight v gestational age



Weight v gestational age



Priors

Consider a simple model of weight v gestational age (logged)

$$\log(y_i) \sim N(\beta_0 + \beta_1 \log(x_i), \sigma^2)$$

Vague priors:

- β's $\sim N(0, 100)$
- $\sigma \sim$ InvGamma$(1, 100)$

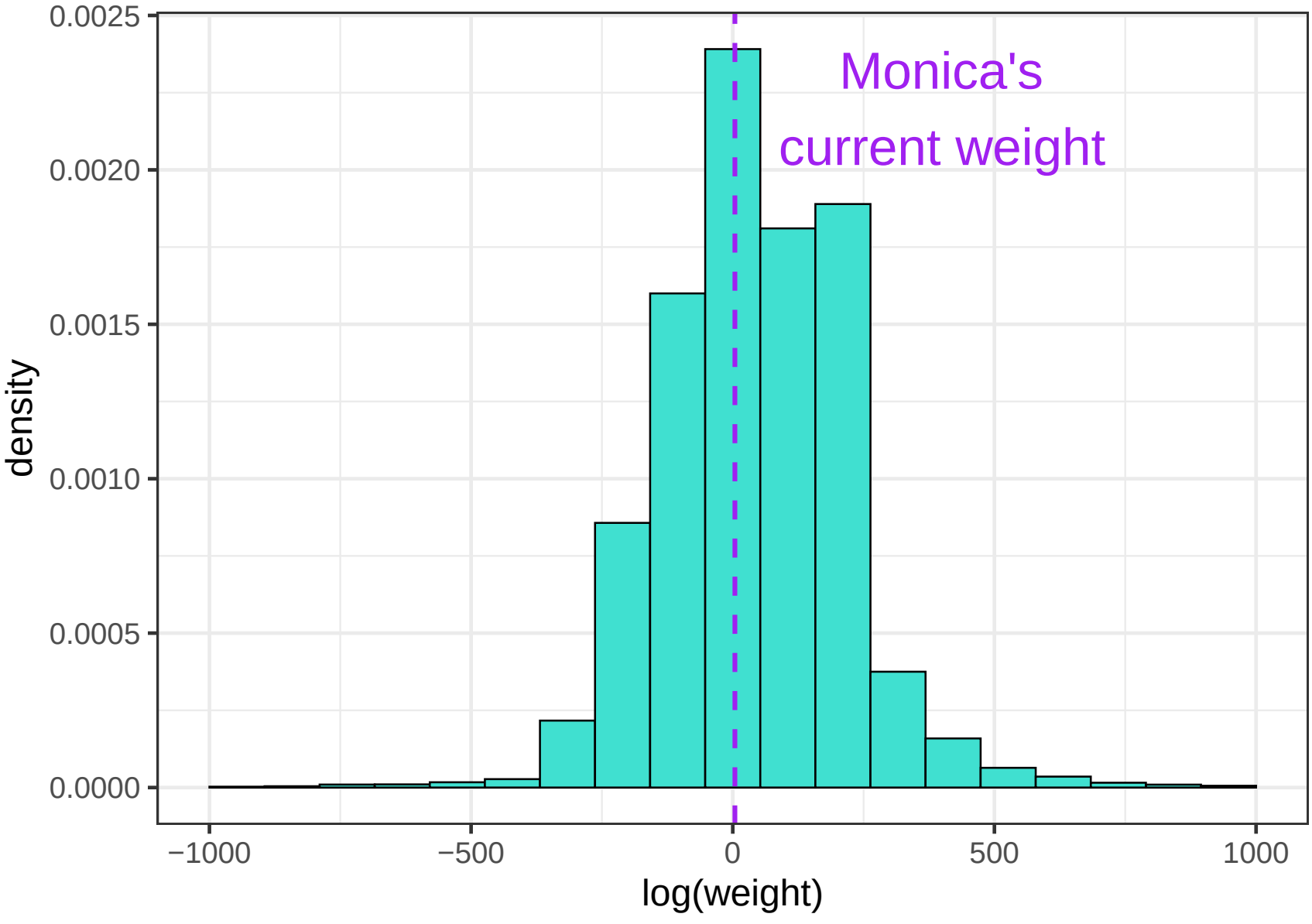
Weakly informative priors:

- β's $\sim N(0, 1)$
- $\sigma \sim$ Half Normal$(0, 1)$

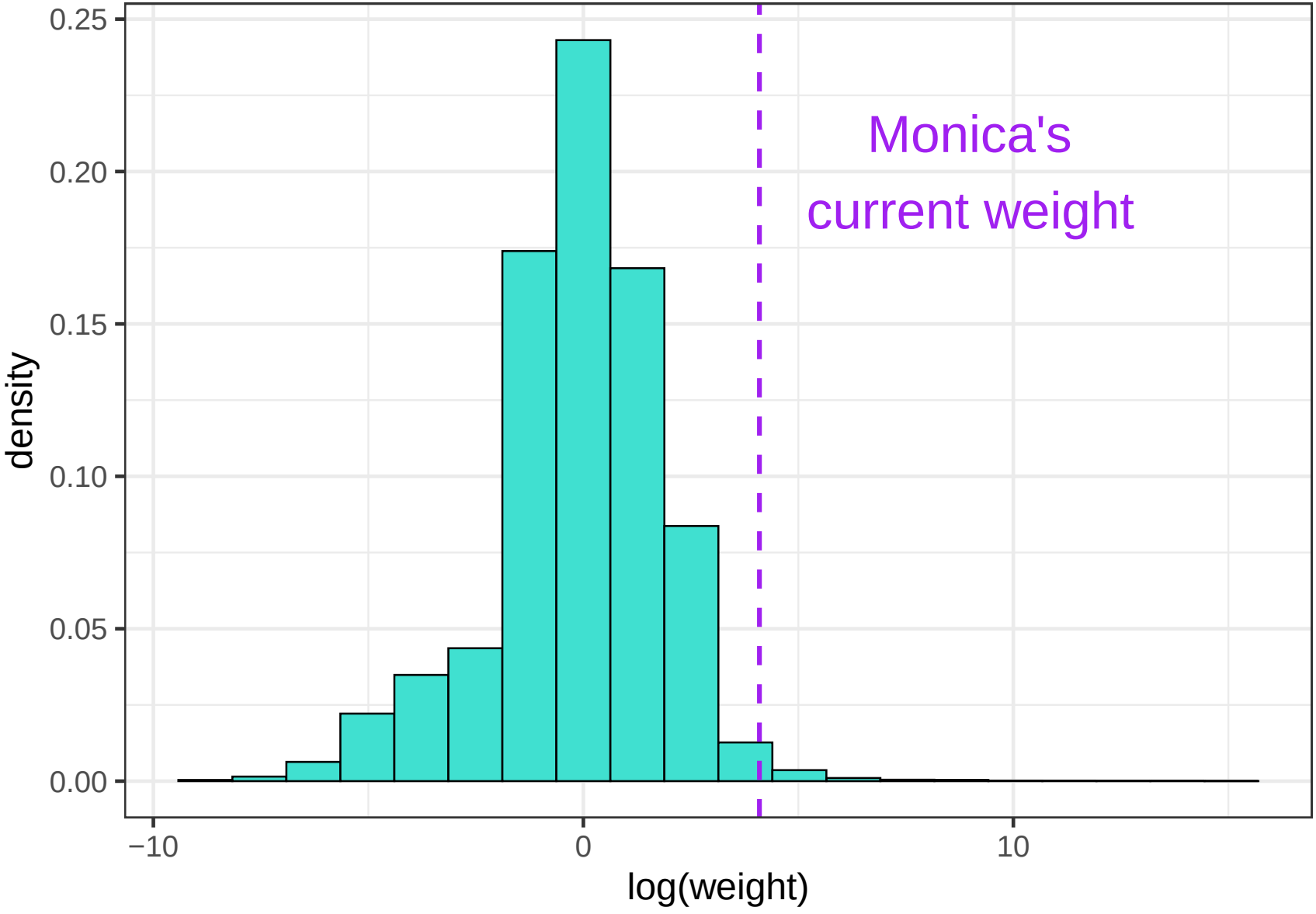
Check these in each case by:

- Simulating parameters from priors
- Simulating data y_i from likelihood
- Plot histogram of implied weights

Vague priors



Weakly informative priors



Posterior predictive checks

Posterior predictive checks

Now we've run a candidate model, how do we explore and check how the model is doing? The idea of **posterior predictive checks** is to compare our observed data to replicated data from the model.

If our model is a good fit, we should be able to use it to generate a dataset that resembles the observed data.

Posterior predictive checks

Posterior predictive distribution for new $\tilde{y}$

$$p(\tilde{y}|y) = \int_{\Theta} p(\tilde{y}|\theta, y)p(\theta|y)d\theta$$

To obtain samples from this distribution, we need to

- Get posterior samples of our parameters $\theta^{(s)}$ (MCMC output!)
- For each posterior sample, we obtain one replicated dataset $\tilde{y}^{(s)}$ by sampling from the likelihood $p(\tilde{y}|\theta^{(s)})$. Can do this in R or within Stan.

Generated quantities in Stan

For each posterior sample, we obtain one replicated dataset $\tilde{y}^{(s)}$ by sampling from the likelihood $p(\tilde{y}|\theta^{(s)})$. Can do this in R or within Stan.

```
model {
  // Log-likelihood
  target += normal_lpdf(log_weight | beta0 + beta1 * log_gest, sigma);

  // Log-priors
  target += normal_lpdf(sigma | 0, 1)
          + normal_lpdf(beta0 | 0, 1)
          + normal_lpdf(beta1 | 0, 1);
}
generated quantities {
  vector[N] log_weight_rep; // replications from posterior predictive dist

  for (n in 1:N) {
    real log_weight_hat_n = beta0 + beta1 * log_gest[n];
    log_weight_rep[n] = normal_rng(log_weight_hat_n, sigma);
  }
}
```

PPCs

Now that we have a set of replicated datasets, can decide on a test statistic $t(\theta)$ that is a summary of interest

- Things like: median, skew, min, max, proportion under 2500 grams (low birth weight)
- Calculate test statistic for our data $t(y)$ and for each replicated dataset $t(y_{rep})$ and compare
- Appropriate test statistic is context dependent
- Bad test statistics are highly dependent on parameters in the model (e.g. mean, variance)

Example: birthweight

Model 1:

$$\log(y_i) \sim (\beta_0 + \beta_1 \log(x_i), \sigma^2)$$

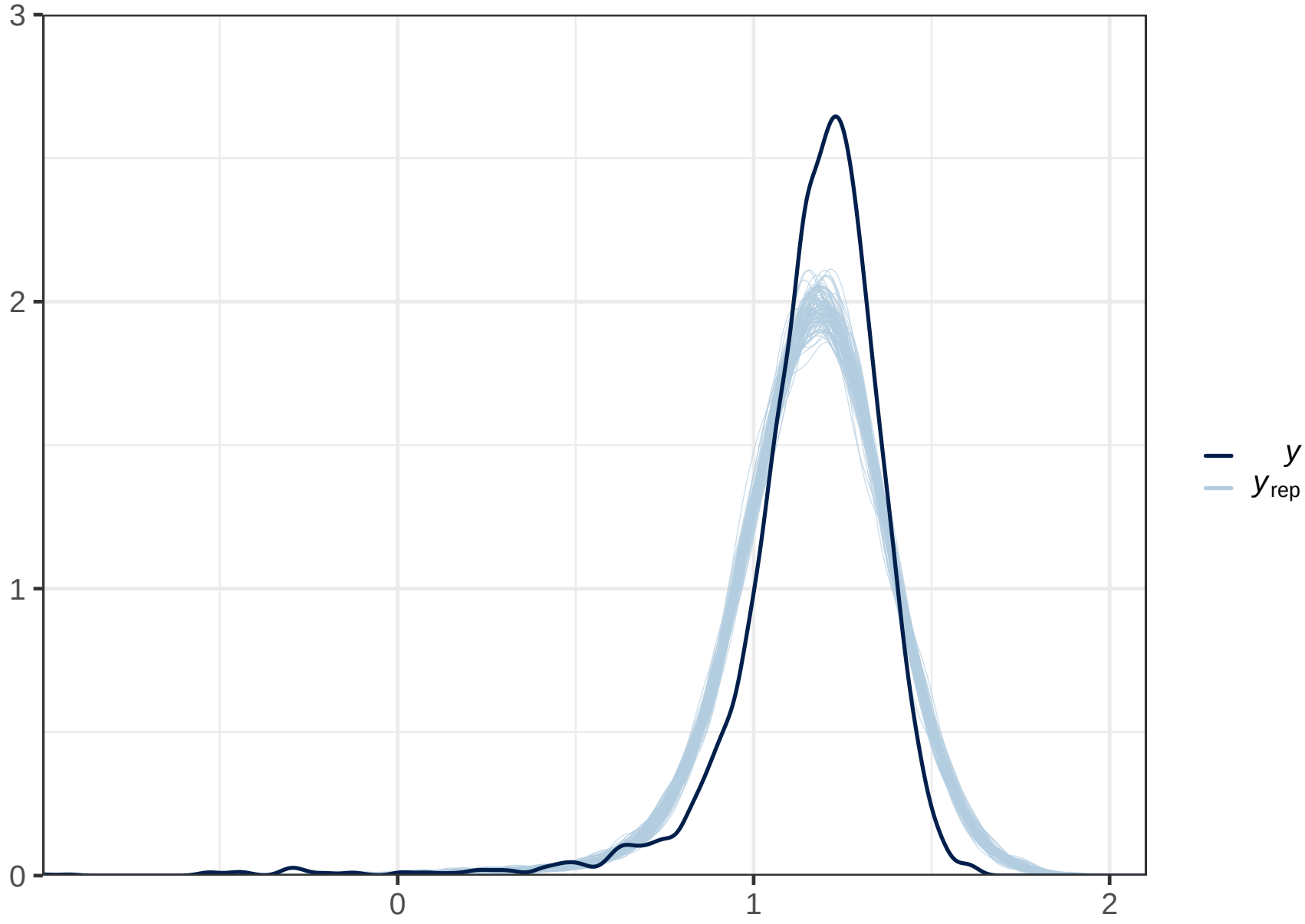
Model 2: preterm + interaction

$$\log(y_i) \sim (\beta_0 + \beta_1 \log(x_i) + \gamma_0 z_i + \gamma_1 \log(x_i) z_i, \sigma^2)$$

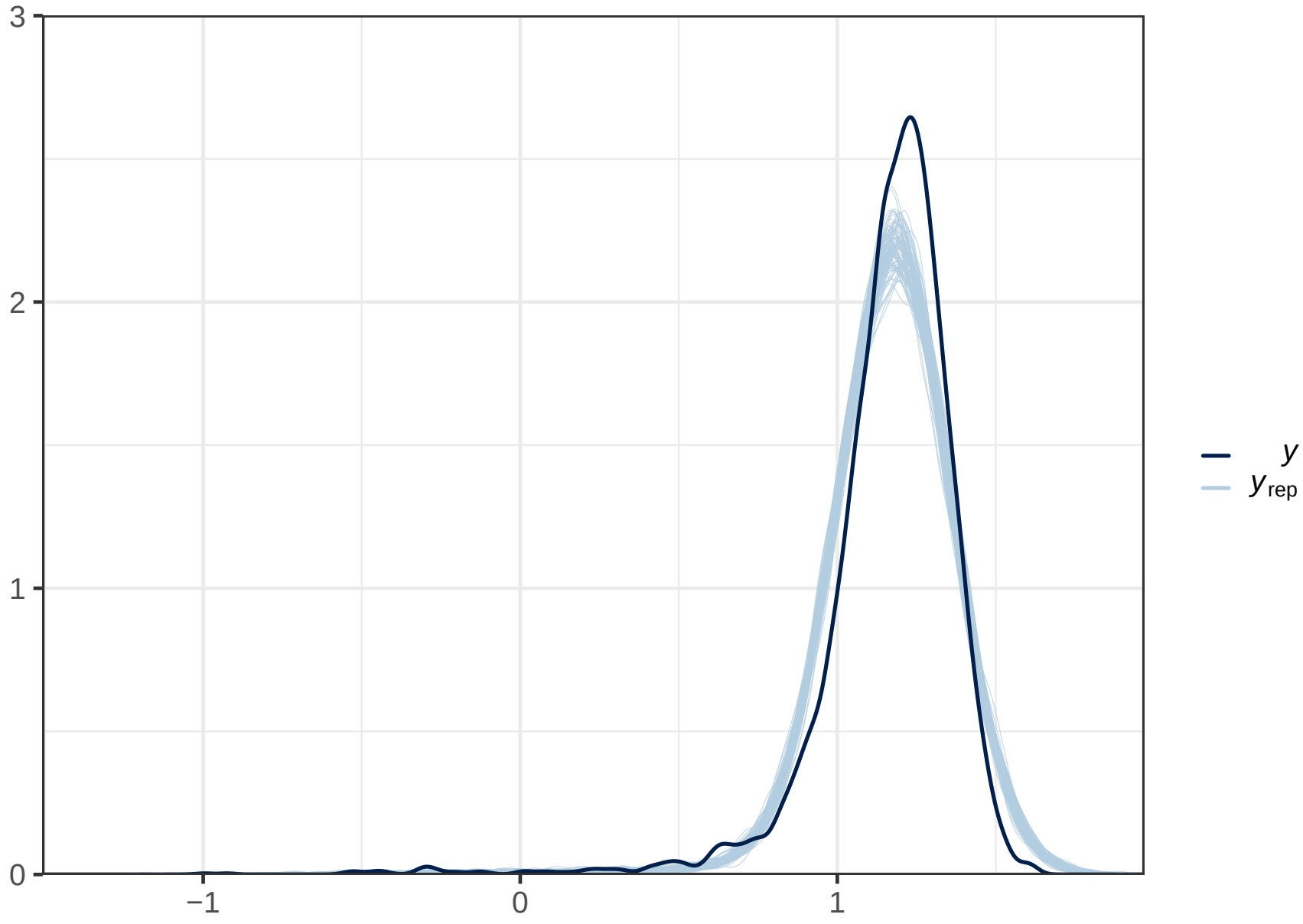
- y_i is weight in kg
- x_i is gestational age in weeks
- z_i is preterm (0 or 1, if gestational age is less than 30 weeks)

PPCs: Compare our dataset with 100 replicates

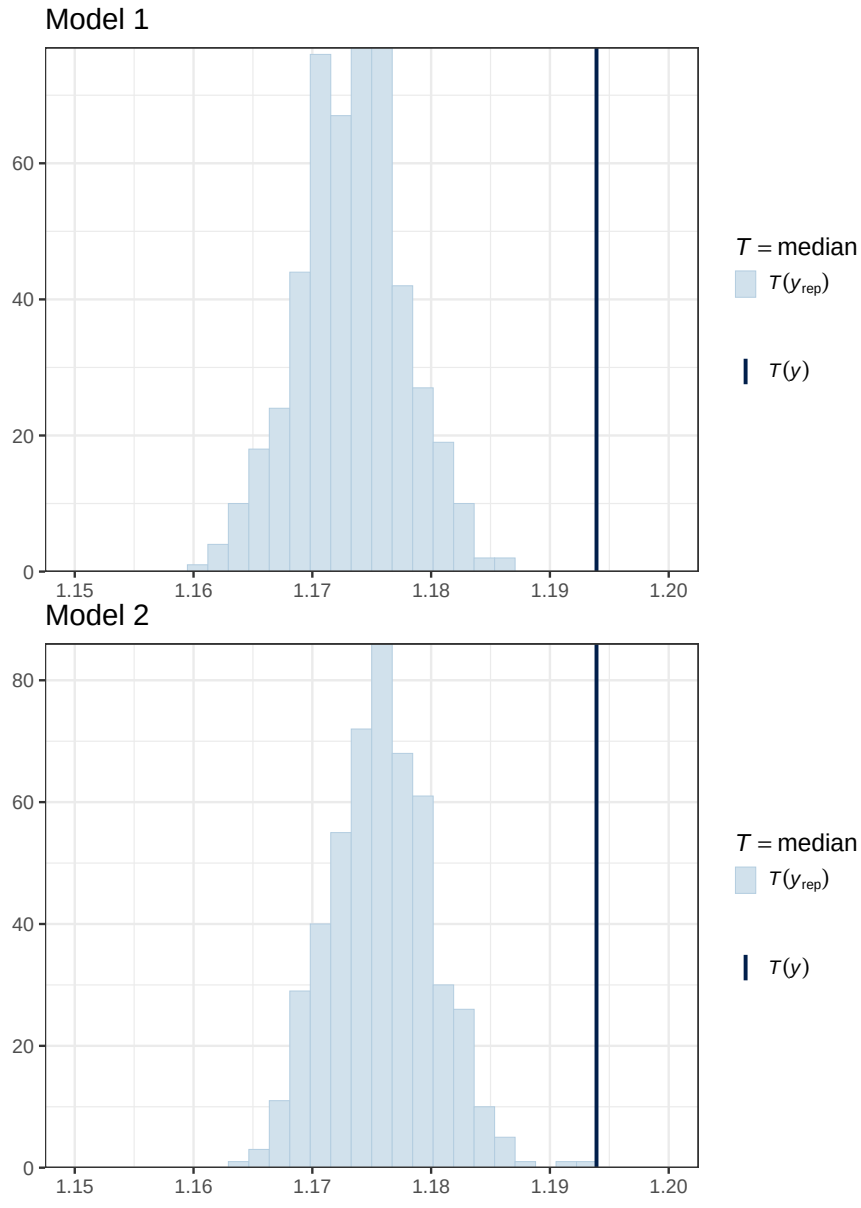
Model 1:



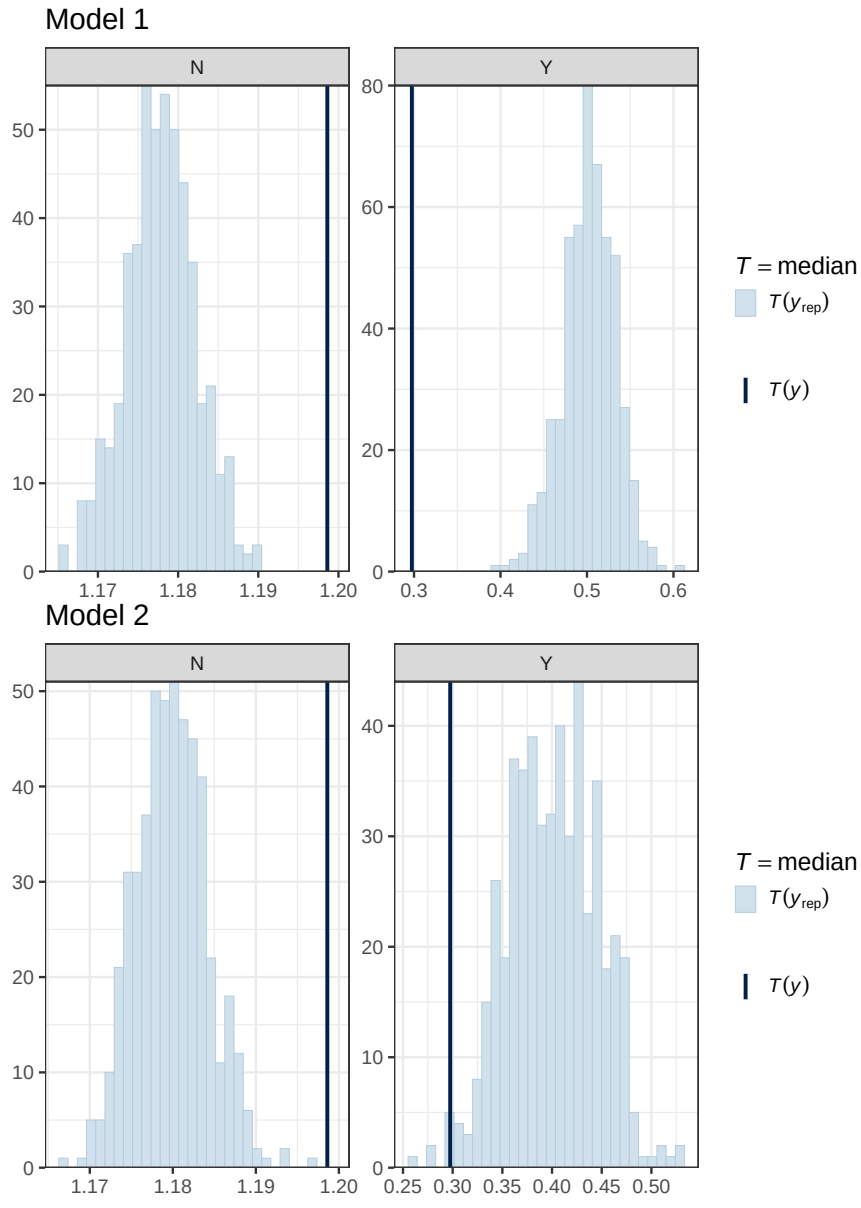
Model 2



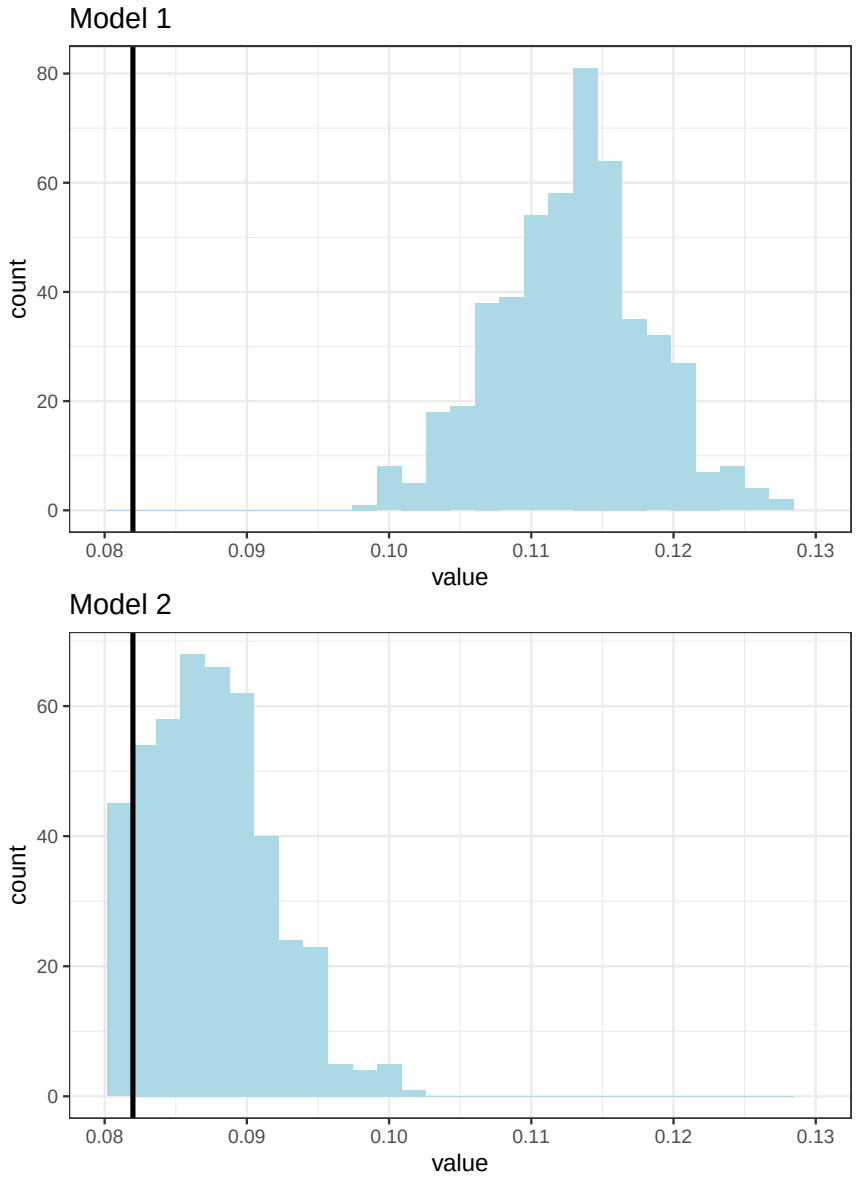
Look at median



Look at median by preterm



Look at proportion low birthweight (< 2.5kg)



LOO-CV

Compare data to itself

- In PPC we are using the data twice: once to fit model and once to check
- It would be nice to know how well the model would do fitting to a new dataset
- i.e. interested in **out of sample** prediction accuracy
- We usually don't have a new dataset

Idea: split dataset into **train** and **test** datasets (e.g. 80/20% split)

- Fit the model using training set
- Check the model using testing set
  - check based on some metric e.g. MSE

Training and testing over and over

- An issue with just doing a train/test split once is that the metric is highly dependent on the test set chosen
- One way to get around this is to split the data into train/test multiple times
- This is called **cross validation**
- **Leave-one-out cross validation** (LOO-CV) uses single observations as test sets.

Idea:

- Use all data except i, i.e. use $\boldsymbol{y}_{-i}$ to predict y_i.
- Ideally, we would fit the model to $\boldsymbol{y}_{-i}$ and get $p\left(y_i|\boldsymbol{y}_{-i}\right)$, the **leave-one-out predictive density**.

LOO-CV

Ideally, we would fit the model to $\boldsymbol{y}_{-i}$ and get $p\left(y_i|\boldsymbol{y}_{-i}\right)$, the **leave-one-out predictive density**.

If we had infinite time and resources, we could for $i = 1, \ldots, n$

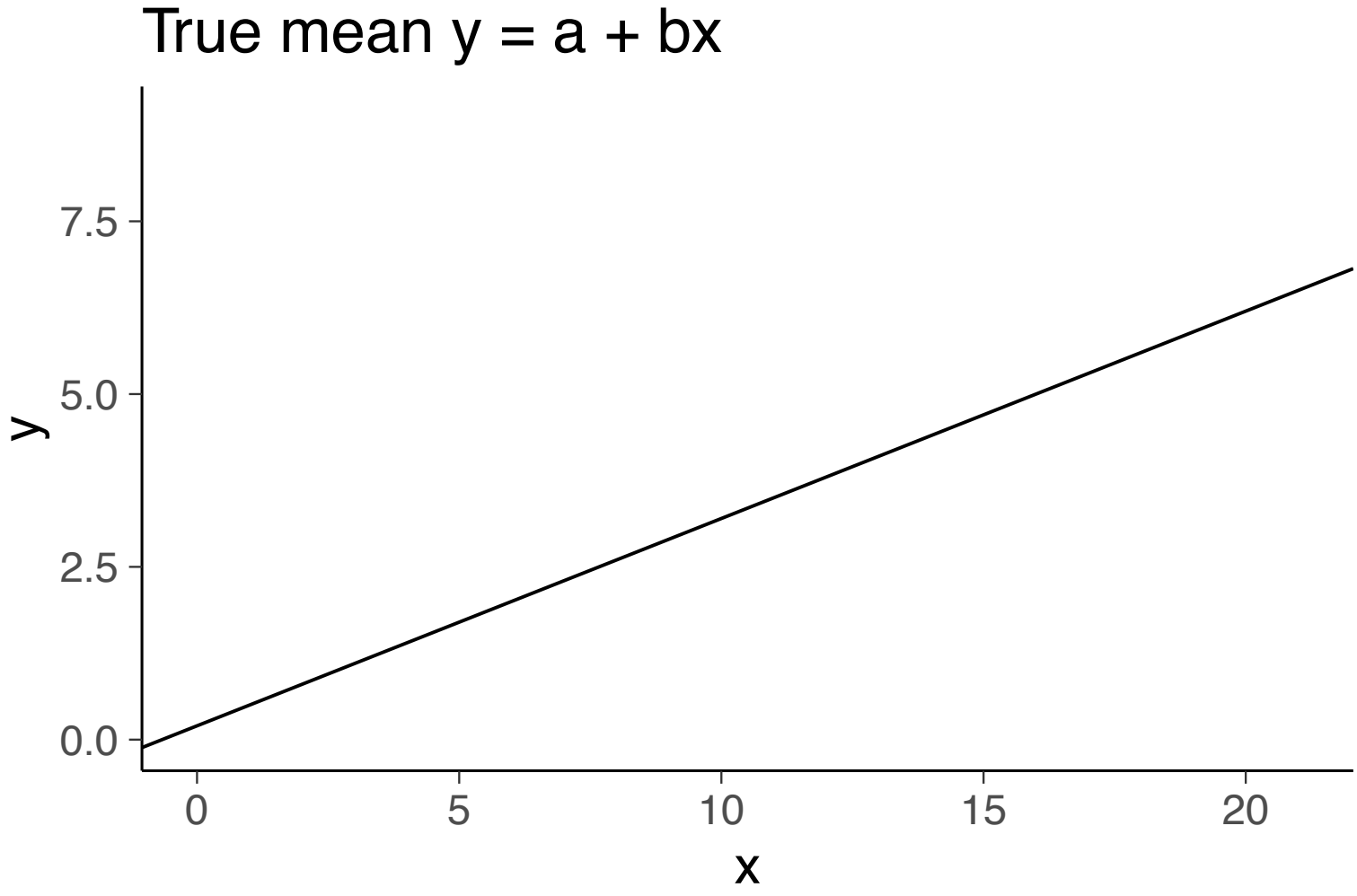
1. Remove the ith data point
2. Rerun the model
3. Calculate $p\left(y_i|\boldsymbol{y}_{-i}\right)$

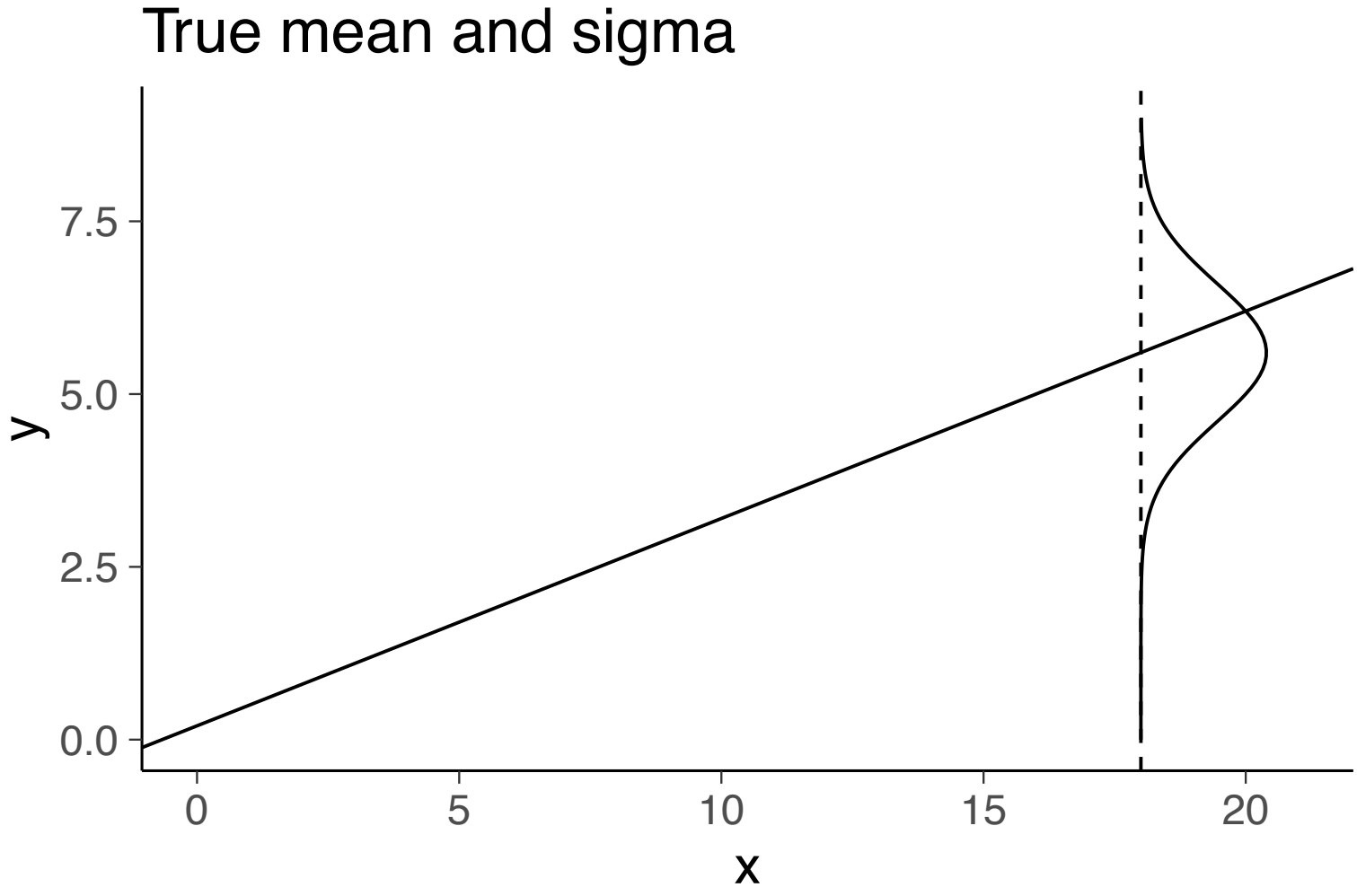
Then calculate the **expected log pointwise predictive density**

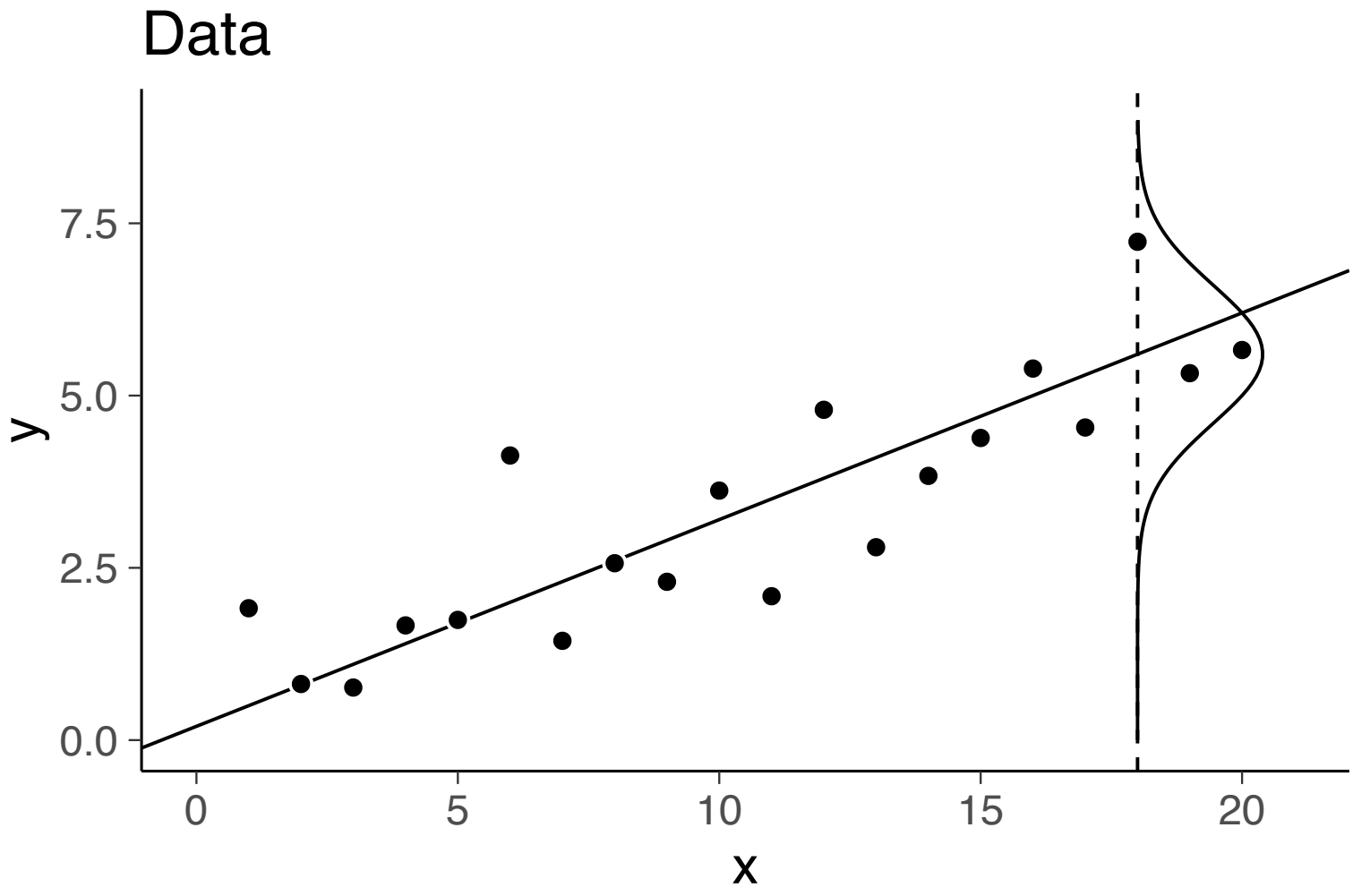
$$\text{elpd}_{\text{LOO}} = \sum_{i=1}^{n} \log p\left(y_i|\boldsymbol{y}_{-i}\right)$$

Then can compare elpd_{LOO} across different models, etc. The bigger the better.

Visualizing $p\left(y_i | \boldsymbol{y}_{-i}\right)$ (Source)


True mean y = a + bx
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


True mean and sigma
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


Data
7.5
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y
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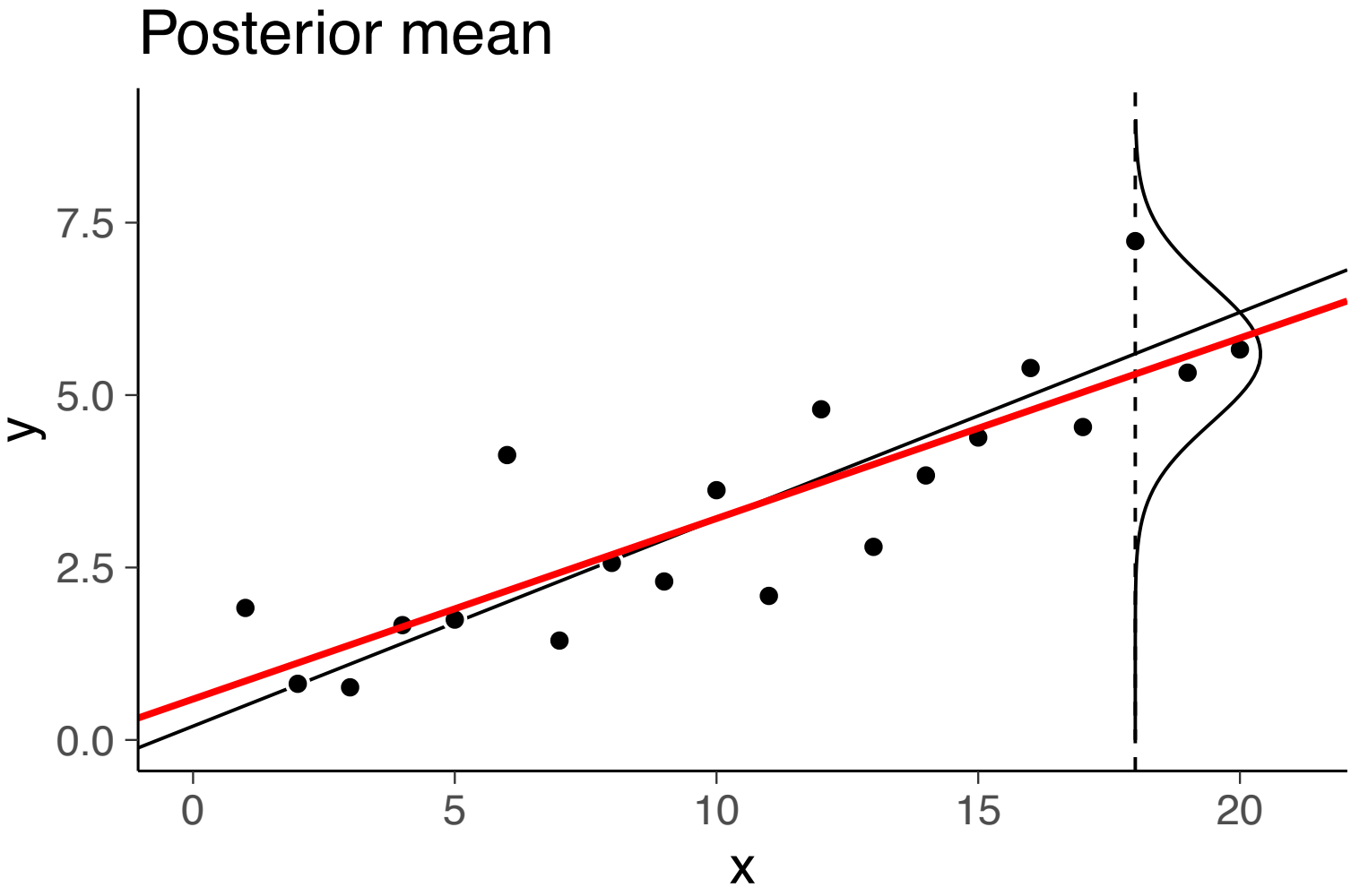
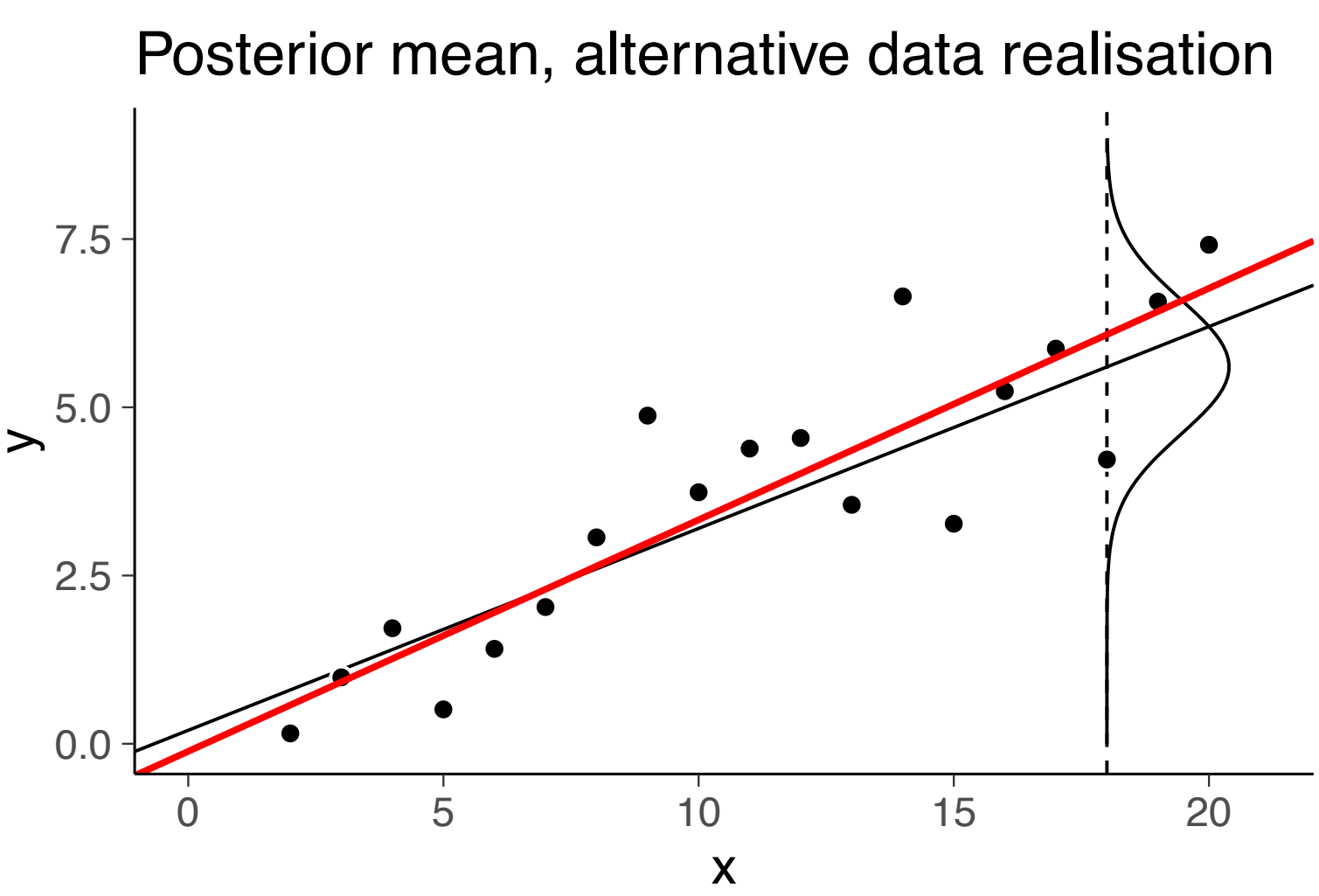
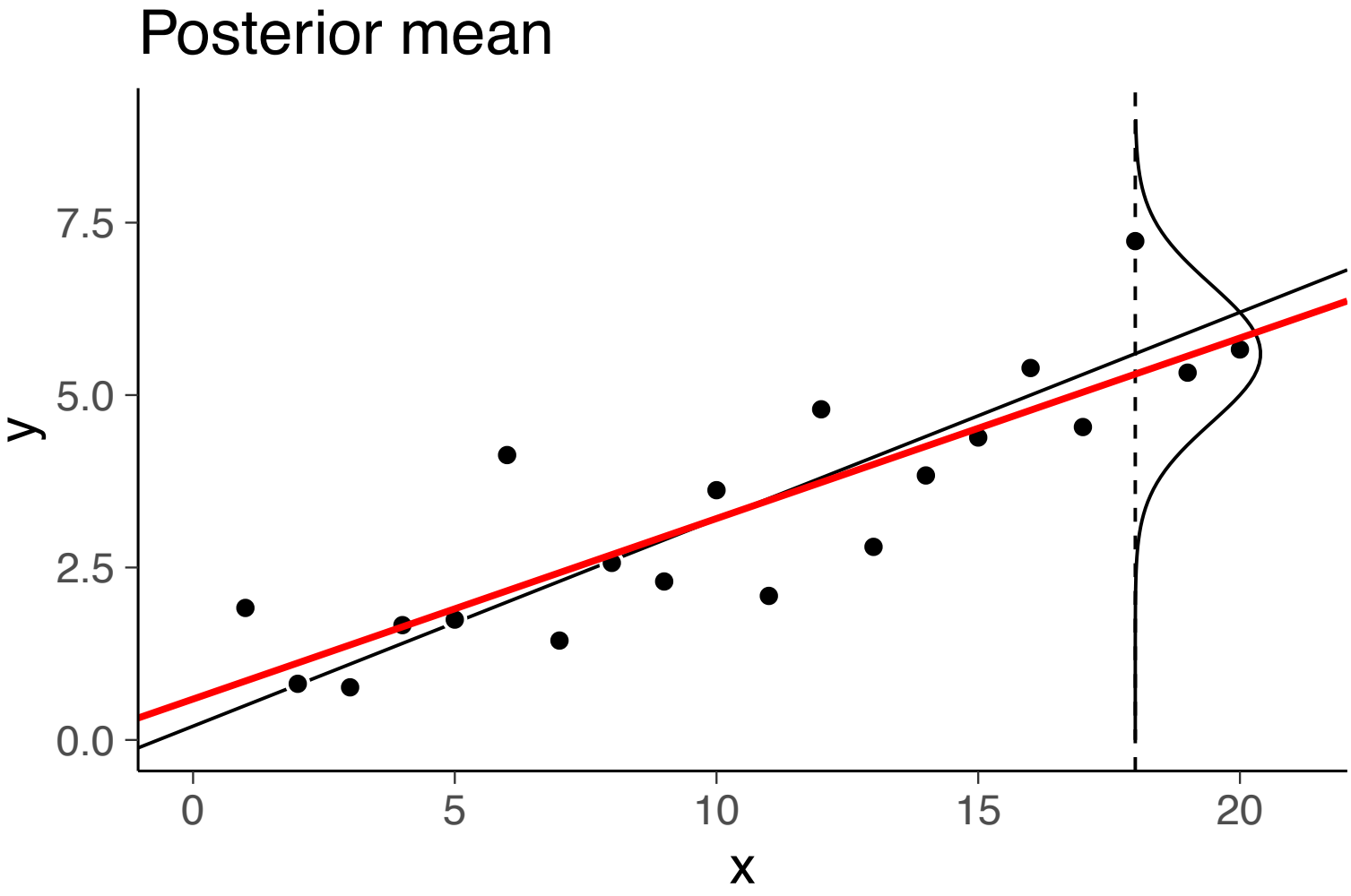
10
15
20
x


Posterior mean
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


Posterior mean, alternative data realisation
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


Posterior mean
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5.0
2.5
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y
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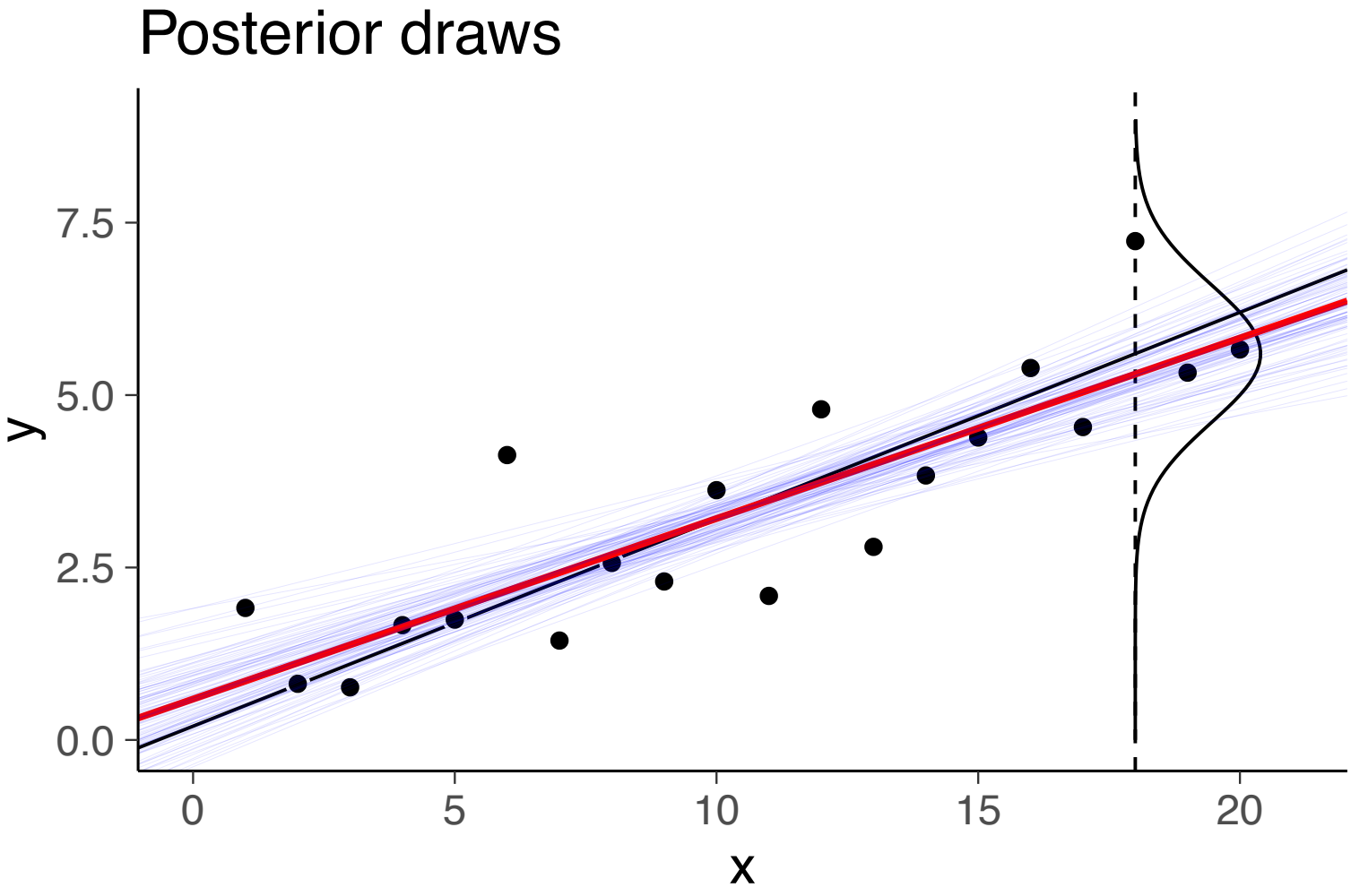
10
15
20
x


Posterior draws
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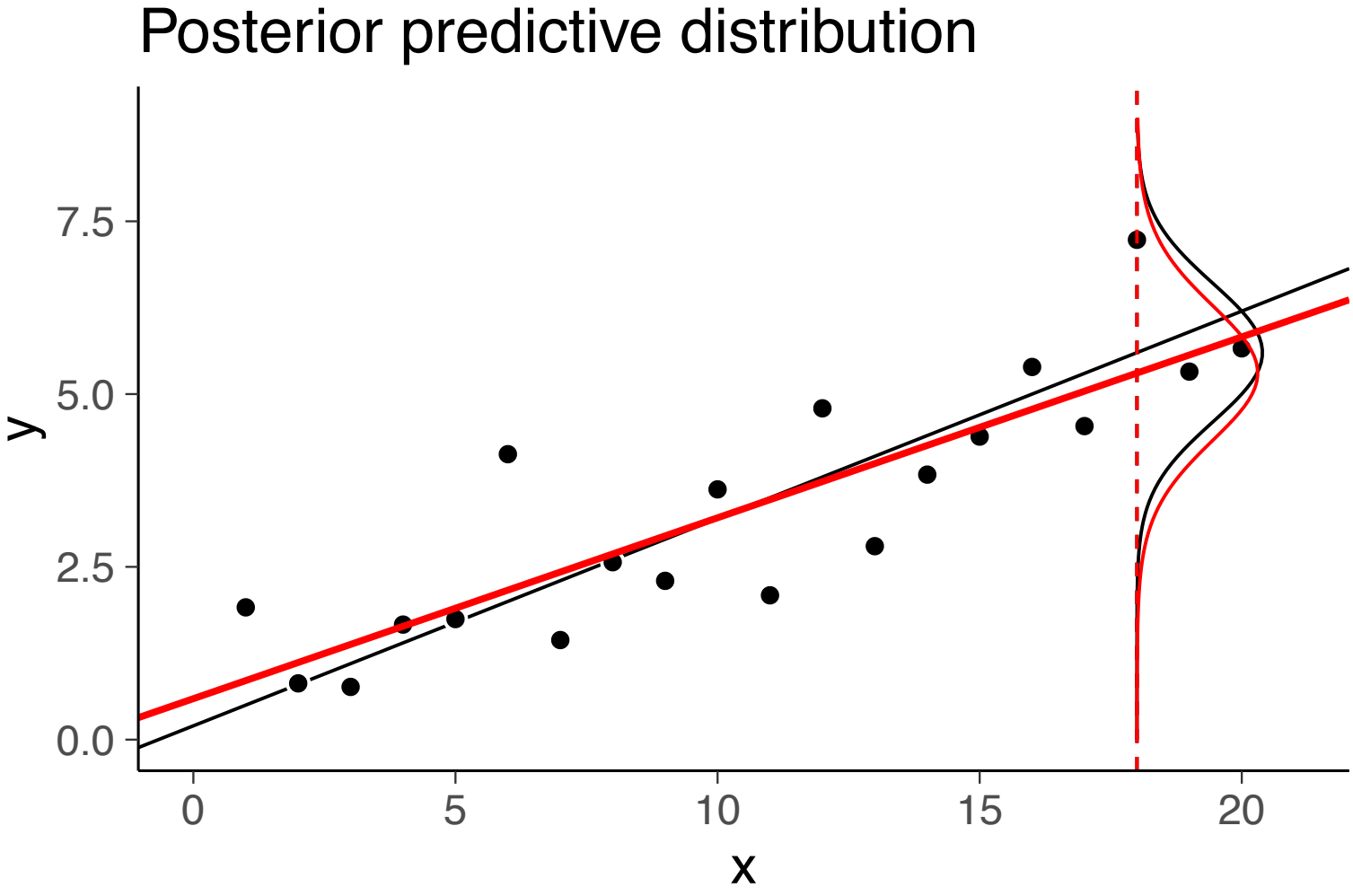
Posterior predictive distribution
7.5
5.0
2.5
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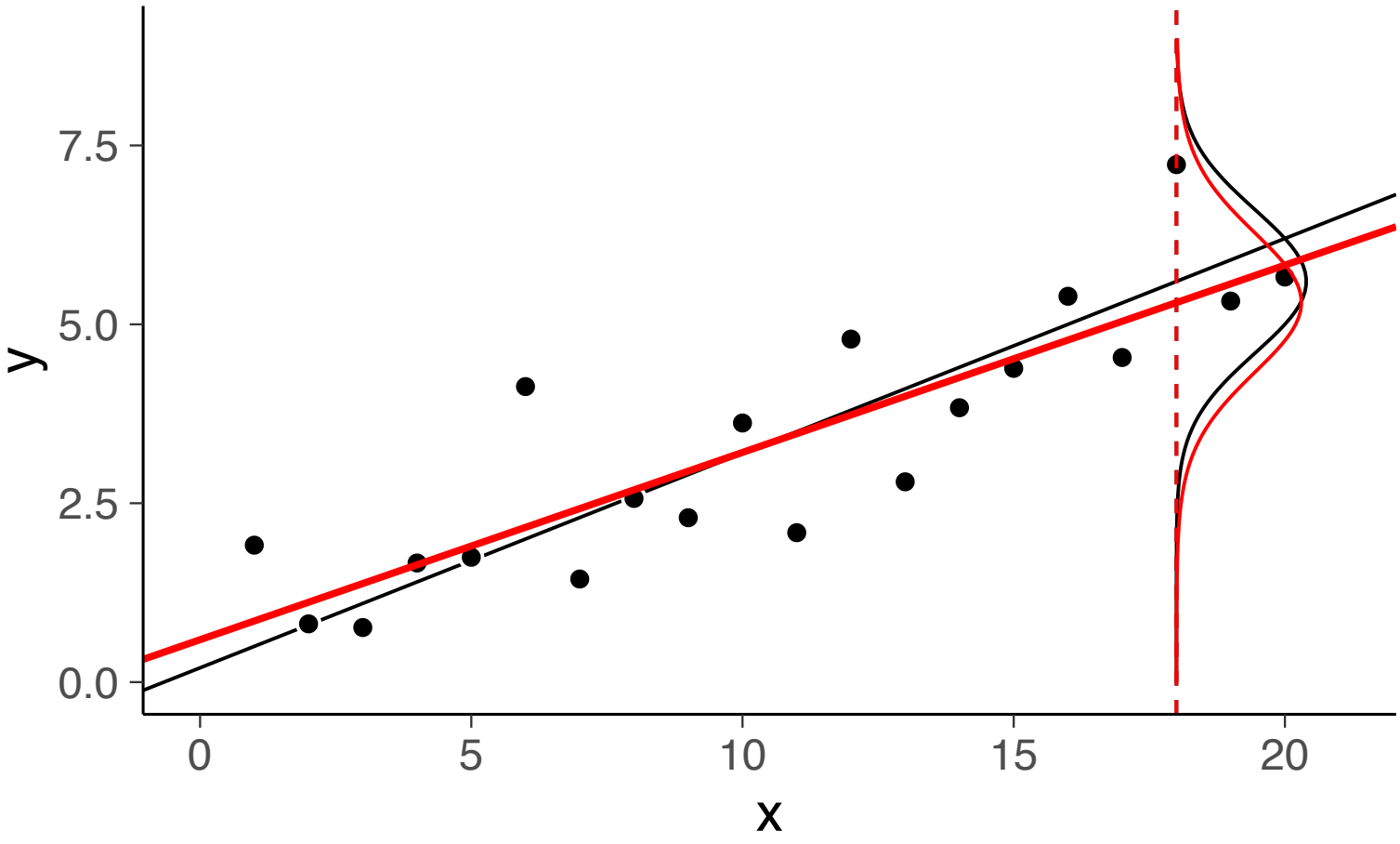
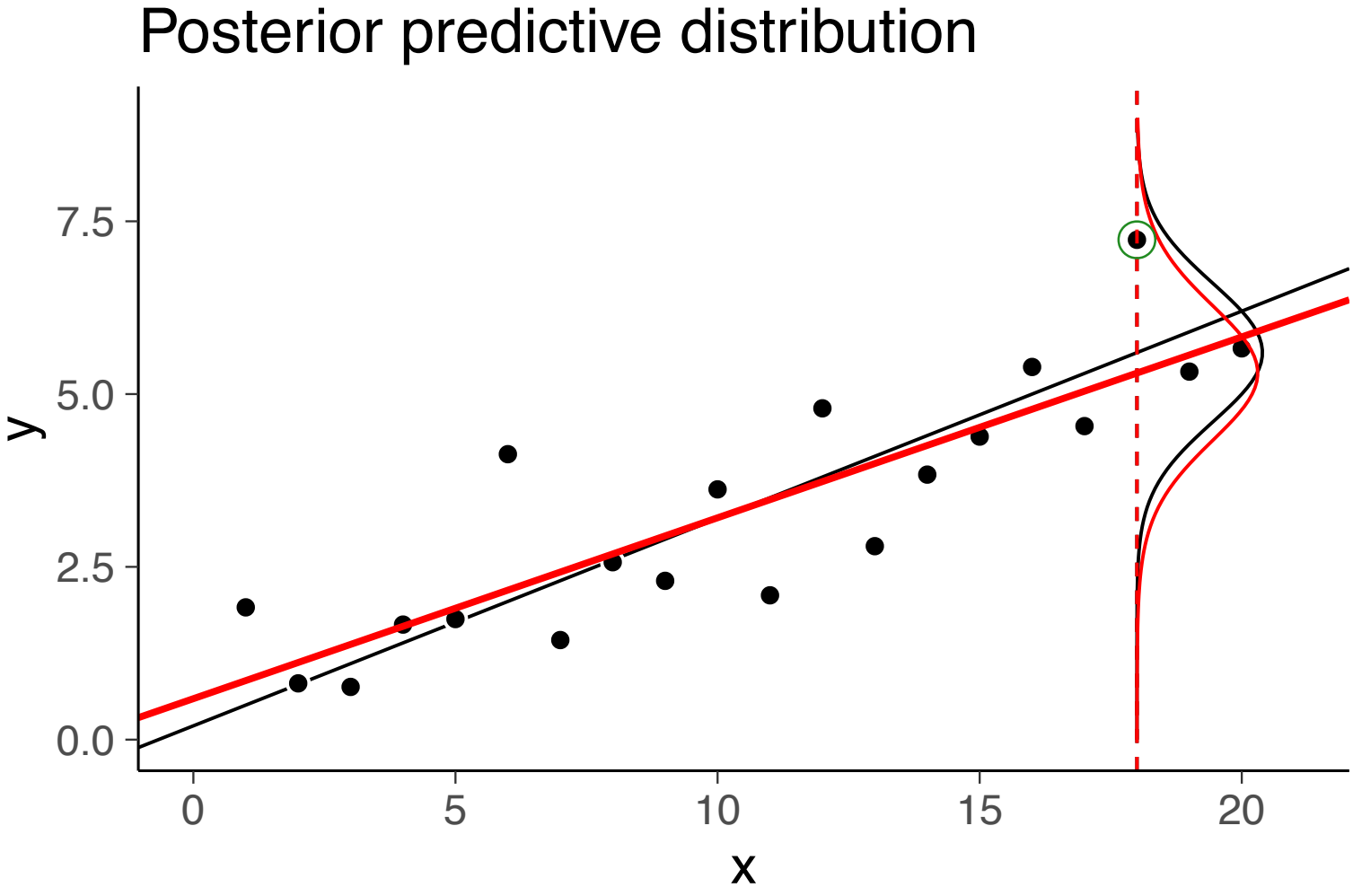
Posterior predictive distribution



$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta) p(\theta|x, y) d\theta$$


Posterior predictive distribution
7.5
5.0
2.5
0.0
y
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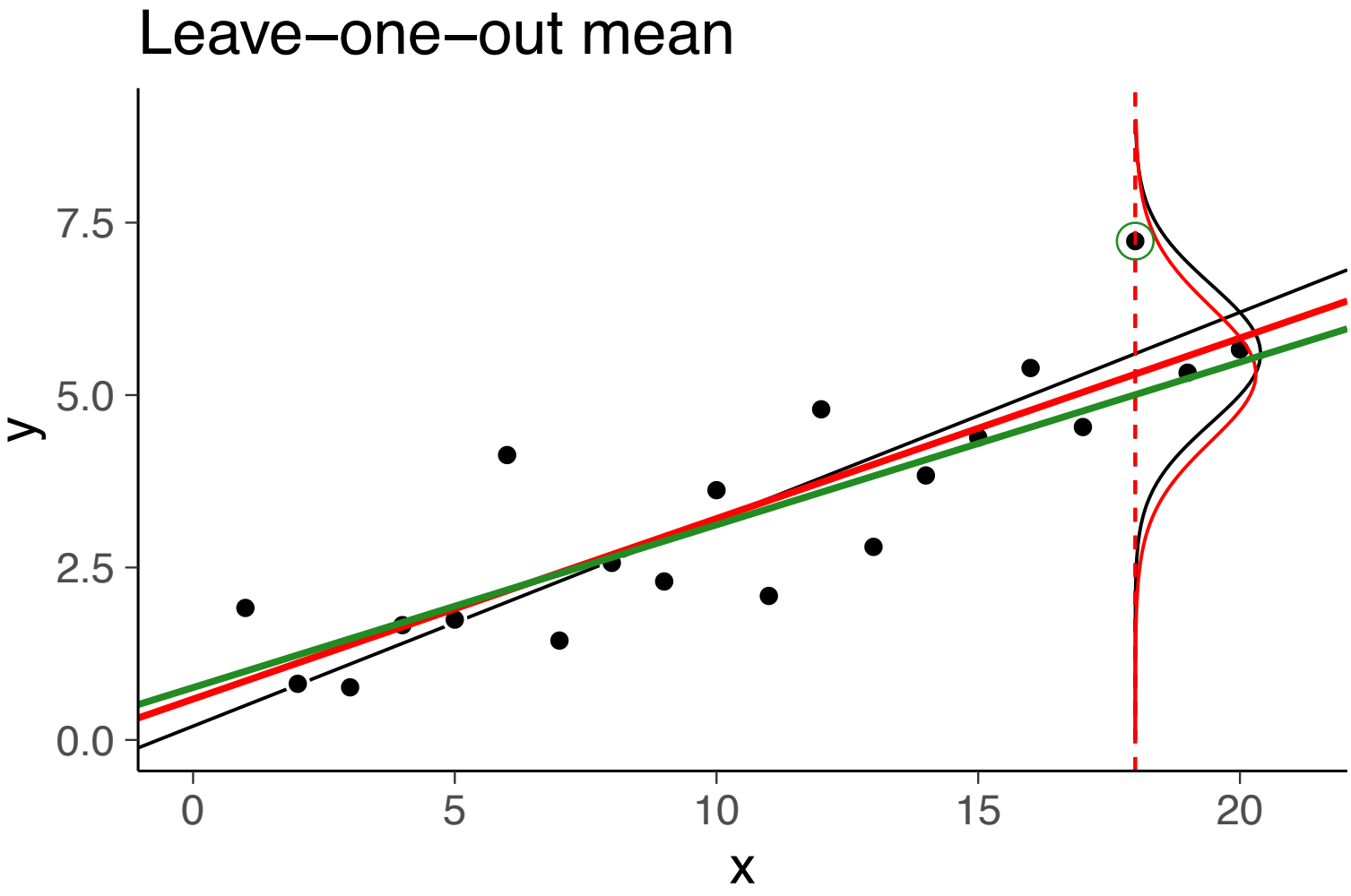
15
20
x


Leave–one–out mean
7.5
5.0
2.5
0.0
y
0
5
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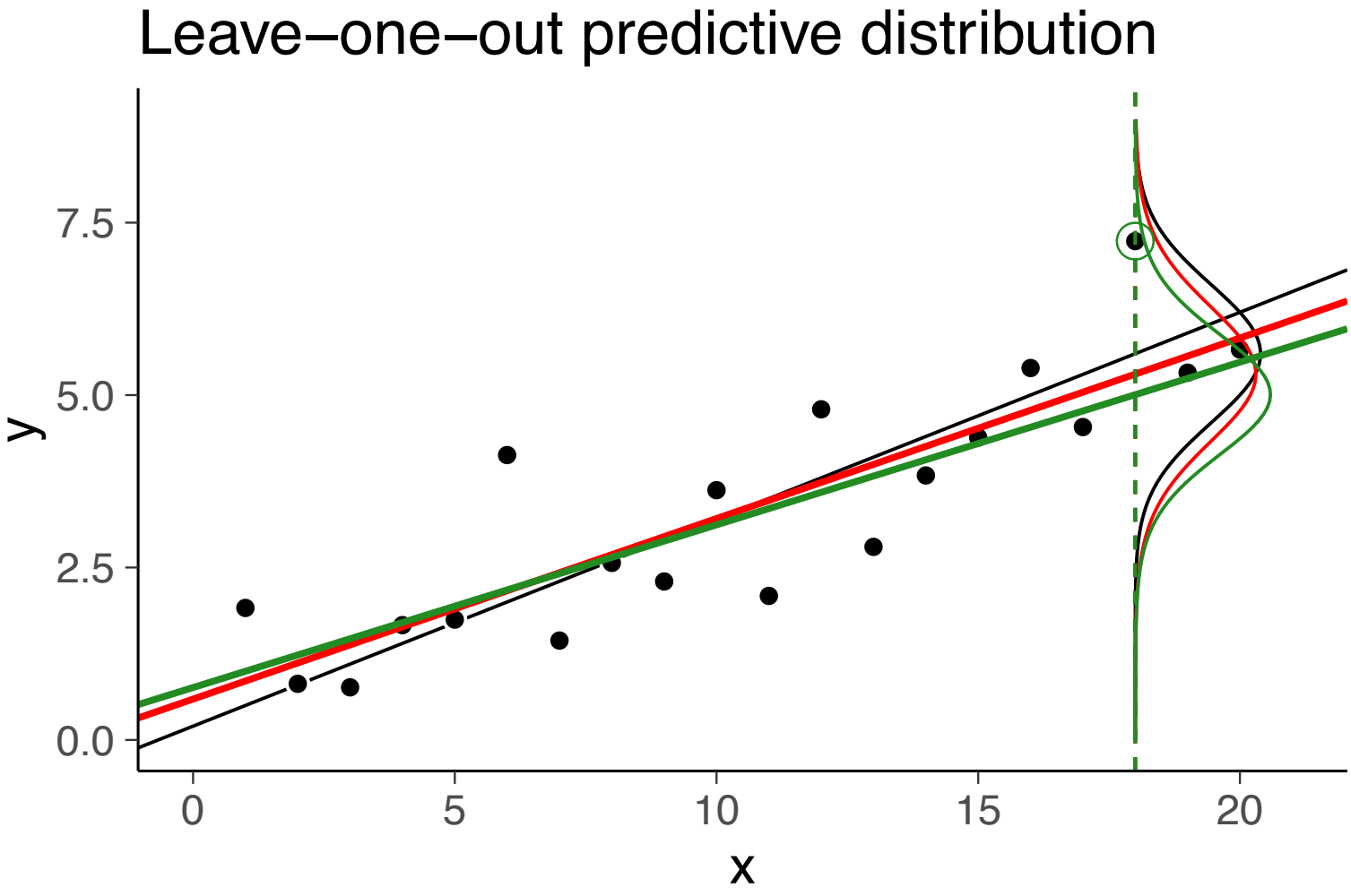
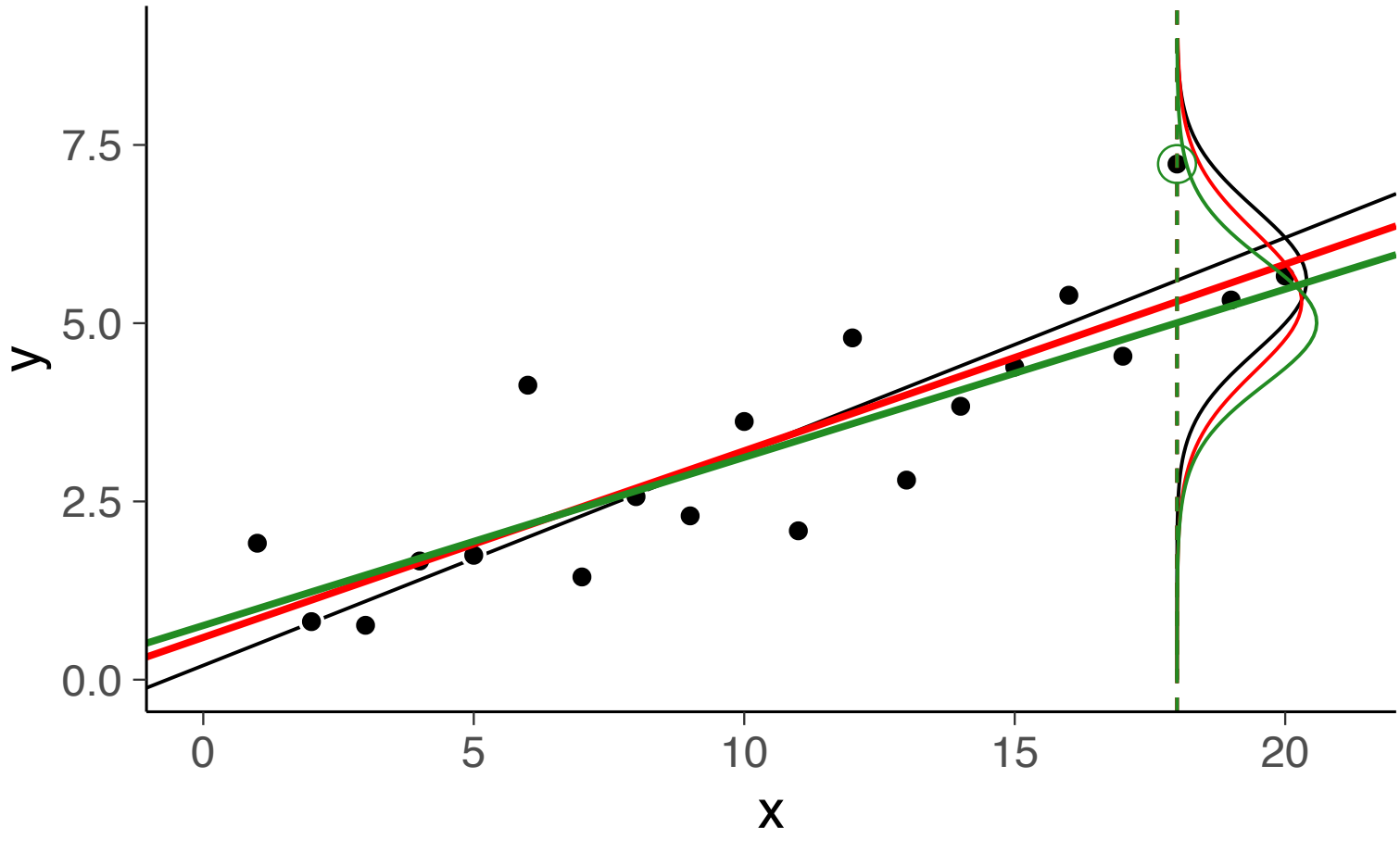
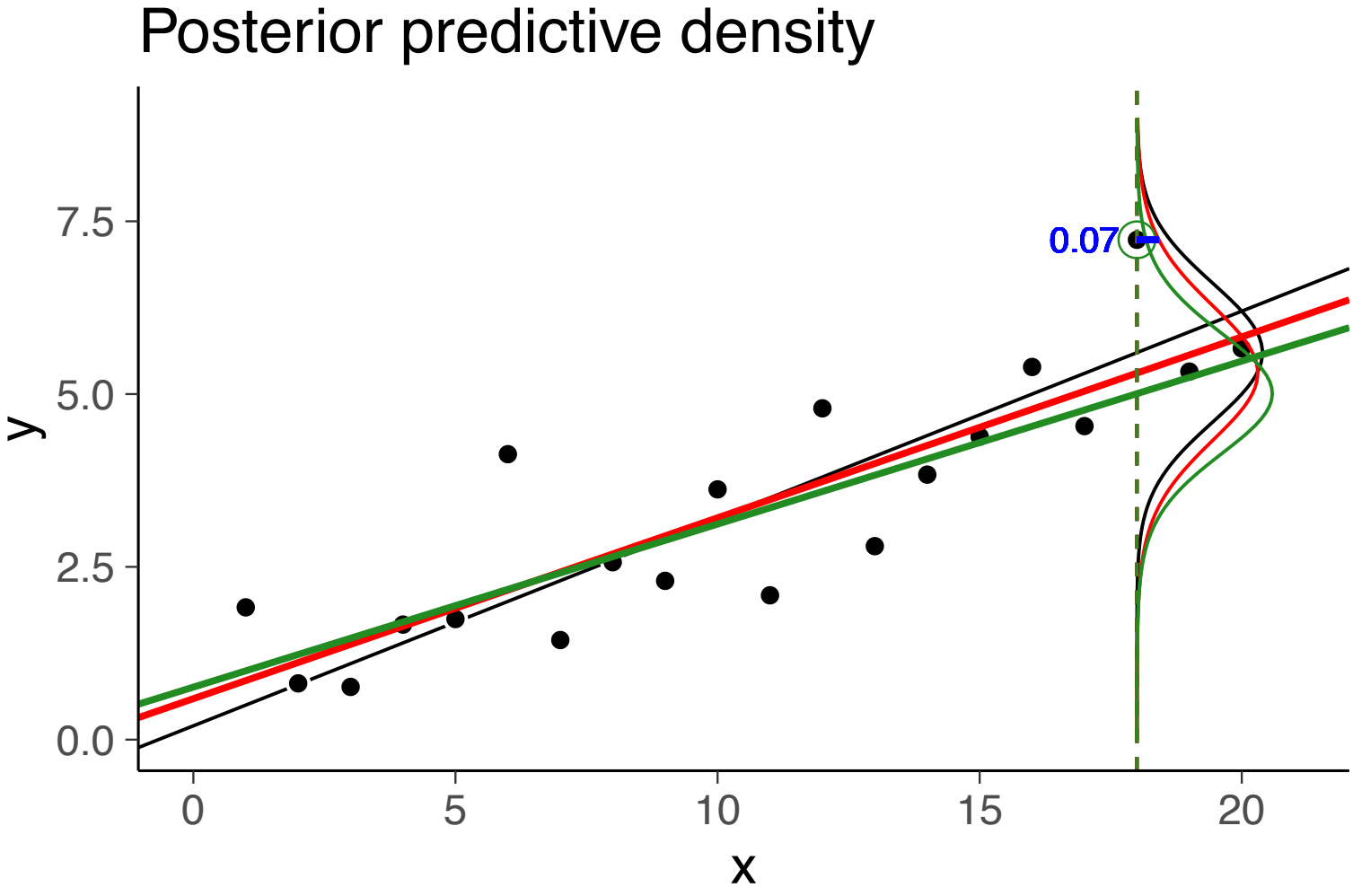
x


Leave–one–out predictive distribution
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

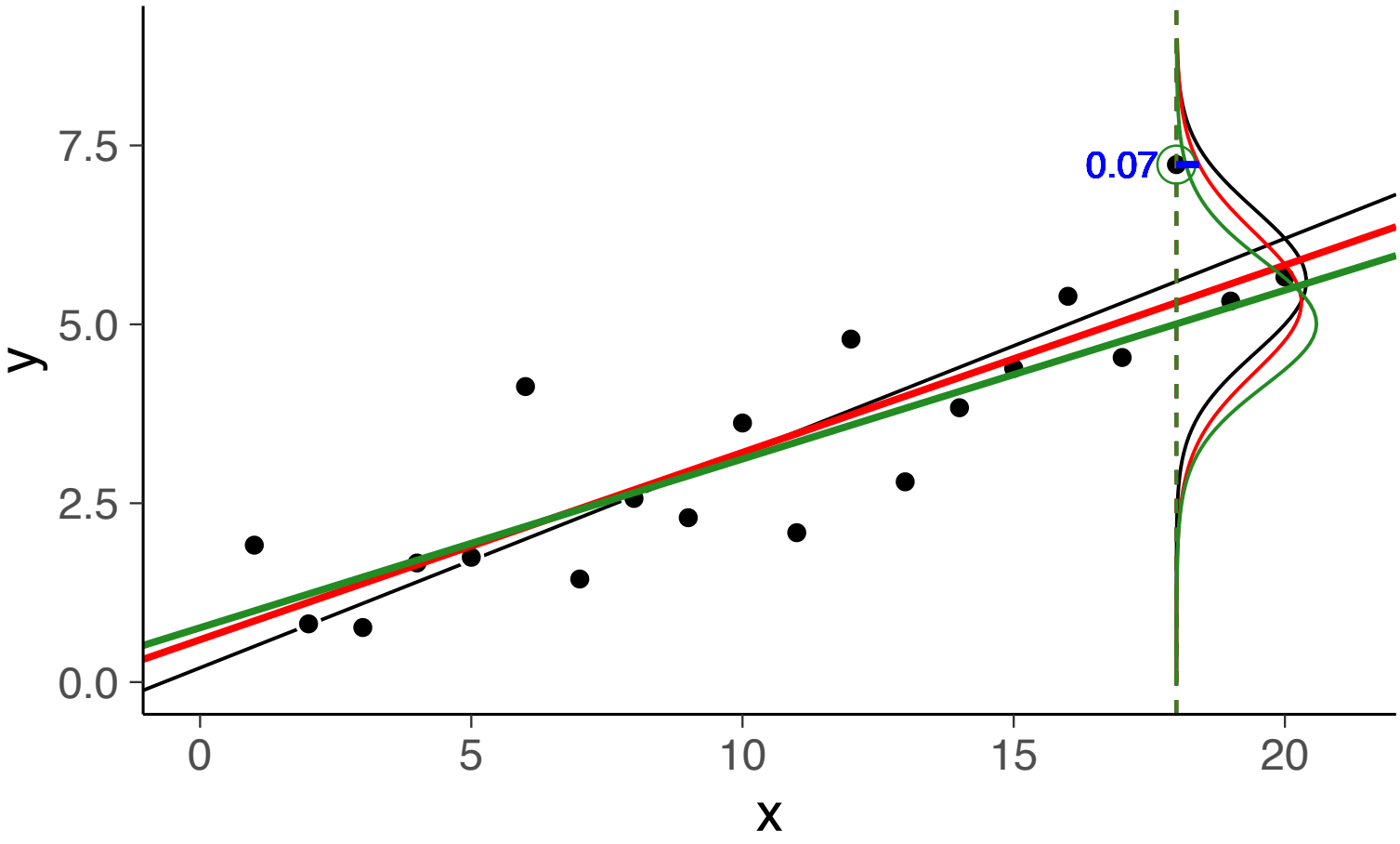
Leave–one–out predictive distribution



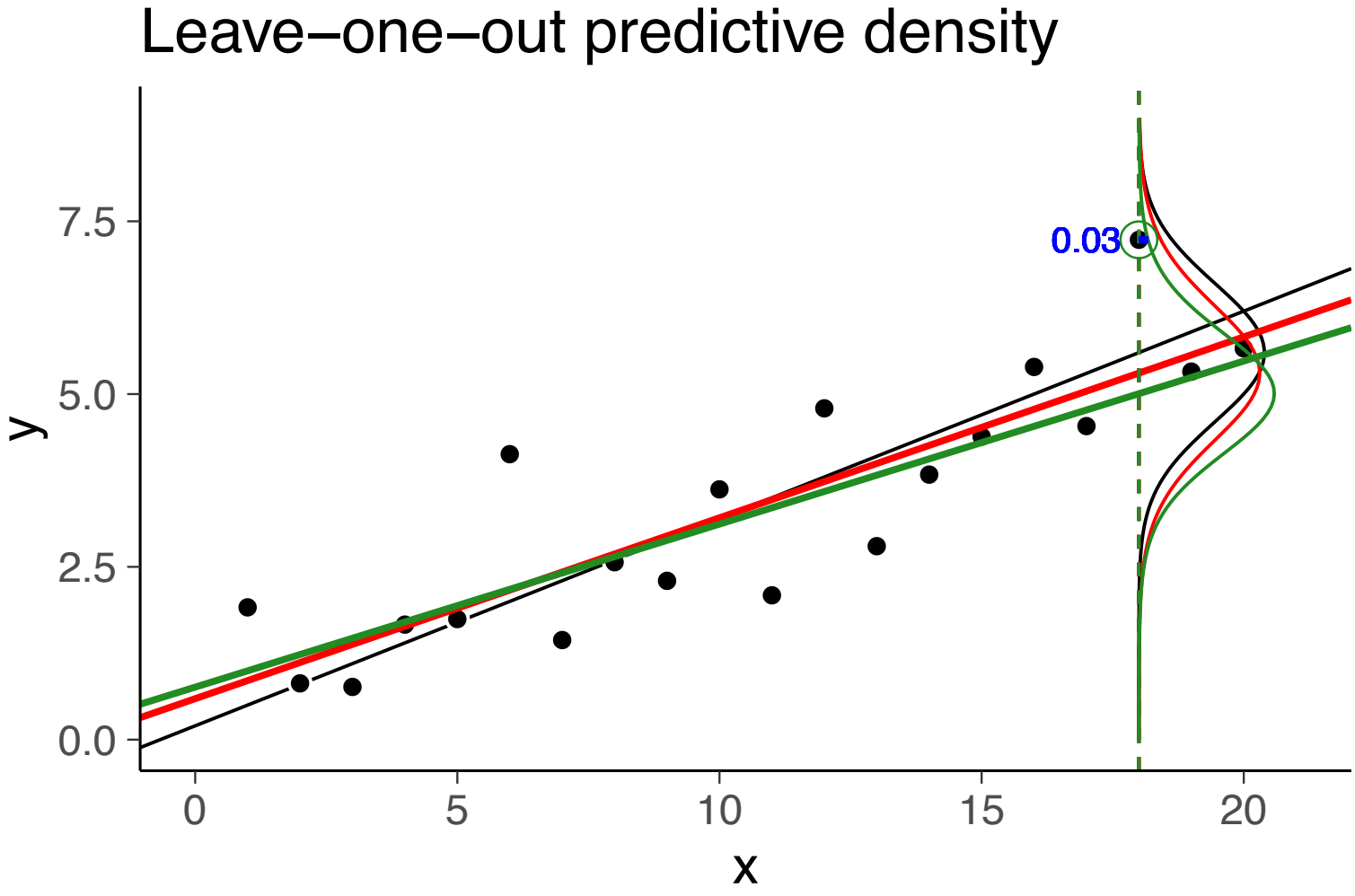
$$p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x} = 18, \theta) p(\theta|x_{-18}, y_{-18}) d\theta$$


Posterior predictive density
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x
0.07

Posterior predictive density



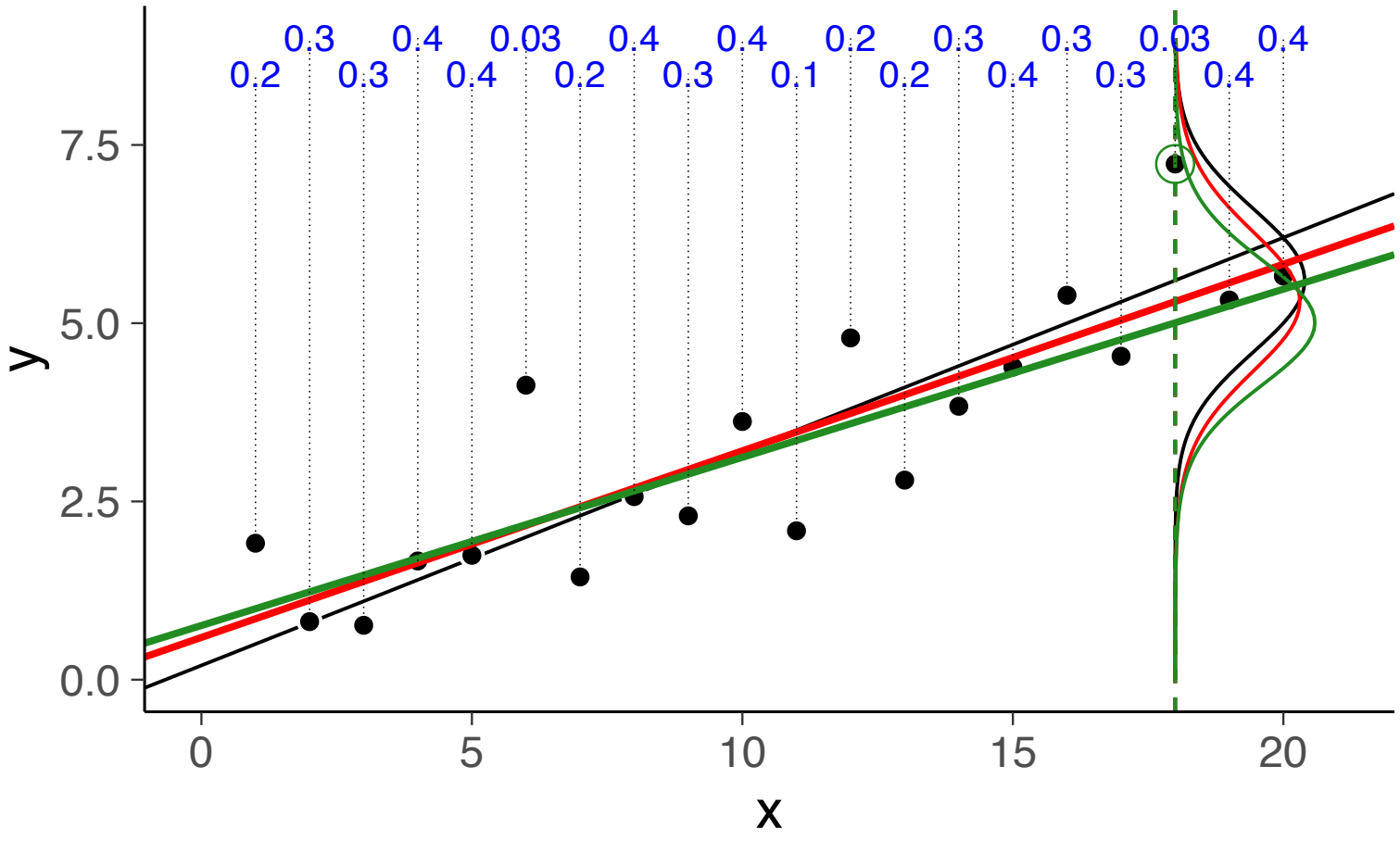
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$



$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$

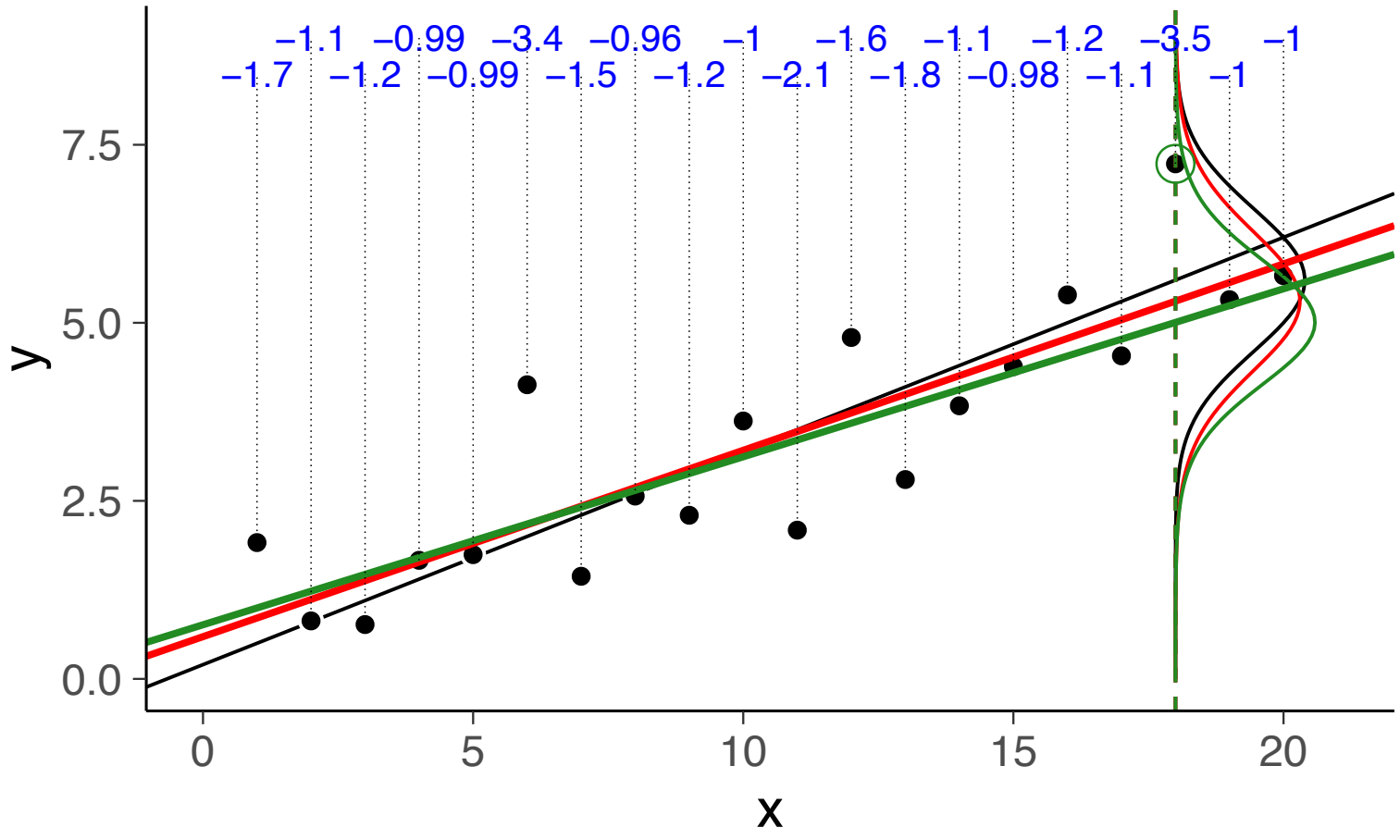
$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$

Leave–one–out predictive densities



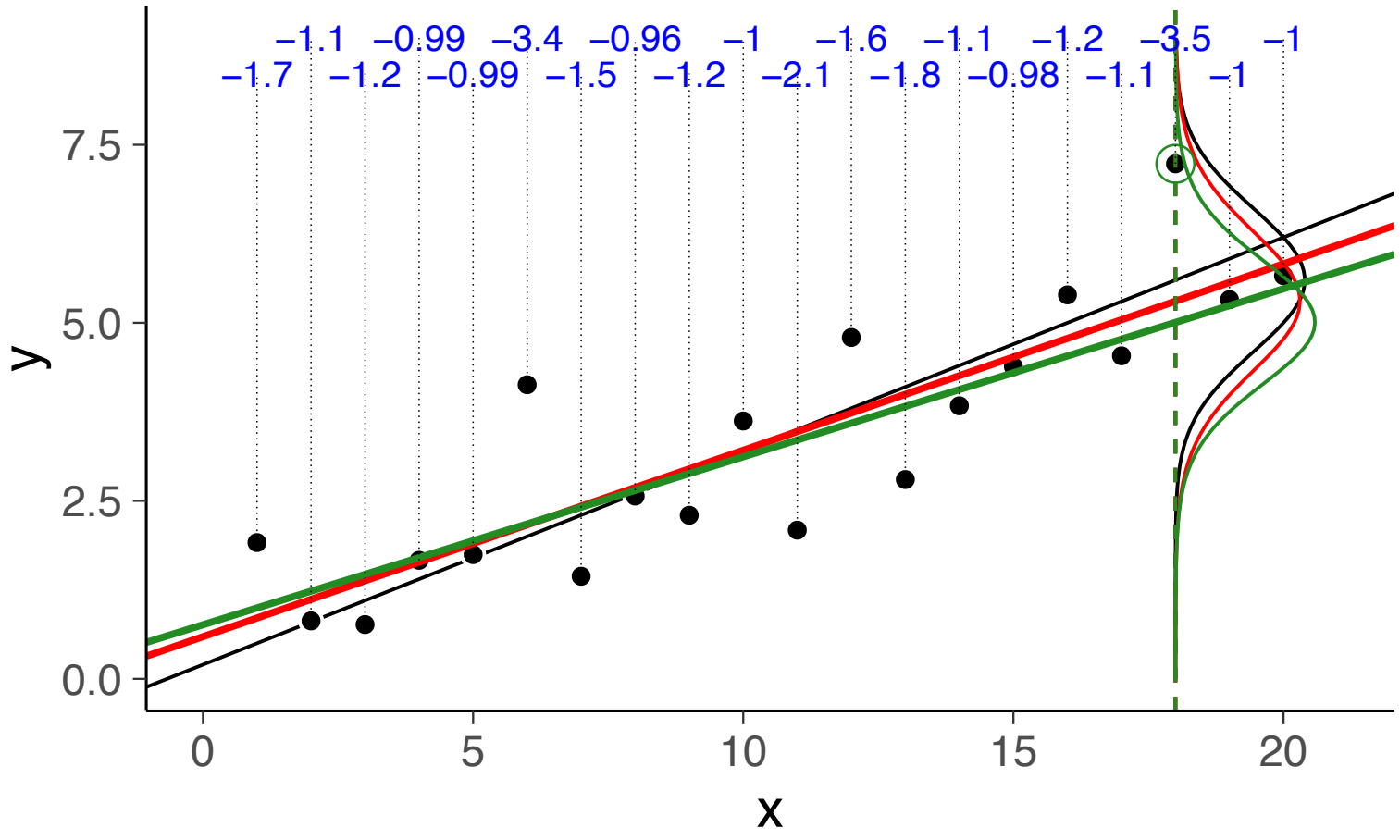
$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave–one–out log predictive densities



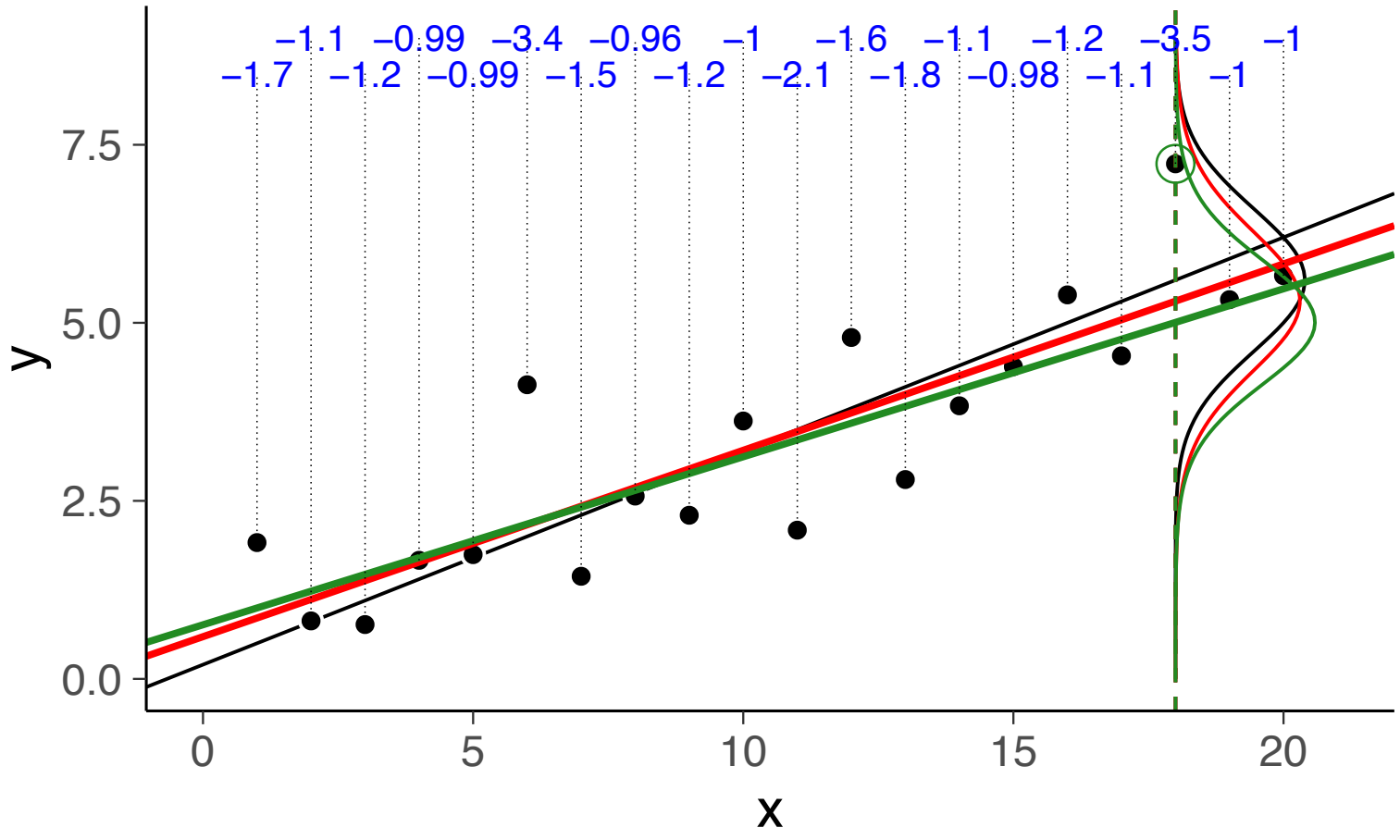
$\log p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave–one–out log predictive densities



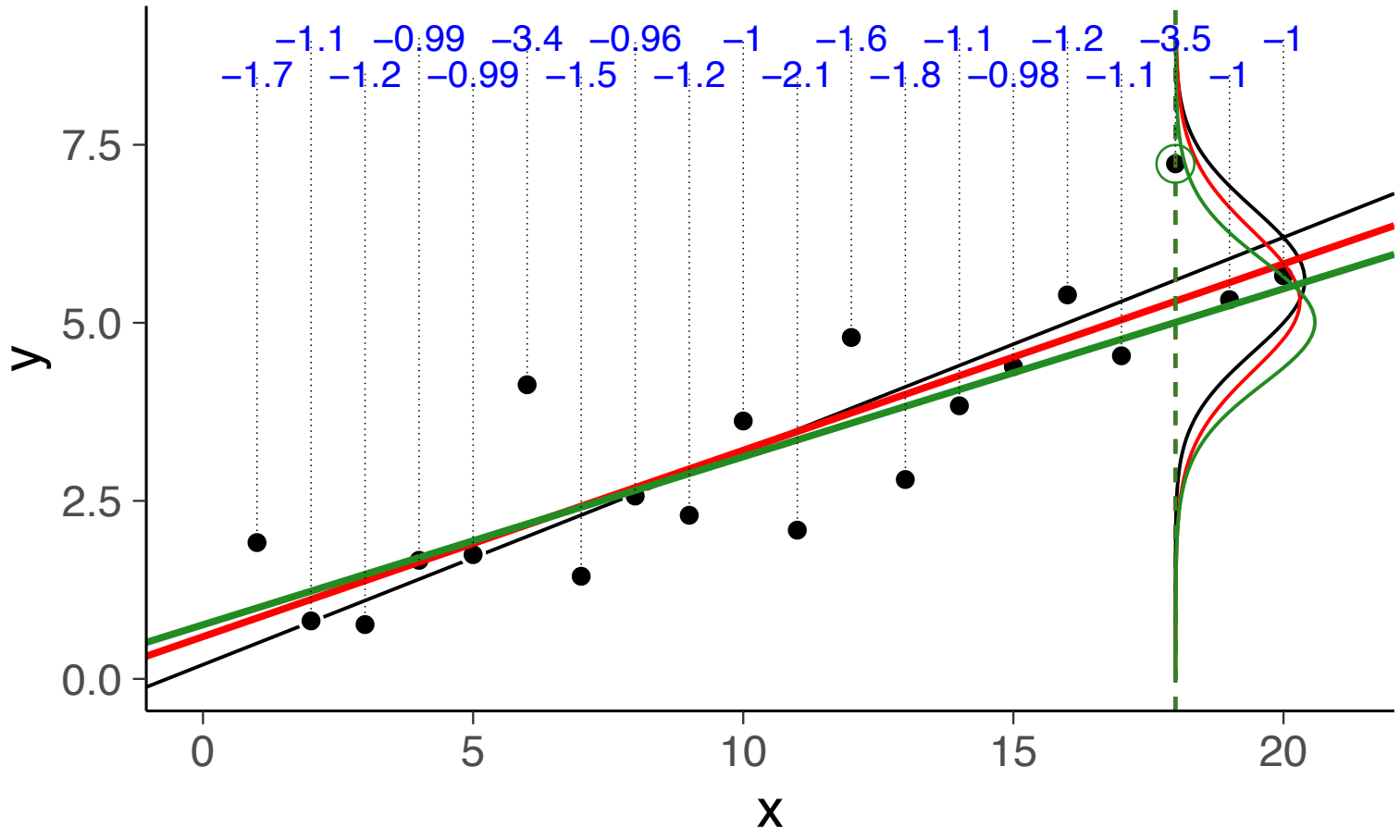
$\sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

Leave–one–out log predictive densities



$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

Leave–one–out log predictive densities



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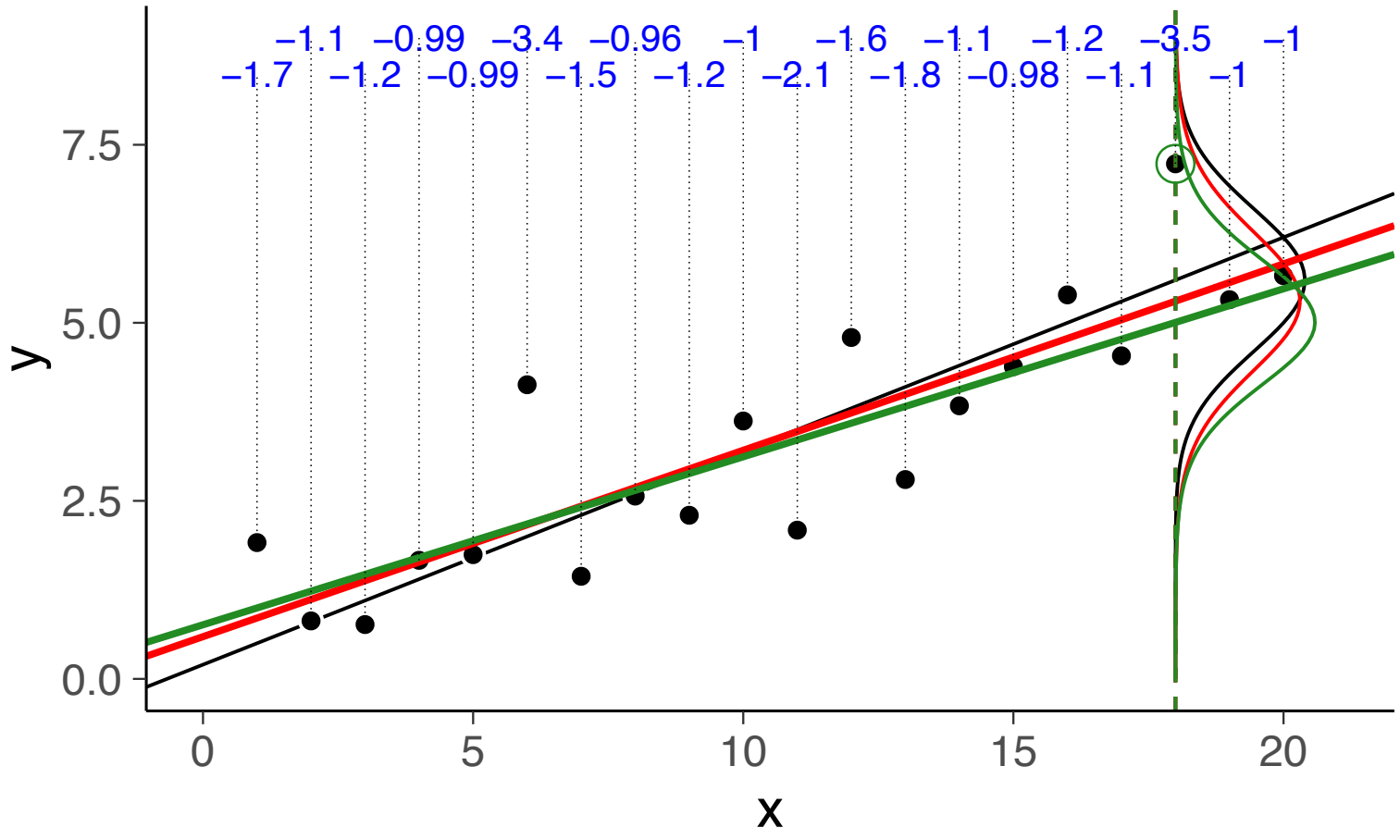
Leave–one–out log predictive densities



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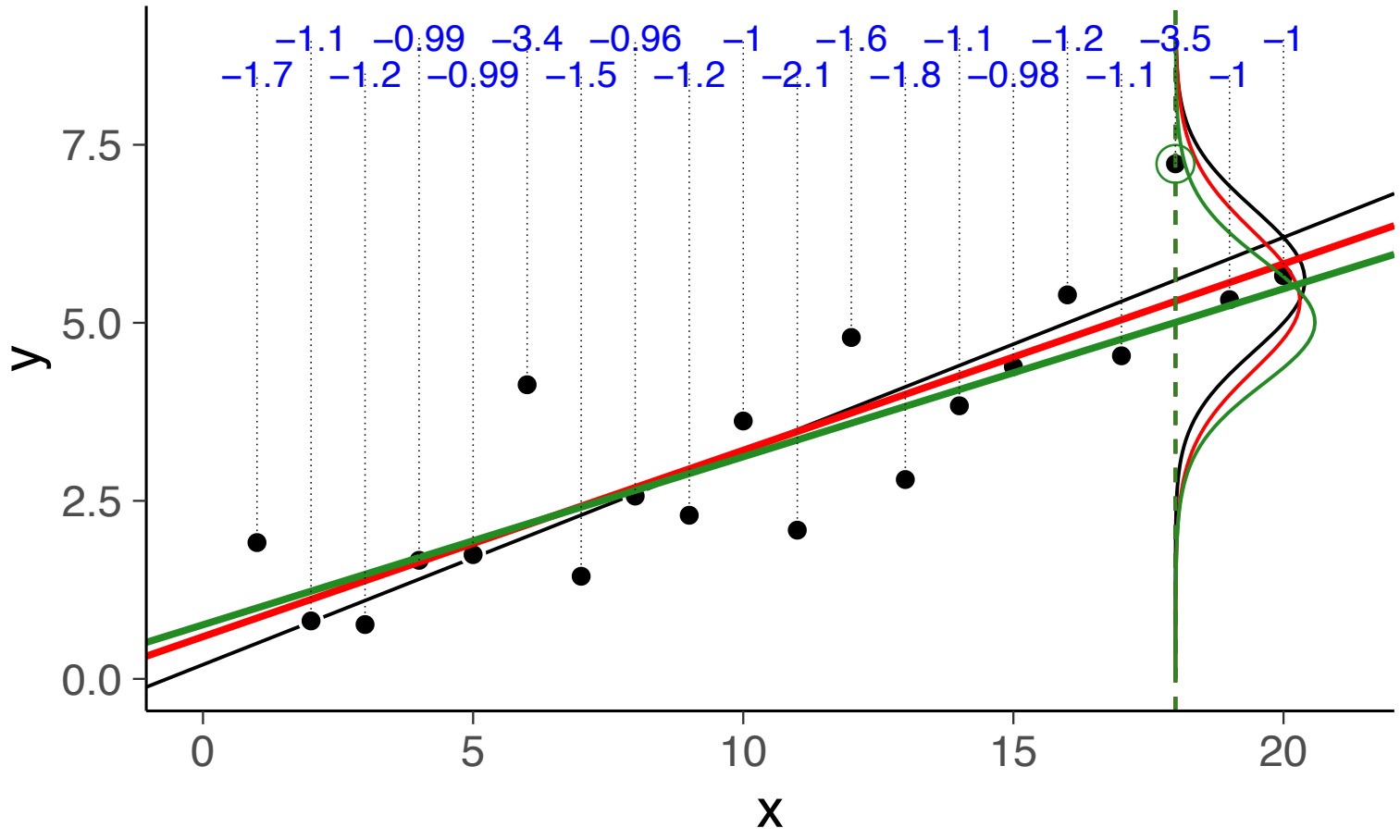
$\text{p\_loo} = \text{lpd} - \text{elpd\_loo} \approx 2.7$

Leave–one–out log predictive densities



$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$

PSIS-LOO

PSIS-LOO

- But we don't generally have infinite time and resources, so want to estimate $p\left(y_i|\boldsymbol{y}_{-i}\right)$.
- PSIS-LOO refers to using Pareto-smoothed importance sampling to do this

Details in Vehtari et al (2017) but broadly...

This IS bit

Estimating properties of one distribution using samples from another distribution.

We want to know about the LOO predictive distribution

$$p\left(y_i|\boldsymbol{y}_{-i}\right) = \int p\left(y_i|\theta\right) p\left(\theta|y_{-i}\right) d\theta = \int p\left(y_i|\theta\right) \frac{p\left(\theta|y_{-i}\right)}{p\left(\theta|y\right)} p\left(\theta|y\right) d\theta$$

We can evaluate above with draws from the full posterior and using importance ratios

$$r_i^s = \frac{1}{p\left(y_i|\theta^s\right)} \propto \frac{p\left(\theta^s|y_{-i}\right)}{p\left(\theta^s|y\right)}$$

which implies

$$p\left(y_i|y_{-i}\right) \approx \frac{\sum_{s=1}^{S} r_i^s p\left(y_i|\theta^s\right)}{\sum_{s=1}^{S} r_i^s}$$

The PS bit

- The direct use of the importance ratios/weights can lead to instability because the ratios can have high or infinite variance.
- To get around this, weights are smoothed by fitting a generalized Pareto distribution to the upper tail (largest 20%) of the importance weights.
- With new weights w_i^s we can calculate the PSIS estimate of the LOO expected log pointwise predictive density

$$\widehat{\text{elpd}}_{\text{psis}-\text{loo}} = \sum_{i=1}^{n} \log \left(\frac{\sum_{s=1}^{S} w_i^s p\left(y_i|\theta^s\right)}{\sum_{s=1}^{S} w_i^s} \right)$$

- Vehtari et al 2017 show that PSIS performs better than other existing methods, and they provide a check to see if the result is reliable or whether you should obtain $p\left(y_i|\boldsymbol{y}_{-i}\right)$ by fitting the model to $\boldsymbol{y}_{-i}$ instead.

An added bonus

The generalized Pareto distribution has the form

$$p(z) = \frac{1}{\sigma}(1 + kz)^{-1/k-1}$$

- The key parameter here is k, which controls how many moments the tail distribution has
- If the estimate of k is large, there are more outlying weights, and the LOO predictive distribution for point i is very different from the full predictive distribution
- So point i is 'influential' in some sense.
- $\hat{k}$ is larger than 0.7 then
  - point is flagged as influential
  - PSIS-LOO approximation of $p\left(y_i|\boldsymbol{y}_{-i}\right)$ may not be very good, it is recommended to get $p\left(y_i|\boldsymbol{y}_{-i}\right)$ directly

PSIS-LOO in R

- This is what the `loo` package in R uses
- In practice, what do we need from the model?

```
model {
  // Log-likelihood
  target += normal_lpdf(log_weight | beta0 + beta1 * log_gest, sigma);

  // Log-priors
  target += normal_lpdf(sigma | 0, 1)
          + normal_lpdf(beta0 | 0, 1)
          + normal_lpdf(beta1 | 0, 1);
}
generated quantities {
  vector[N] log_lik;    // pointwise log-likelihood for LOO
  vector[N] log_weight_rep; // replications from posterior predictive dist

  for (n in 1:N) {
    real log_weight_hat_n = beta0 + beta1 * log_gest[n];
    log_lik[n] = normal_lpdf(log_weight[n] | log_weight_hat_n, sigma);
    log_weight_rep[n] = normal_rng(log_weight_hat_n, sigma);
  }
}
```

PSIS-LOO in R

```
library(loo)
loglik1 <- as.matrix(mod1, pars = "log_lik")
loglik2 <- as.matrix(mod2, pars = "log_lik")
loo1 <- loo(loglik1, save_psis = TRUE)
loo2 <- loo(loglik2, save_psis = TRUE)
loo2
```

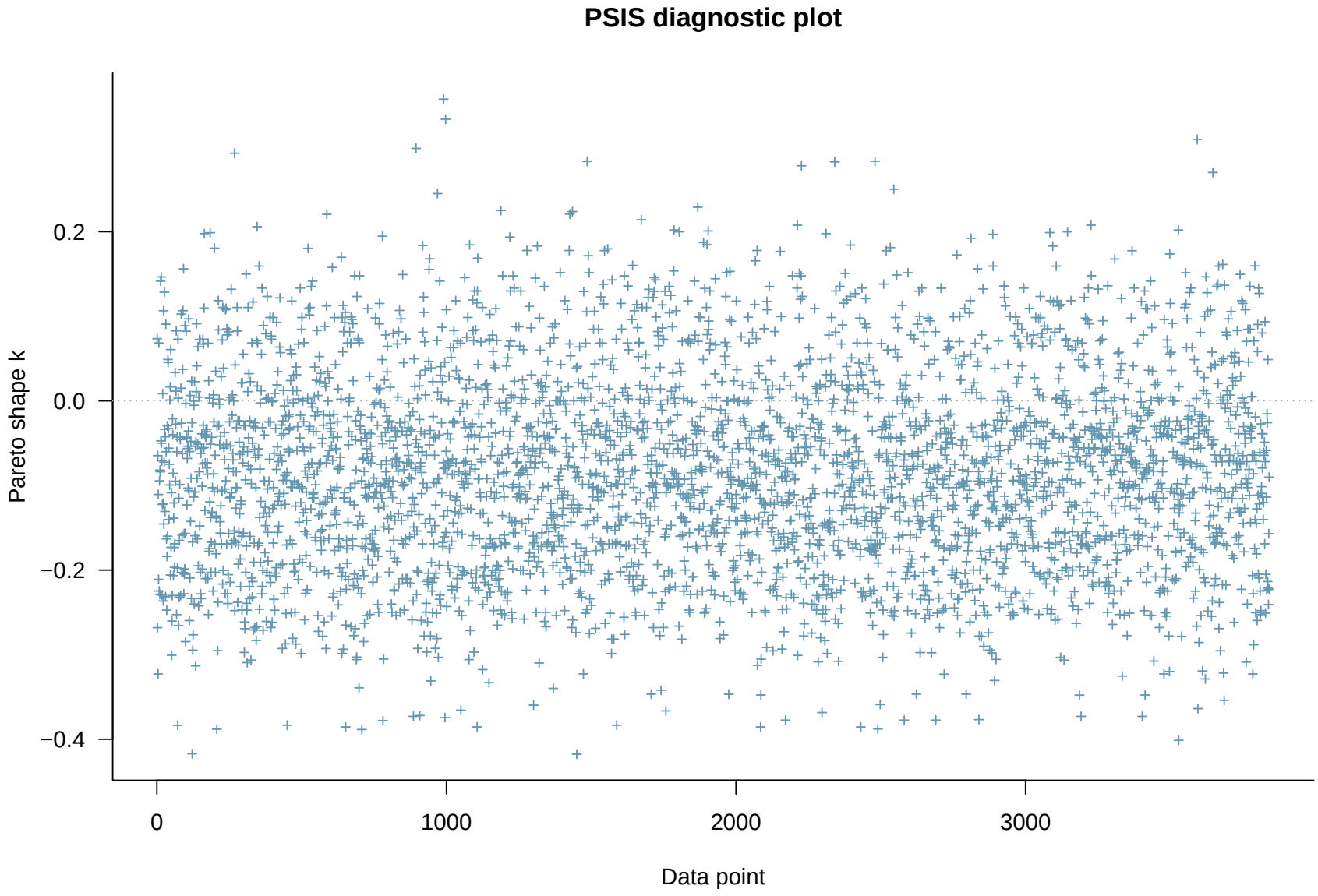
```
##
## Computed from 500 by 3842 log-likelihood matrix
##
##          Estimate    SE
## elpd_loo   1552.8  70.0
## p_loo        14.8   2.3
## looic     -3105.6 139.9
## ------
## Monte Carlo SE of elpd_loo is 0.2.
##
## All Pareto k estimates are good (k < 0.5).
## See help('pareto-k-diagnostic') for details.
```

Compare

```
loo_compare(loo1, loo2)
```

```
##        elpd_diff se_diff
## model2    0.0       0.0
## model1 -175.3      36.0
```

Plot k values: Model 2

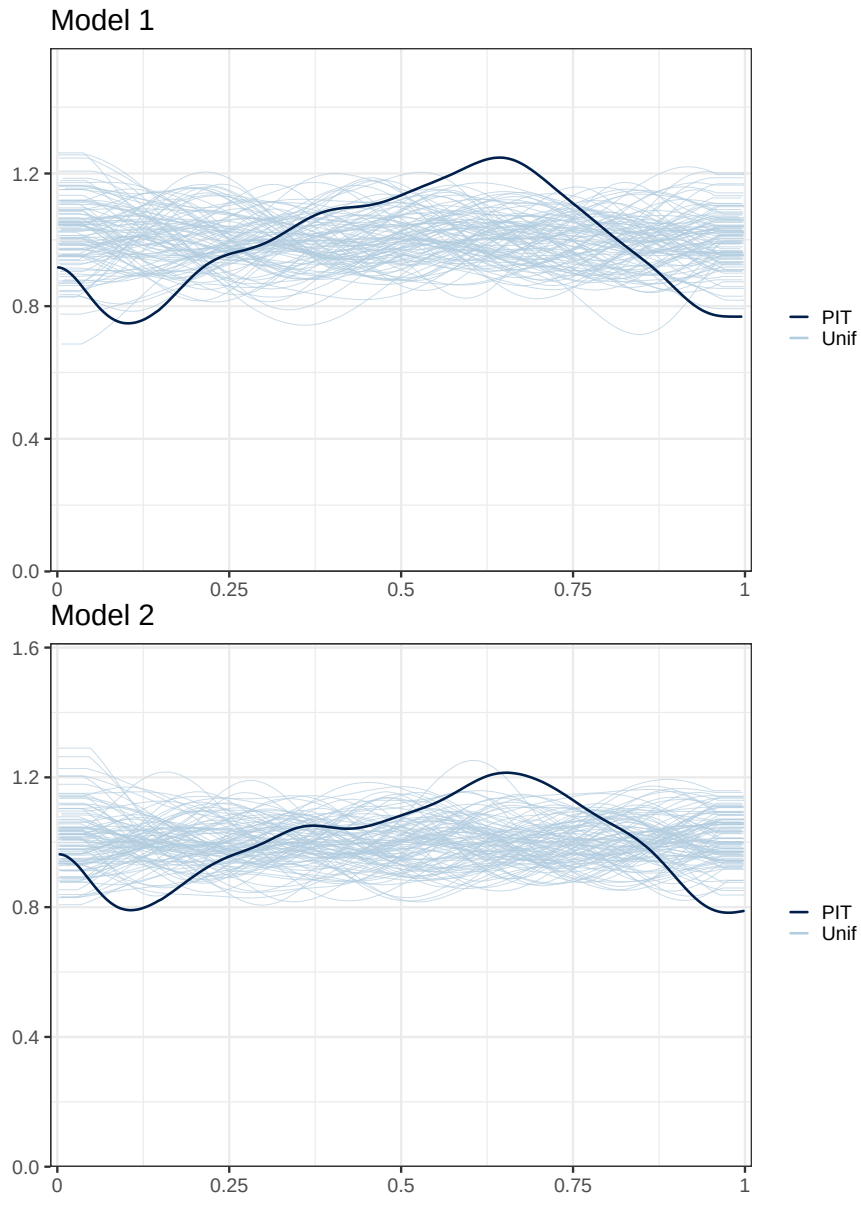


All outliers are extremely preterm.

LOO probability integral transform (PIT)

- LOO-PIT$_i = P\left(\tilde{y}_i \leq y_i | \boldsymbol{y}_{-i}\right)$ i.e. where does y_i fall in its LOO predictive distribution
- If $y_i \sim p\left(\tilde{y}_i | \boldsymbol{y}_{-i}\right)$ then LOO-PIT$_i \sim U(0, 1)$
- So can compare PITs to uniforms

LOO probability integral transform (PIT)



Briefly: Information Criteria

- You are probably used to seeing the Akaike Information Criterion to compare models, $AIC = -2\log(p(\boldsymbol{y}|\widehat{\boldsymbol{\theta}(\boldsymbol{y})})) + 2 \cdot k$ where k is the number of parameters and $\widehat{\boldsymbol{\theta}(\boldsymbol{y})}$ is the MLE.
- Bayesian setting requires estimation of an 'effective number of parameters' to replace k that takes prior info into account
- E.g. Widely Applicable Information Criterion (WAIC)

$$WAIC = -2\widehat{\text{lpd}} + 2p_{WAIC}$$

Where lpd is the log pointwise predictive density,

$$\text{lpd} = \sum_{i=1}^{n} \log p\left(y_i|y\right) = \sum_{i=1}^{n} \log \int p\left(y_i|\theta\right) p(\theta|y) d\theta$$

estimated as $= \sum_{i=1}^{n} \log \left(\frac{1}{S} \sum_{s=1}^{S} p\left(y_i|\theta^s\right) \right)$ and the effective number of parameters is

$$p_{\text{waic}} = \sum_{i=1}^{n} \text{var}_{\text{post}} \left(\log p\left(y_i|\theta\right)\right)$$

Briefly: Information Criteria

- As for the other criteria, WAIC is the combination of predictive accuracy and a bias adjustment.
- WAIC aims to approximate -2elpd
- Asymptotically closest to Bayesian leave-one-out accuracy
- Veharti et al 2017 shows that PSIS-LOO tends to perform better than WAIC in terms of estimating $\sum_i \log\left(p\left(y_i|\boldsymbol{y}_{-i}\right)\right)$

Briefly: Actually training and testing

Set-up: Fit the model to a training set and validate predictive accuracy of the model for the left-out test data

- Bad: how to split, variable results, computationally intensive
- Good: actual predictions for new data, can be more convincing

May make sense especially with temporal data (neonatal mortality example)

Briefly: Actually training and testing

Measures given by some summary of errors, e.g. relative error

$$e_i = (y_i - \hat{y}_i) / \hat{y}_i$$

- could look at mean error, median error, mean squared error, median absolute error
- could also look at coverage of prediction intervals, % above and below prediction intervals.
- Can still look at PITs

Validation measures, model comparison

	Expected	$\leq$ 2005	$>$ 2005
Mean absolute relative error	–	0.05	0.09
80% coverage	$\geq$ 0.80	0.90	0.77
90% coverage	$\geq$ 0.90	0.94	0.84
95% coverage	$\geq$ 0.95	0.96	0.90

PSIS-LOO: issues in the wild

- If the estimate of k is large, there are more outlying weights, and the LOO predictive distribution for point i is very different from the full predictive distribution
- In data sparse contexts, essentially every point is influential
- So makes more sense to fall back to train/test, out-of-sample validation
- An open question: model validation in data-sparse contexts

Table 2: Top 30 observations with Pareto k > 0.7

source	iso	country	year	ABO	DIR	EMB	HEM	SEP	IND	HYP	MDG	Pareto k	ID
Grey (National)	USA	United States of America	2013	NA	36	84	65	68	150	81	Developed regions	3.1	78
Grey (National)	GTM	Guatemala	2015	20	NA	NA	167	27	106	72	Latin America and Caribbean	1.8	37
Grey (National)	CHN	China	2015	NA	NA	400	888	29	888	488	Eastern Asia	1.5	27
Studies (ADM1 and above)	NGA	Nigeria	2011	2	27	NA	61	28	55	149	Sub-Saharan Africa	1.5	84
Grey (National)	CHN	China	2011	NA	NA	801	1212	NA	648	470	Eastern Asia	1.5	23

Paper: https://arxiv.org/abs/2101.05240

Summary

What are all these things?

- $p(\tilde{y})$
- $p(\tilde{y}|\boldsymbol{y})$
- $p(y_i|\boldsymbol{y})$
- $p(y_i|\boldsymbol{y}_{-i})$
- lpd
- $\widehat{\text{lpd}}$
- elpd_{LOO}
- $\widehat{\text{elpd}}_{PSIS-LOO}$

Summary

General advice for model checking:

Plot, plot, plot

- Check your priors
- PPCs by different groups of interest
- LOO to not only compare models but also to inform model specification (influential points)

Also not discussed today, but plot

- Data and model fit
- residuals, grouped by whatever characteristics of data/predictors you can think of, or a scatter against predictors