Diagnostics and Model Evaluation

Lecture 03

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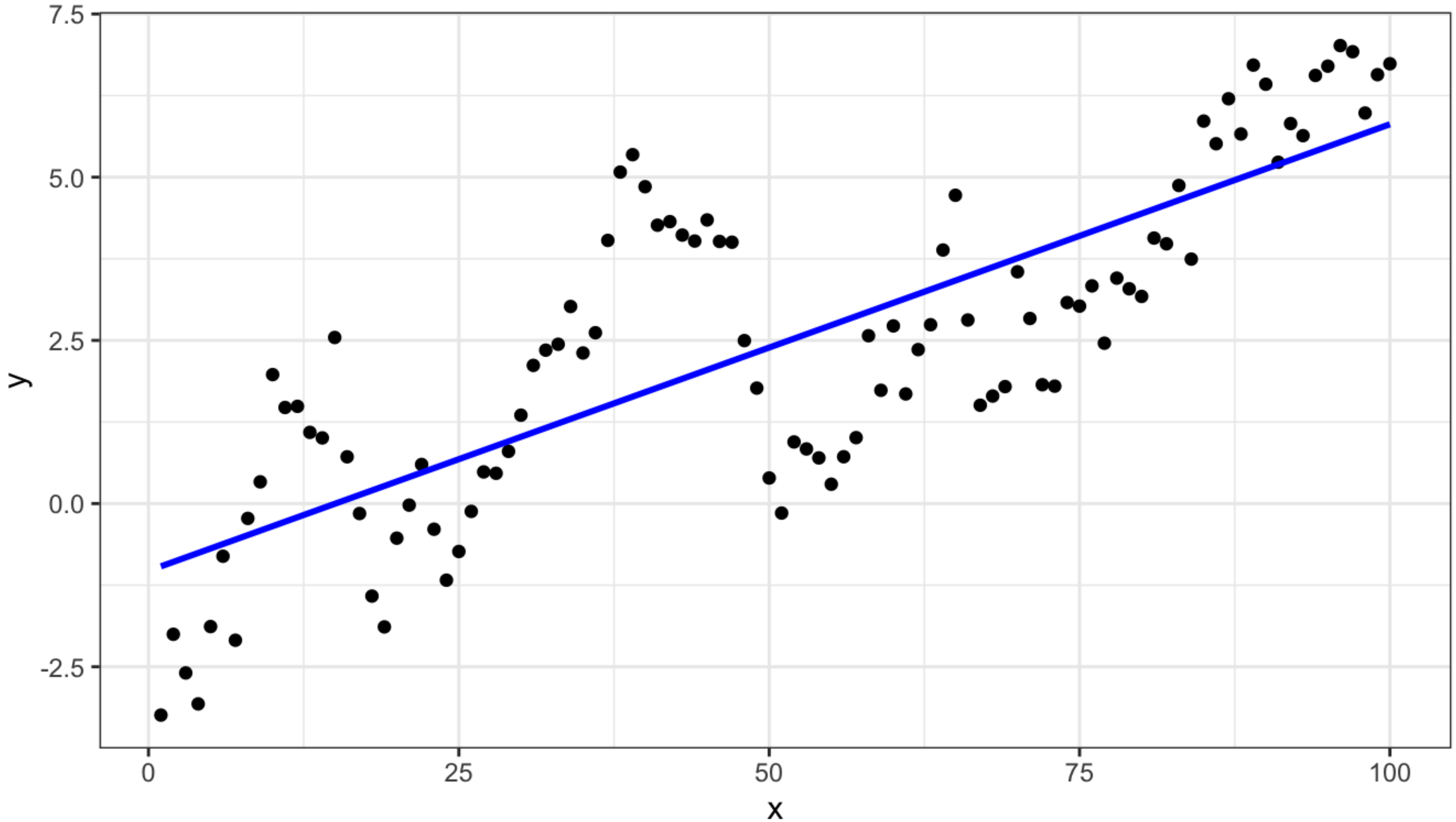
Some more linear models

Linear model and data

```r
ggplot(d, aes(x=x,y=y)) +
  geom_point() +
  geom_smooth(method="lm", color="blue", se = FALSE)
```



Linear model

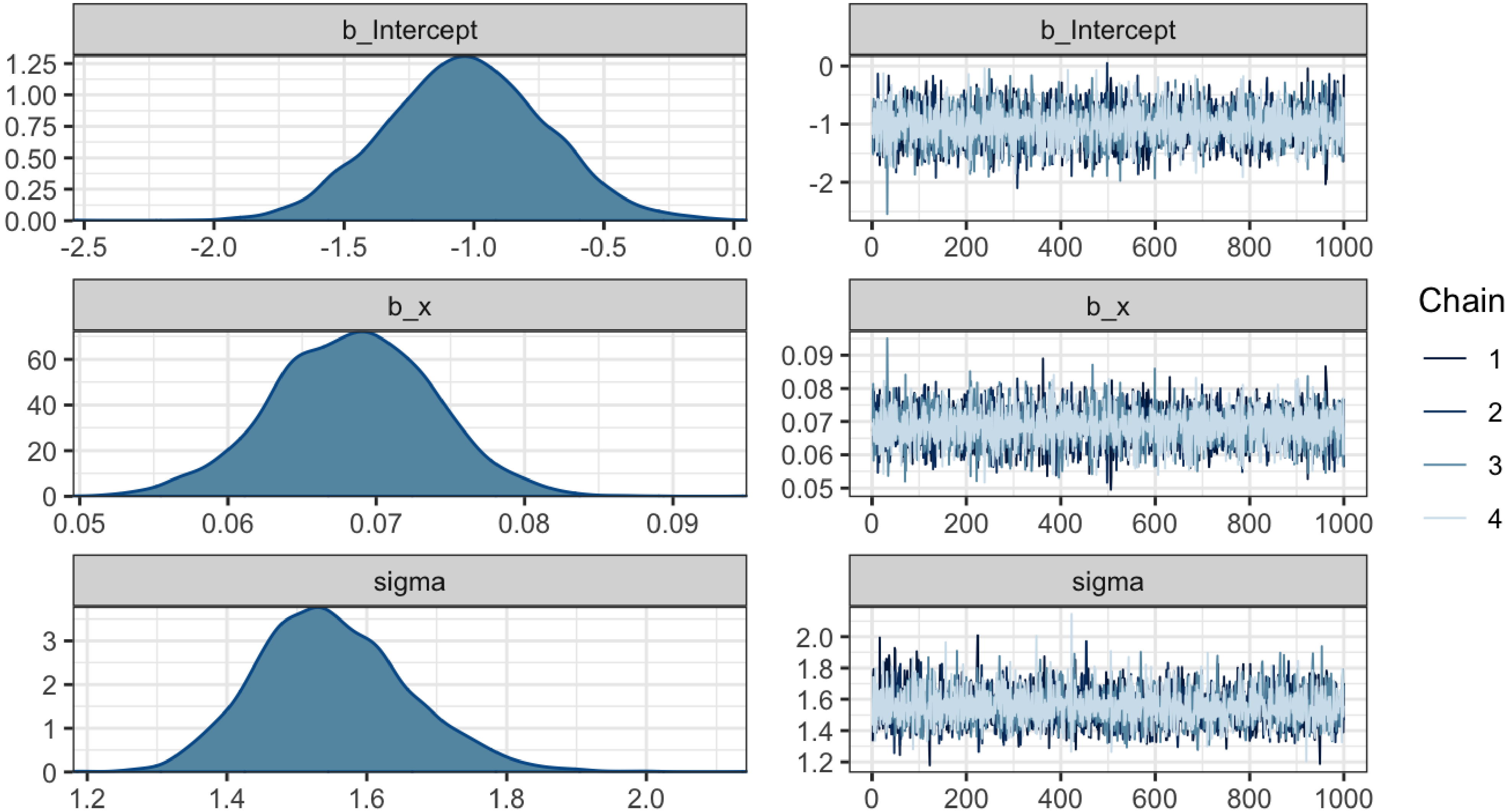
```r
l = lm(y ~ x, data=d)
summary(l)
## 
## Call:
## lm(formula = y ~ x, data = d)
## 
## Residuals:
##     Min      1Q  Median      3Q     Max 
## -2.6041 -1.2142 -0.1973  1.1969  3.7072 
## 
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)    
## (Intercept) -1.030315   0.310326   -3.32  0.00126 ** 
## x            0.068409   0.005335   12.82  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 1.54 on 98 degrees of freedom
## Multiple R-squared:  0.6266, Adjusted R-squared:  0.6227 
## F-statistic: 164.4 on 1 and 98 DF,  p-value: < 2.2e-16
```

Bayesian model (brms)

```
( b = brms::brm(
    y ~ x, data=d,
    prior = c(
      brms::prior(normal(0, 100), class = Intercept),
      brms::prior(normal(0, 10),  class = b),
      brms::prior(cauchy(0, 2),   class = sigma)
    ),
    silent = 2, refresh = 0
  )
)
## Running /opt/homebrew/Cellar/r/4.2.1_2/lib/R/bin/R CMD SHLIB foo.c
## clang -I"/opt/homebrew/Cellar/r/4.2.1_2/lib/R/include" -DNDEBUG   -I"/Users/rundel/Library/R/
## In file included from <built-in>:1:
## In file included from /Users/rundel/Library/R/arm64/4.2/library/StanHeaders/include/stan/math
## In file included from /Users/rundel/Library/R/arm64/4.2/library/RcppEigen/include/Eigen/Dense
## In file included from /Users/rundel/Library/R/arm64/4.2/library/RcppEigen/include/Eigen/Core:
## /Users/rundel/Library/R/arm64/4.2/library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:
## namespace Eigen {
## ^
## /Users/rundel/Library/R/arm64/4.2/library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:
## namespace Eigen {
##                 ^
```

Parameter estimates

```
plot(b)
```



tidybayes - gather_draws (long)

```
b_post = b |>
  tidybayes::gather_draws(b_Intercept, b_x, sigma)

b_post
## # A tibble: 12,000 × 5
## # Groups:   .variable [3]
##    .chain .iteration .draw .variable   .value
##     <int>      <int> <int> <chr>        <dbl>
##  1      1          1     1 b_Intercept -0.961
##  2      1          2     2 b_Intercept -1.24
##  3      1          3     3 b_Intercept -1.29
##  4      1          4     4 b_Intercept -0.763
##  5      1          5     5 b_Intercept -0.980
##  6      1          6     6 b_Intercept -1.13
##  7      1          7     7 b_Intercept -0.810
##  8      1          8     8 b_Intercept -1.33
```

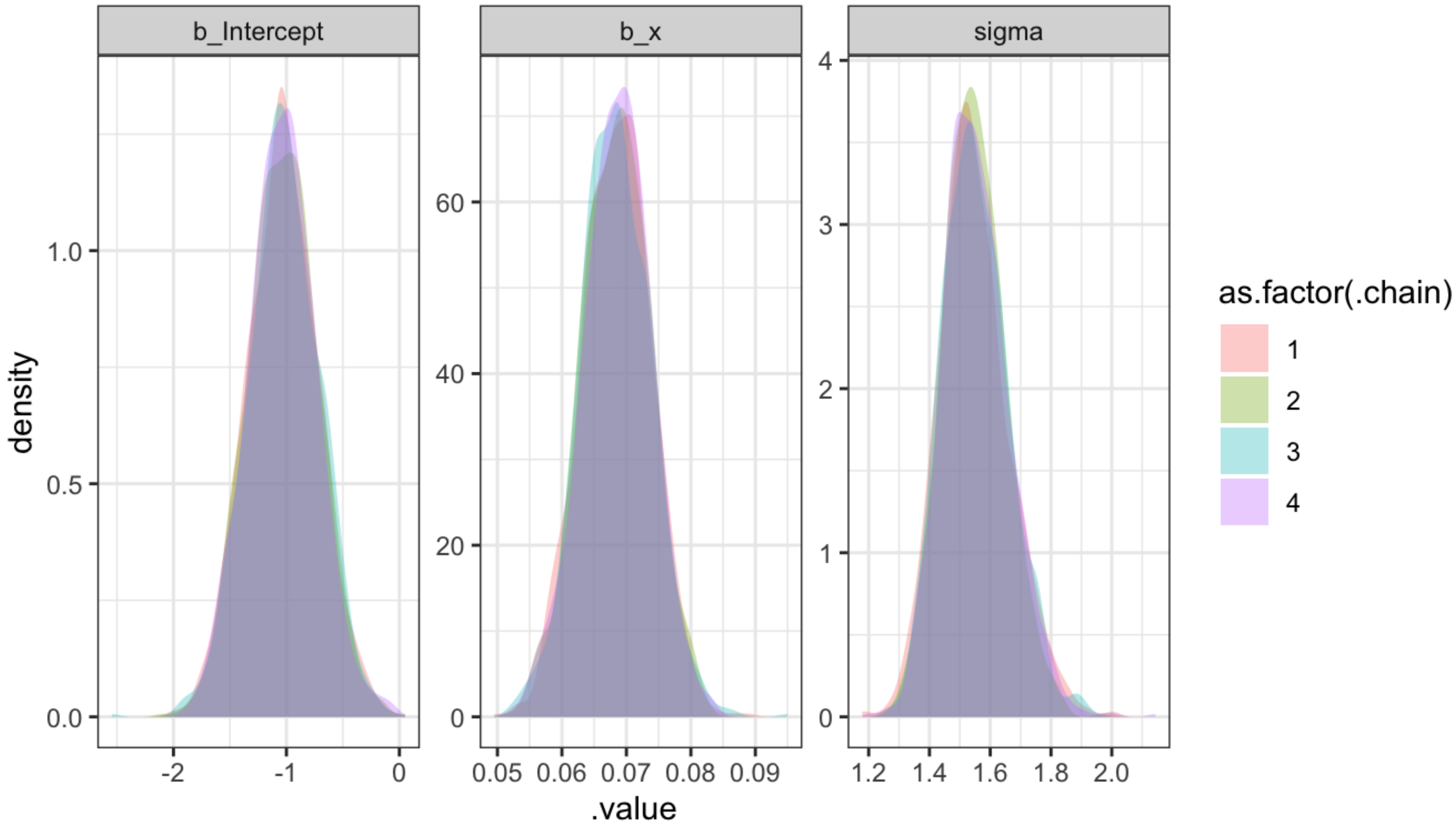
tidybayes - spread_draws (wide)

```r
b_post_wide = b |>
  tidybayes::spread_draws(b_Intercept, b_x, sigma)

b_post_wide
## # A tibble: 4,000 × 6
##    .chain .iteration .draw b_Intercept    b_x sigma
##     <int>      <int> <int>       <dbl>  <dbl> <dbl>
##  1      1          1     1      -0.961 0.0671  1.33
##  2      1          2     2      -1.24  0.0726  1.75
##  3      1          3     3      -1.29  0.0736  1.79
##  4      1          4     4      -0.763 0.0639  1.35
##  5      1          5     5      -0.980 0.0697  1.53
##  6      1          6     6      -1.13  0.0692  1.53
##  7      1          7     7      -0.810 0.0637  1.52
##  8      1          8     8      -1.33  0.0726  1.47
##  9      1          9     9      -1.22  0.0728  1.65
```

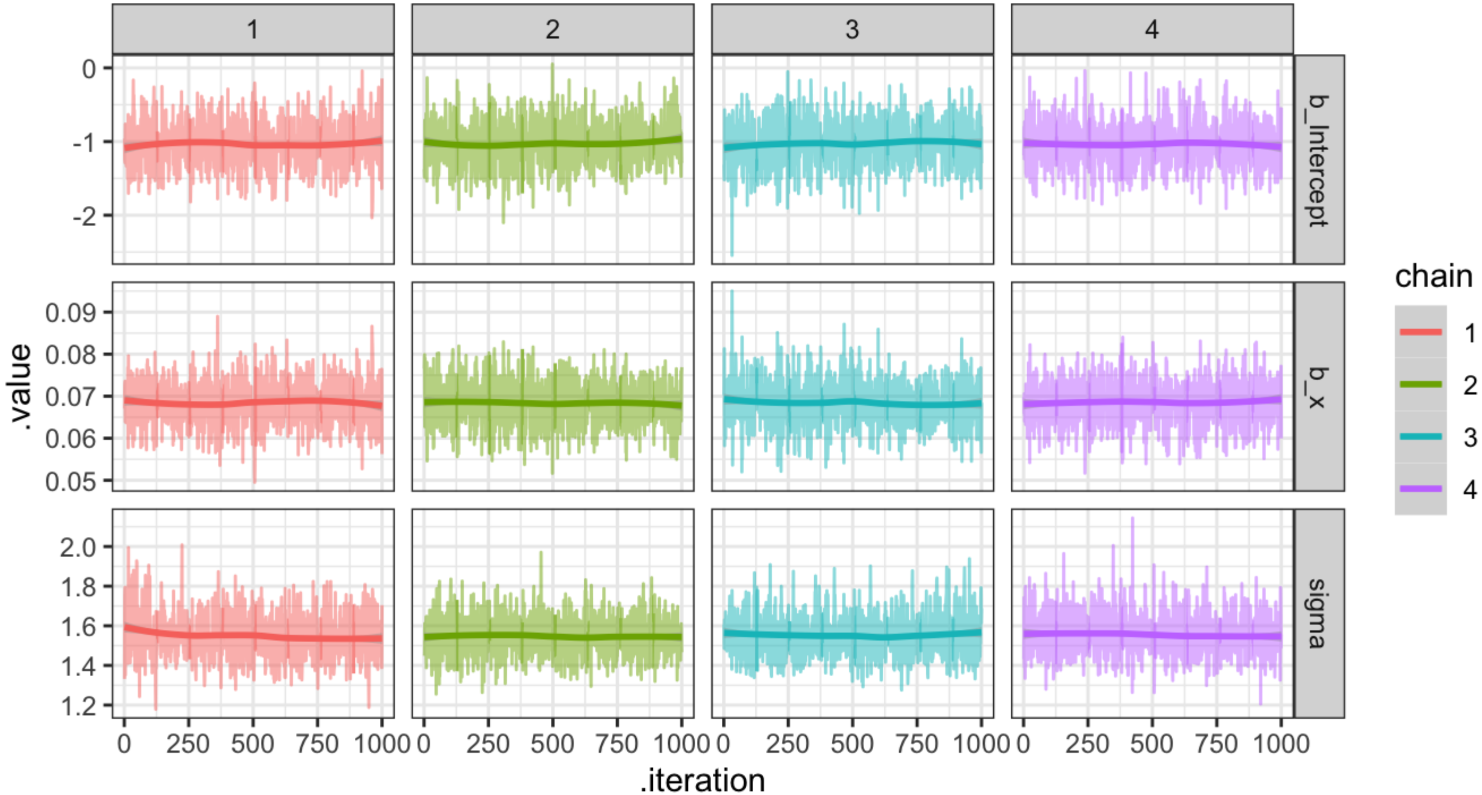
Posterior plots

```r
b_post |>
  ggplot(aes(fill=as.factor(.chain), group=.chain, x=.value)) +
  geom_density(alpha=0.33, color=NA) +
  facet_wrap(~.variable, scales = "free")
```



Trace plots

```
b_post %>%
  ggplot(aes(x=.iteration, y=.value, color=as.factor(.chain))) +
  geom_line(alpha=0.5) +
  facet_grid(.variable~.chain, scale="free_y") +
  geom_smooth(method="loess") + labs(color="chain")
```

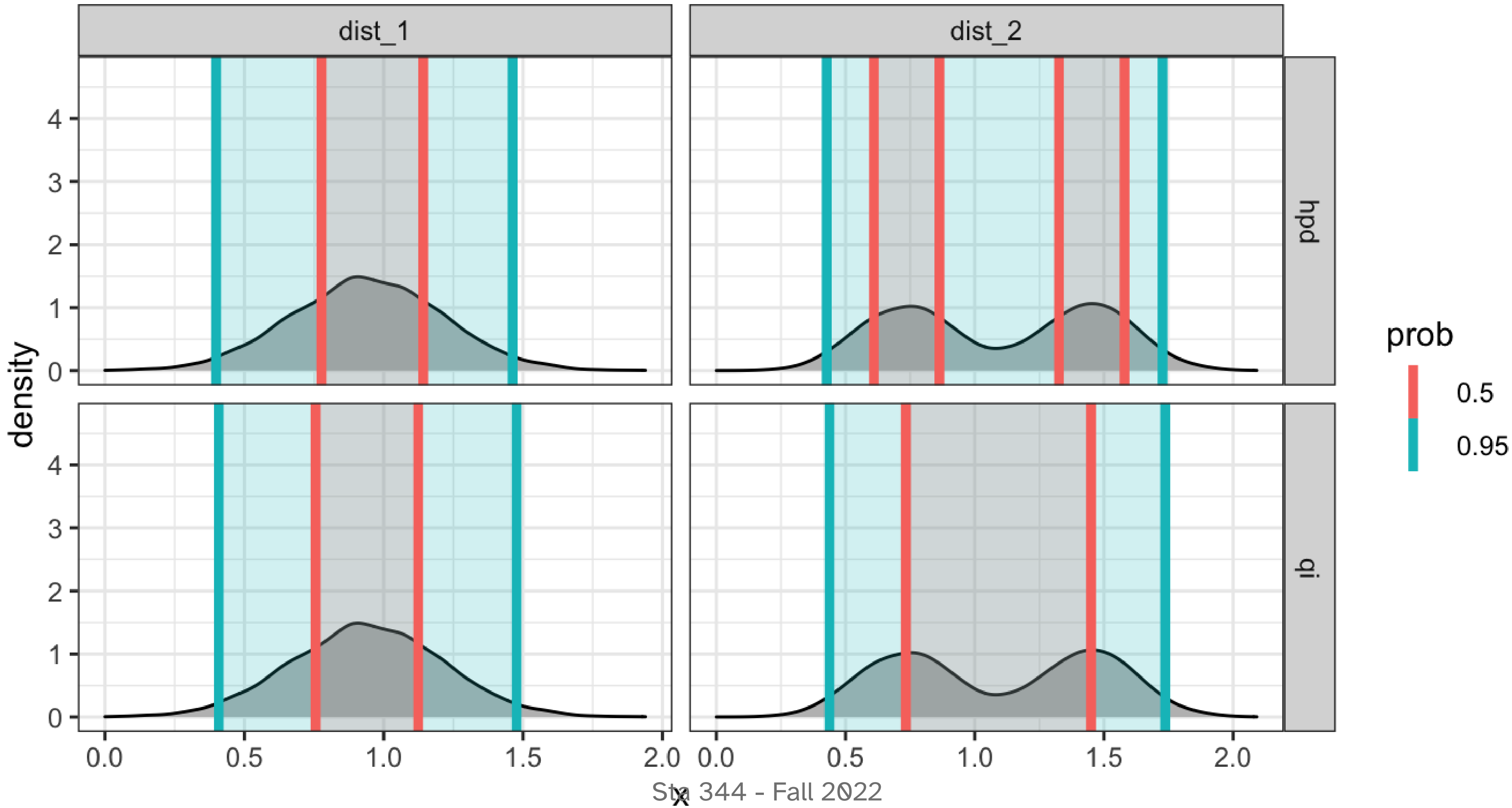


Credible Intervals

```
( b_ci = b_post |>
    group_by(.chain, .variable) |>
    tidybayes::mean_hdi(.value, .width=c(0.8, 0.95))
)
## # A tibble: 24 × 8
##    .chain .variable    .value  .lower  .upper .width .point .interval
##     <int> <chr>         <dbl>   <dbl>   <dbl>  <dbl> <chr>  <chr>
##  1      1 b_Intercept -1.03   -1.40   -0.624     0.8 mean   hdi
##  2      1 b_x          0.0685  0.0624  0.0761    0.8 mean   hdi
##  3      1 sigma        1.55    1.40    1.69      0.8 mean   hdi
##  4      2 b_Intercept -1.03   -1.41   -0.621     0.8 mean   hdi
##  5      2 b_x          0.0684  0.0620  0.0753    0.8 mean   hdi
##  6      2 sigma        1.55    1.43    1.69      0.8 mean   hdi
##  7      3 b_Intercept -1.02   -1.40   -0.604     0.8 mean   hdi
##  8      3 b_x          0.0684  0.0615  0.0749    0.8 mean   hdi
##  9      3 sigma        1.55    1.42    1.69      0.8 mean   hdi
## 10      4 b_Intercept -1.04   -1.40   -0.637     0.8 mean   hdi
## # … with 14 more rows
```

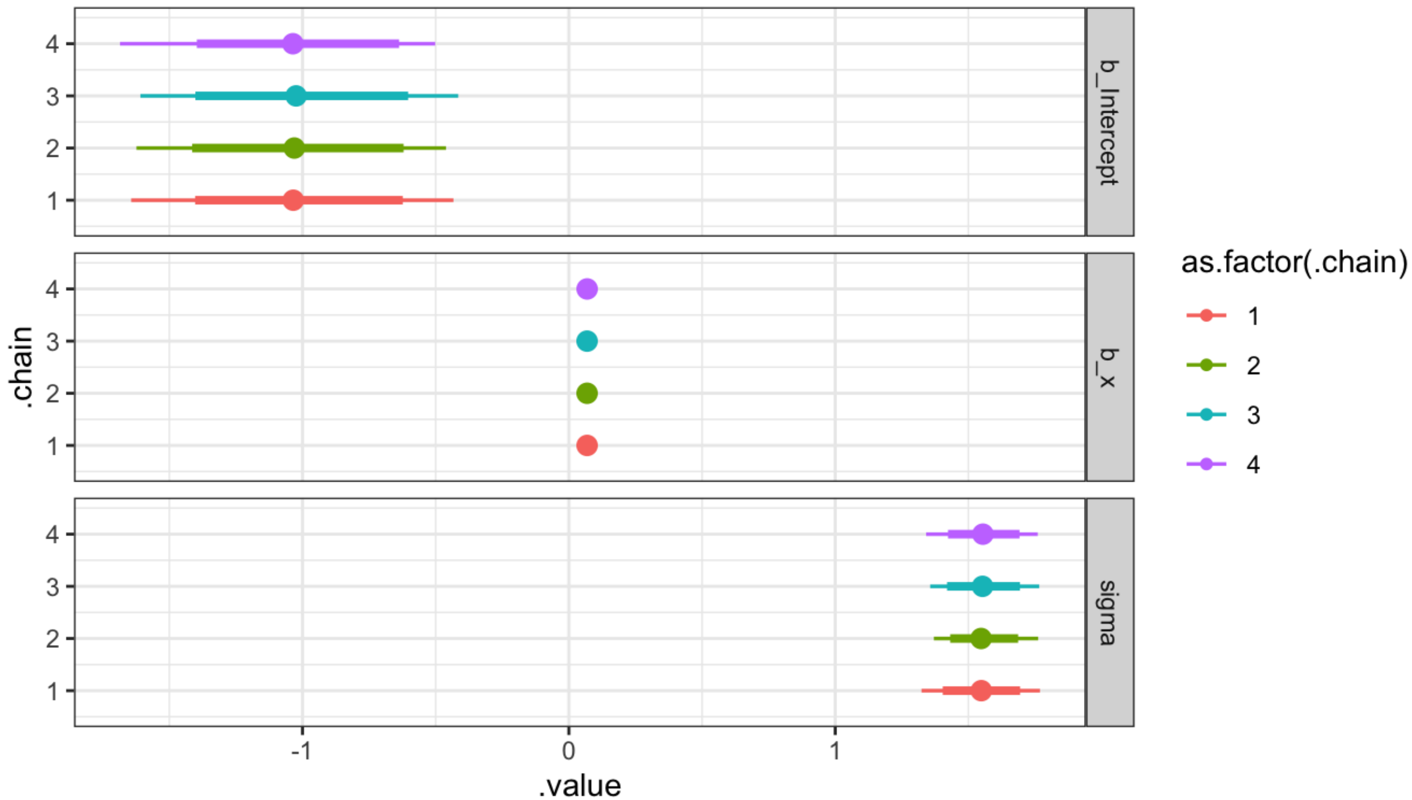
Aside - `mean_qi()` vs `mean_hdi()`

These differ in the use of the quantile interval vs. the highest-density interval.



Caterpillar Plots

```r
b_ci %>%
  ggplot(aes(x=.value, y=.chain, color=as.factor(.chain))) +
  facet_grid(.variable ~ .) +
  tidybayes::geom_pointintervalh() +
  ylim(0.5, 4.5)
```



Predictions

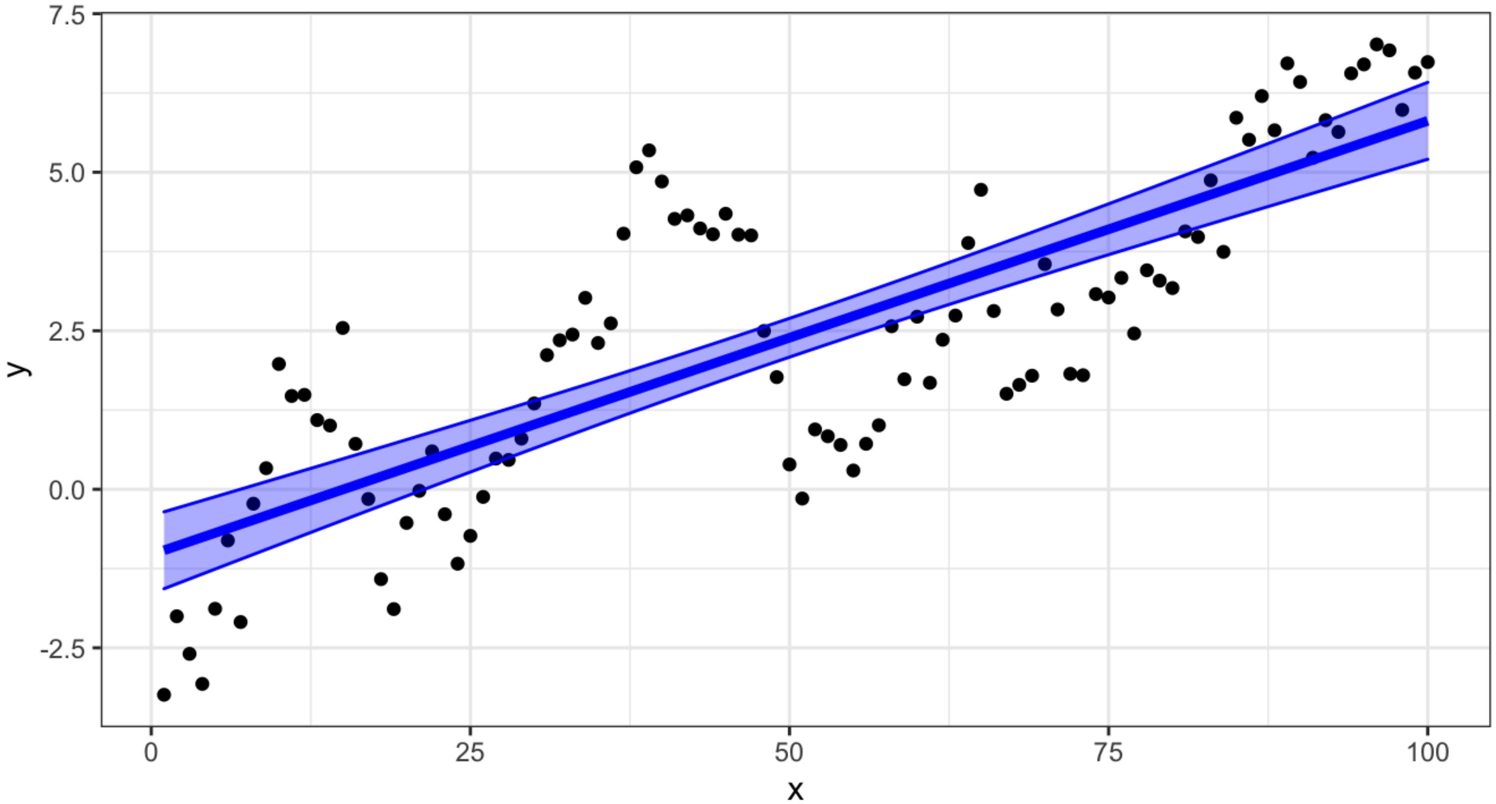
lm predictions

```
(l_pred = broom::augment(l, interval="confidence"))
## # A tibble: 100 × 10
##         y     x .fitted .lower   .upper .resid   .hat .sigma   .cooksd .std.re
##     <dbl> <int>   <dbl>  <dbl>    <dbl>  <dbl>  <dbl>  <dbl>     <dbl>      <c
##  1 -3.24      1  -0.962 -1.57  -0.355   -2.28  0.0394   1.53 0.0467       -1.
##  2 -2.00      2  -0.893 -1.49  -0.296   -1.11  0.0382   1.54 0.0107       -0.
##  3 -2.59      3  -0.825 -1.41  -0.237   -1.77  0.0371   1.54 0.0264       -1.
##  4 -3.07      4  -0.757 -1.34  -0.177   -2.31  0.0359   1.53 0.0436       -1.
##  5 -1.88      5  -0.688 -1.26  -0.118   -1.20  0.0348   1.54 0.0113       -0.
##  6 -0.807     6  -0.620 -1.18  -0.0583  -0.187 0.0338   1.55 0.000266     -0.
##  7 -2.09      7  -0.551 -1.10   0.00127 -1.54  0.0327   1.54 0.0175       -1.
##  8 -0.227     8  -0.483 -1.03   0.0609   0.256 0.0317   1.55 0.000466      0.
##  9  0.333     9  -0.415 -0.950  0.121    0.747 0.0307   1.55 0.00384       0.
## 10  1.98     10  -0.346 -0.873  0.180    2.32  0.0297   1.53 0.0358        1.
## # … with 90 more rows
```

There are the same values you would get from `predict(l, se.fit = TRUE)` just combined with `d`

Confidence interval

```
l_pred |>
  ggplot(aes(x=x,y=y)) +
   geom_point() +
   geom_line(aes(y=.fitted), col="blue", size=1.5) +
   geom_ribbon(aes(ymin=.lower, ymax=.upper), col="blue", fill="blue", a
```

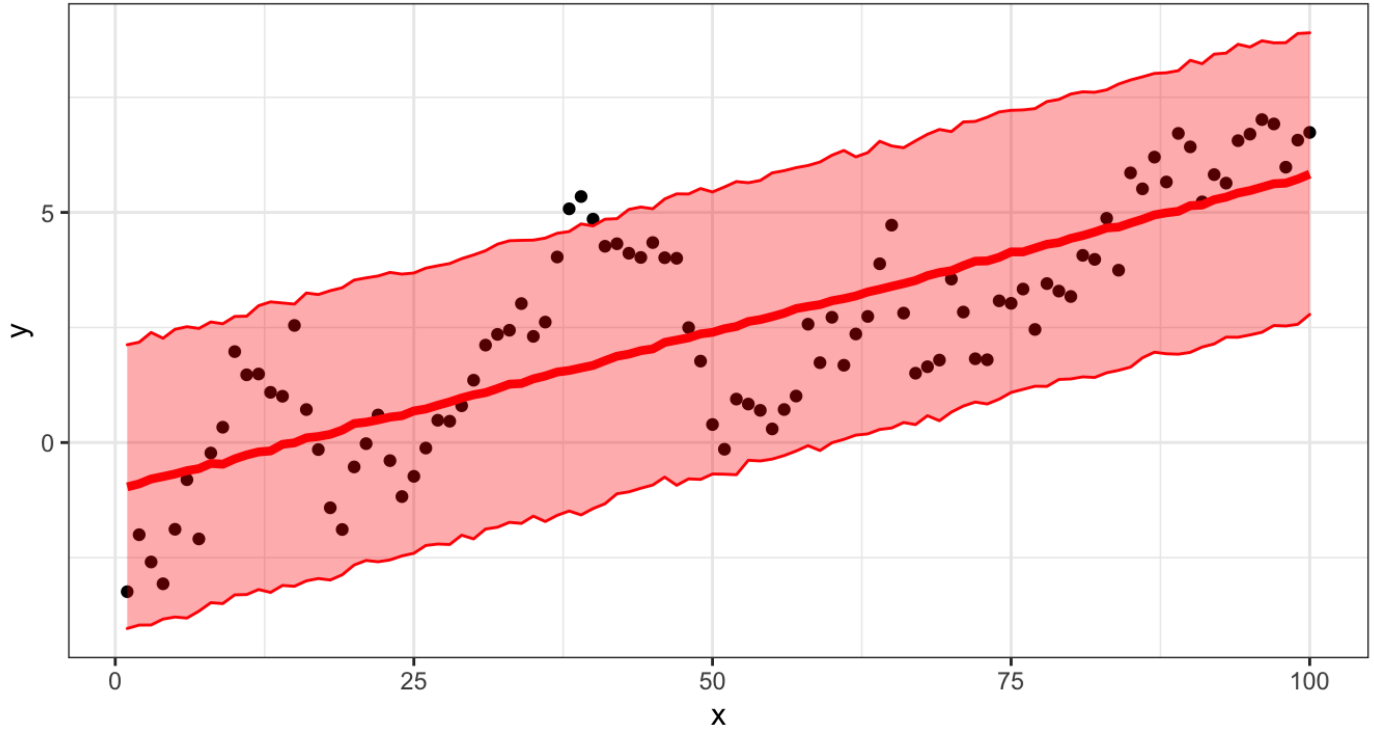


brms predictions

```
(b_pred = predict(b))
##          Estimate Est.Error       Q2.5    Q97.5
##   [1,] -0.96419044  1.553634 -4.04028547 2.124732
##   [2,] -0.89721849  1.593799 -3.96603496 2.179769
##   [3,] -0.79179315  1.594565 -3.96413800 2.391643
##   [4,] -0.73859326  1.579550 -3.83546564 2.266440
##   [5,] -0.68293418  1.579669 -3.79089154 2.460559
##   [6,] -0.61155250  1.609090 -3.81348198 2.516711
##   [7,] -0.56675460  1.579506 -3.66369377 2.479165
##   [8,] -0.45334581  1.570071 -3.47909432 2.620280
##   [9,] -0.47151098  1.565524 -3.49855796 2.580172
##  [10,] -0.35537333  1.552547 -3.30957100 2.739897
##  [11,] -0.26908970  1.562577 -3.30266874 2.745822
##  [12,] -0.20382232  1.582830 -3.19318502 2.973233
##  [13,] -0.18236463  1.568774 -3.25612849 3.056613
##  [14,] -0.03840721  1.571181 -3.10470573 3.032293
```

Credible interval

```r
d |>
  bind_cols(b_pred) |>
  ggplot(aes(x=x,y=y)) +
    geom_point() +
    geom_line(aes(y=Estimate), col="red", size=1.5) +
    geom_ribbon(aes(ymin=Q2.5, ymax=Q97.5), col='red', fill='red', alpha
```



Why are the intervals different?

Raw predictions

```
dim( brms::posterior_predict(b) )
## [1] 4000  100
dim( brms::posterior_epred(b) )
## [1] 4000  100
```

Tidy raw predictions

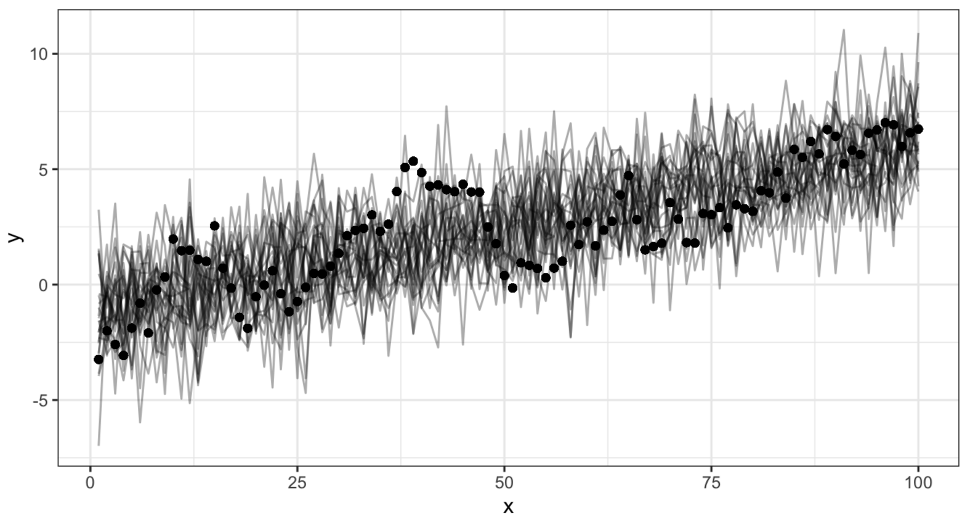
```
( b_post_pred = tidybayes::predicted_draws(
    b, newdata=d
) )
## # A tibble: 400,000 × 7
## # Groups:   x, y, .row [100]
##         x      y  .row .chain .iteration .dr
##     <int> <dbl> <int>  <int>      <int> <in
## 1       1 -3.24     1     NA         NA
## 2       1 -3.24     1     NA         NA
## 3       1 -3.24     1     NA         NA
## 4       1 -3.24     1     NA         NA
## 5       1 -3.24     1     NA         NA
## 6       1 -3.24     1     NA         NA
## 7       1 -3.24     1     NA         NA
## 8       1 -3.24     1     NA         NA
## 9       1 -3.24     1     NA         NA
## 10      1 -3.24     1     NA         NA
## # … with 399,990 more rows
```

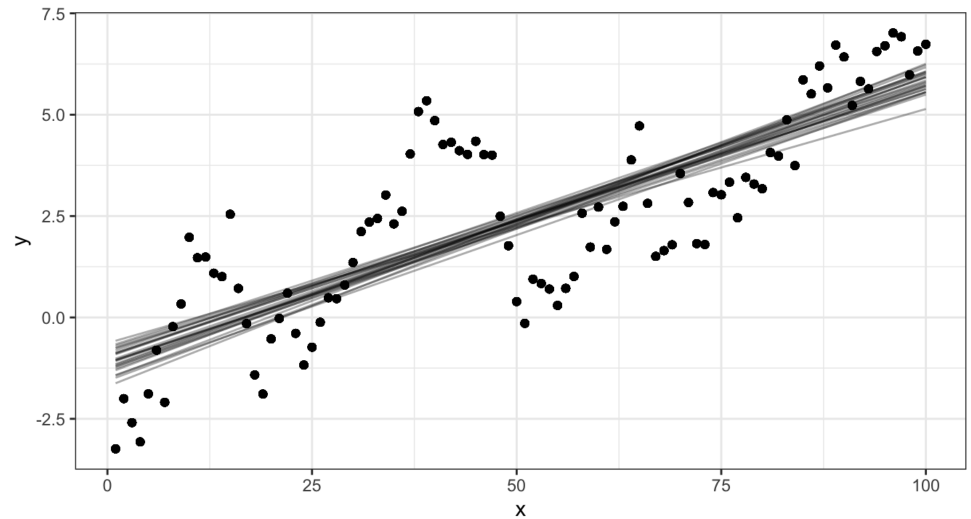
```
( b_post_epred = tidybayes::epred_draws(
    b, newdata=d
) )
## # A tibble: 400,000 × 7
## # Groups:   x, y, .row [100]
##         x      y  .row .chain .iteration .dr
##     <int> <dbl> <int>  <int>      <int> <in
## 1       1 -3.24     1     NA         NA
## 2       1 -3.24     1     NA         NA
## 3       1 -3.24     1     NA         NA
## 4       1 -3.24     1     NA         NA
## 5       1 -3.24     1     NA         NA
## 6       1 -3.24     1     NA         NA
## 7       1 -3.24     1     NA         NA
## 8       1 -3.24     1     NA         NA
## 9       1 -3.24     1     NA         NA
## 10      1 -3.24     1     NA         NA
## # … with 399,990 more rows
```

Posterior predictions vs Expected posterior predictions

```
b_post_pred |>
  filter(.draw <= 25) |>
  ggplot(aes(x=x,y=y)) +
    geom_point() +
    geom_line(
      aes(y=.prediction, group=.draw),
      alpha=0.33
    )
```

```
b_post_epred |>
  filter(.draw <= 25) |>
  ggplot(aes(x=x,y=y)) +
    geom_point() +
    geom_line(
      aes(y=.epred, group=.draw),
      alpha=0.33
    )
```

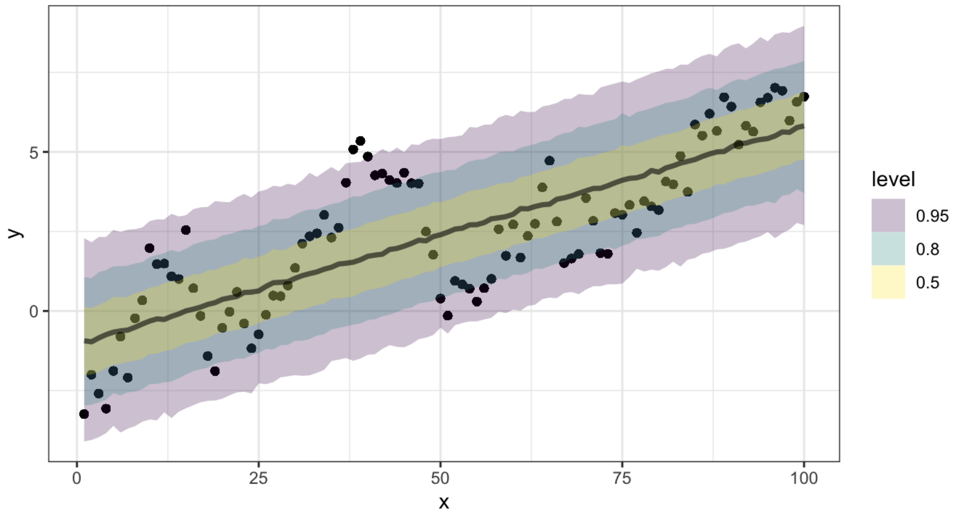


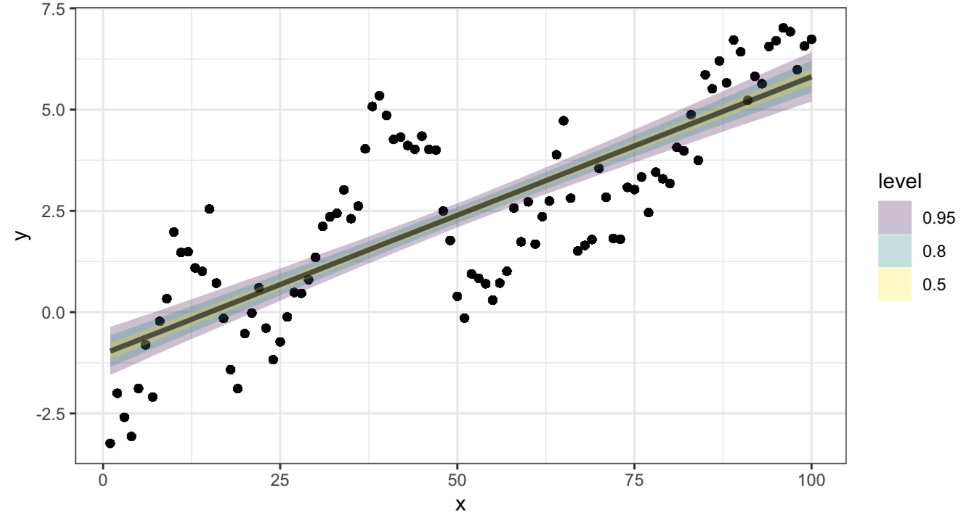


Credible intervals

```r
b_post_pred |>
  ggplot(aes(x=x, y=y)) +
    geom_point() +
    tidybayes::stat_lineribbon(
      aes(y=.prediction), alpha=0.25
    )
```

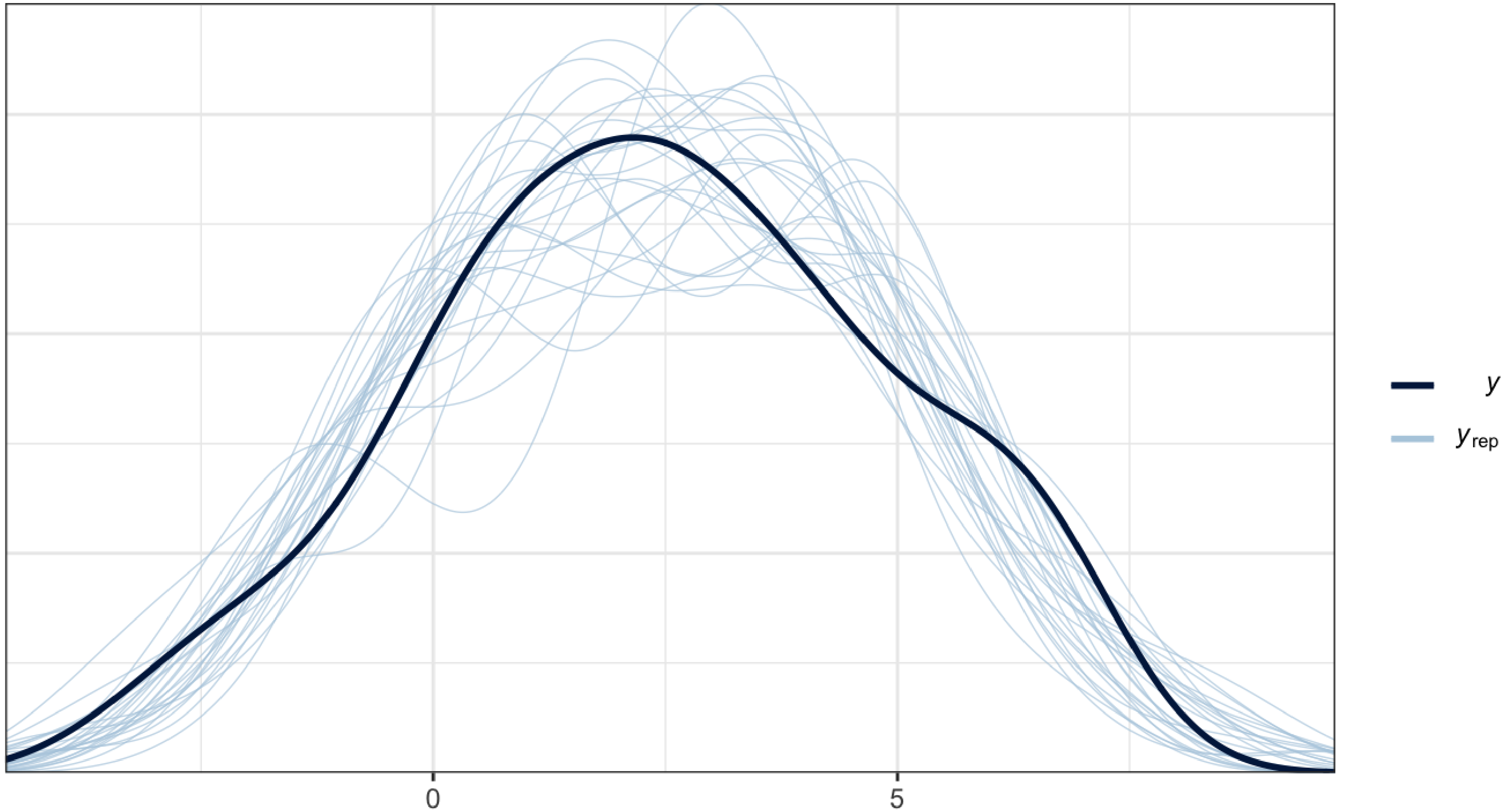
```r
b_post_epred |>
  ggplot(aes(x=x, y=y)) +
    geom_point() +
    tidybayes::stat_lineribbon(
      aes(y=.epred), alpha=0.25
    )
```





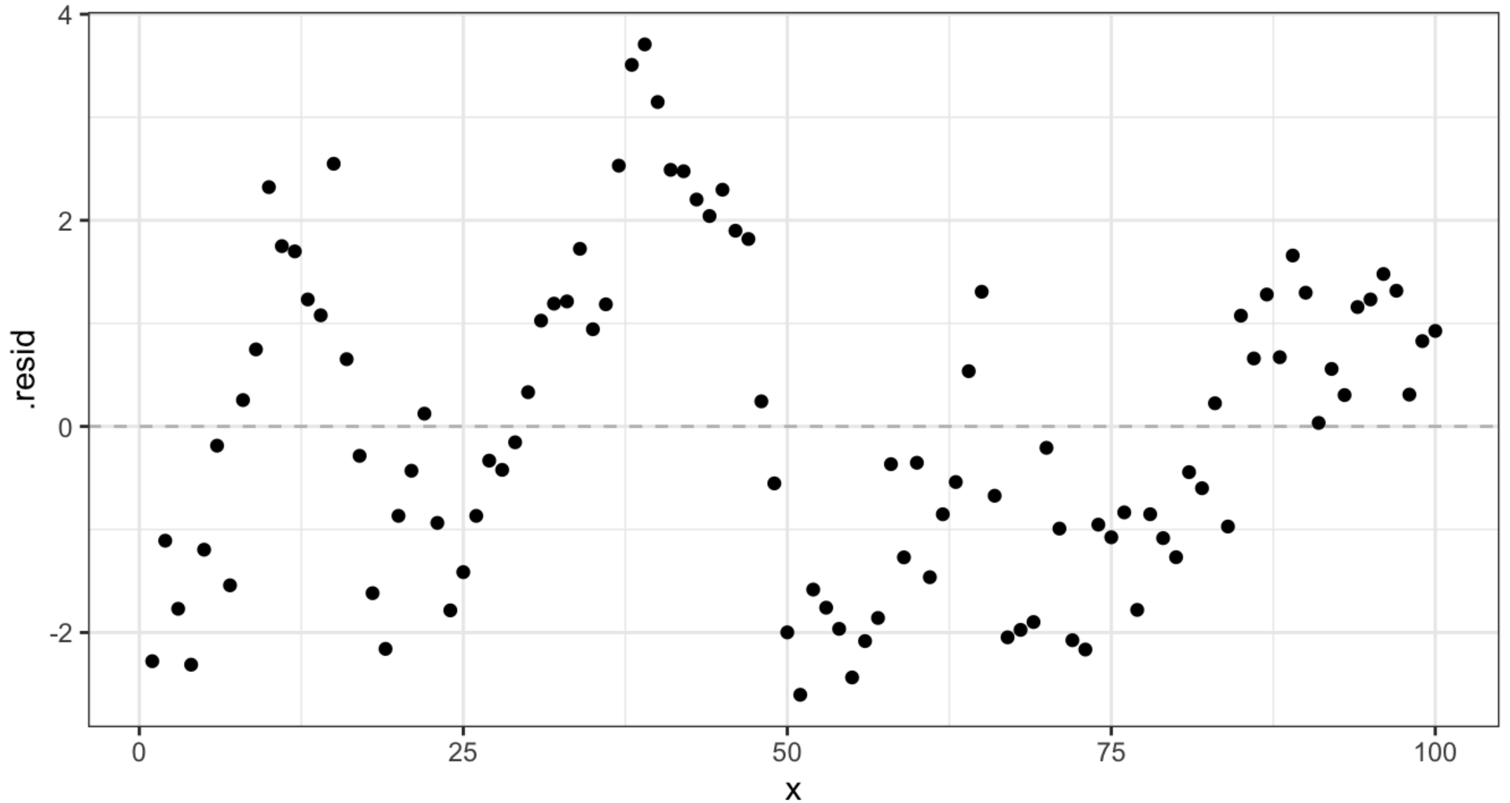
Posterior predictive checks

```r
brms::pp_check(b, ndraws = 25)
```



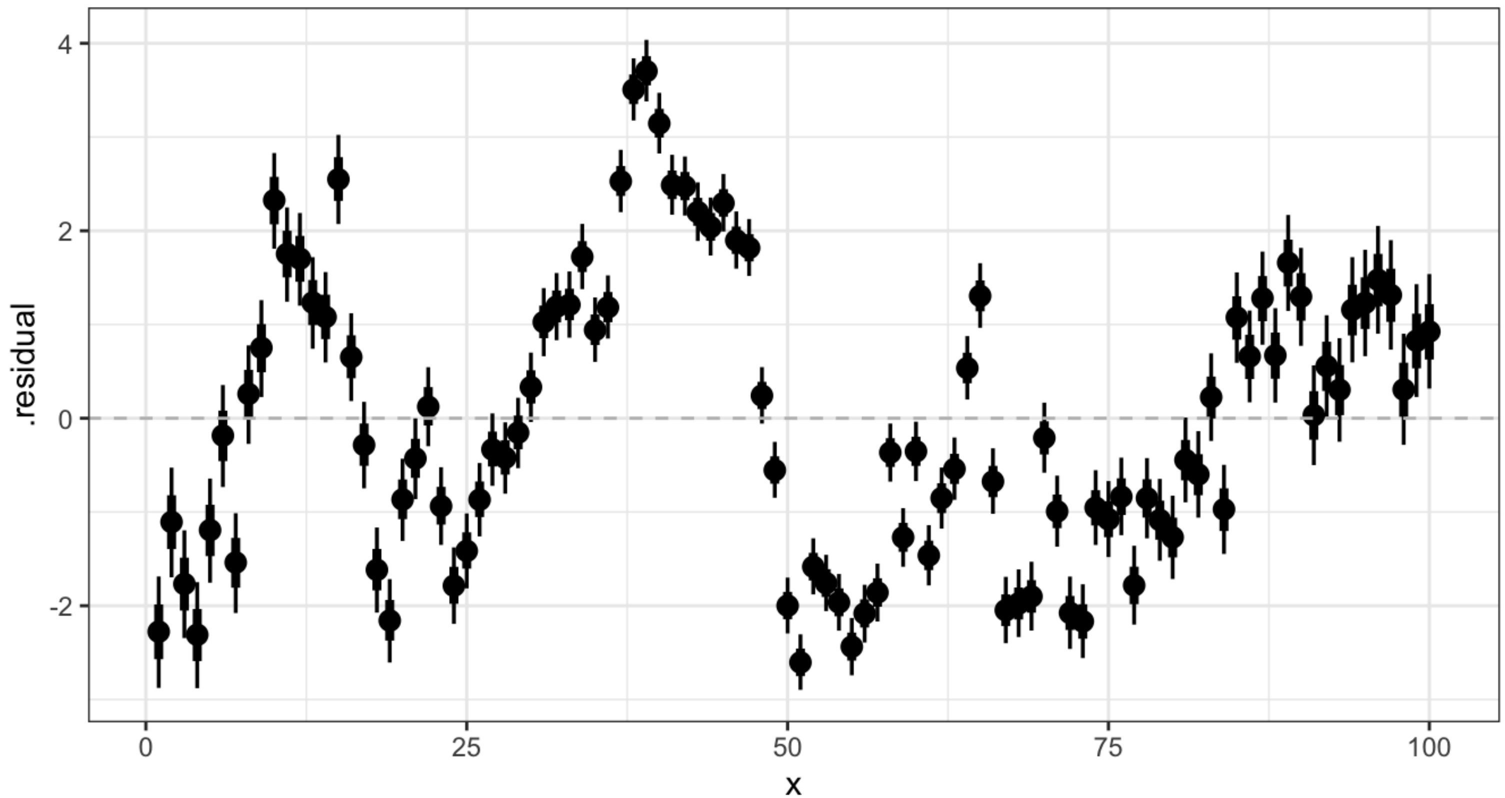
Residuals - lm

```
l |>
  broom::augment() |>
  ggplot(aes(x=x, y=.resid)) +
    geom_point() +
    geom_hline(yintercept=0, color='grey', linetype=2)
```



Residual posteriors - brms

```
b %>%
  tidybayes::residual_draws(newdata=d) |>
  ggplot(aes(x=x, y=.residual, group=x)) +
    tidybayes::stat_pointinterval() +
    geom_hline(yintercept = 0, color='grey', linetype=2)
```



Model Evaluation

Model assessment

If we remember back to our first regression class, one common option is R^2 which gives us the variability in y explained by our model.

Quick review:

$$\underbrace{\sum_{i=1}^{n} (y_i - \bar{y})^2}_{\text{Total}} = \underbrace{\sum_{i=1}^{n} \left(\hat{y}_i - \bar{y}\right)^2}_{\text{Model}} + \underbrace{\sum_{i=1}^{n} \left(y_i - \hat{y}_i\right)^2}_{\text{Error}}$$

$$R^2 = \frac{SS_{model}}{SS_{total}} = \frac{\sum_{i=1}^{n} \left(\hat{Y}_i - \bar{Y}\right)^2}{\sum_{i=1}^{n} \left(Y_i - \bar{Y}\right)^2} = \frac{\text{Var}(\hat{\boldsymbol{Y}})}{\text{Var}(\boldsymbol{Y})} = \text{Cor}(\boldsymbol{Y}, \hat{\boldsymbol{Y}})^2$$

Some data prep

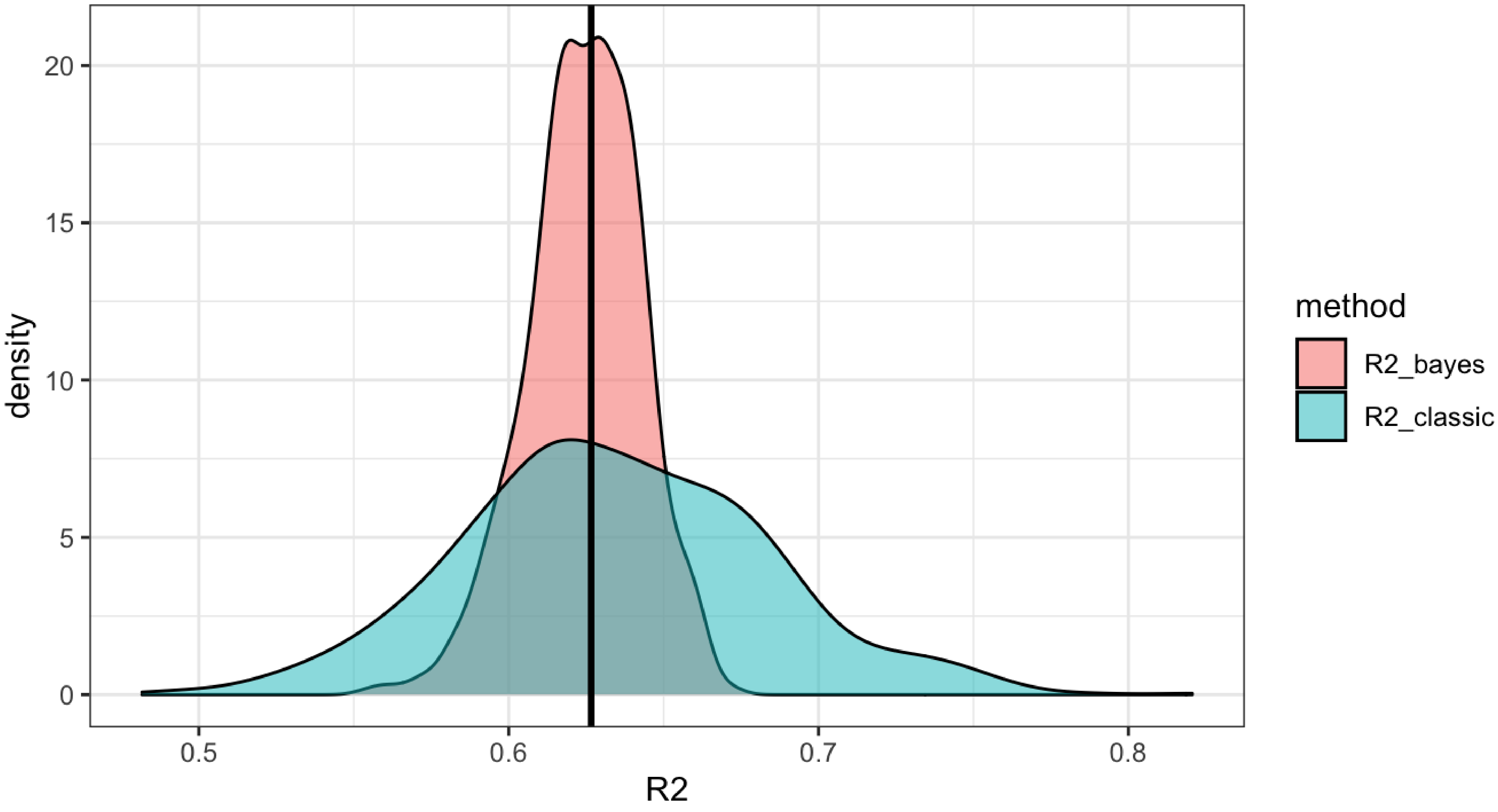
```
( b_post_full = b |>
    tidybayes::spread_draws(b_Intercept, b_x, sigma) |>
    tidyr::expand_grid(d) |>
    mutate(
      y_hat = b_Intercept + b_x * x,
      resid = y - y_hat
    )
)
## # A tibble: 400,000 × 10
##    .chain .iteration .draw b_Intercept    b_x sigma     x      y  y_hat  resi
##     <int>      <int> <int>       <dbl>  <dbl> <dbl> <int>  <dbl>  <dbl>  <dbl
##  1      1          1     1      -0.961 0.0671  1.33     1 -3.24  -0.894 -2.35
##  2      1          1     1      -0.961 0.0671  1.33     2 -2.00  -0.826 -1.18
##  3      1          1     1      -0.961 0.0671  1.33     3 -2.59  -0.759 -1.84
##  4      1          1     1      -0.961 0.0671  1.33     4 -3.07  -0.692 -2.38
##  5      1          1     1      -0.961 0.0671  1.33     5 -1.88  -0.625 -1.26
##  6      1          1     1      -0.961 0.0671  1.33     6 -0.807 -0.558 -0.24
##  7      1          1     1      -0.961 0.0671  1.33     7 -2.09  -0.491 -1.60
```

Bayesian R^2

When we compute any statistic for our model we want to do so at each iteration so that we can obtain the posterior distribution of that particular statistic (e.g. the posterior distribution of R^2 in this case).

```
( b_R2 = b_post_full %>%
    group_by(.iteration) %>%
    summarize(
      R2_classic = var(y_hat) / var(y),
      R2_bayes   = var(y_hat) / (var(y_hat) + var(resid))
    )
)
## # A tibble: 1,000 × 3
##    .iteration R2_classic R2_bayes
##         <int>      <dbl>    <dbl>
##  1          1      0.676    0.642
##  2          2      0.757    0.663
##  3          3      0.593    0.610
##  4          4      0.667    0.637
##  5          5      0.630    0.625
##  6          6      0.627    0.624
##  7          7      0.557    0.593
##  8          8      0.640    0.625
##  9          9      0.730    0.657
```

Uh oh ...



Sanity check

```
( l_pred = broom::augment(l) )
## # A tibble: 100 × 8
##          y     x .fitted .resid   .hat .sig
##      <dbl> <int>   <dbl>  <dbl>  <dbl> <dl
##   1 -3.24      1  -0.962 -2.28  0.0394   1.
##   2 -2.00      2  -0.893 -1.11  0.0382   1.
##   3 -2.59      3  -0.825 -1.77  0.0371   1.
##   4 -3.07      4  -0.757 -2.31  0.0359   1.
##   5 -1.88      5  -0.688 -1.20  0.0348   1.
##   6 -0.807     6  -0.620 -0.187 0.0338   1.
##   7 -2.09      7  -0.551 -1.54  0.0327   1.
##   8 -0.227     8  -0.483  0.256 0.0317   1.
##   9  0.333     9  -0.415  0.747 0.0307   1.
## 10  1.98      10  -0.346  2.32  0.0297   1.
## # … with 90 more rows
```

```
broom::glance(l)$r.squared
## [1] 0.6265565

var(l_pred$.fitted) / var(l_pred$y)
## [1] 0.6265565

var(l_pred$.fitted) / (var(l_pred$.fitted) +
## [1] 0.6265565
```

What if we collapsed first?

Here we calculate the posterior mean of $\hat{y}$ and use that to estimate R^2,

```
b_post_full %>%
  group_by(x) %>%
  summarize(
    y_hat = mean(y_hat),
    y = mean(y),
    resid = mean(y - y_hat),
    .groups = "drop"
  ) %>%
  summarize(
    R2_classic = var(y_hat) / var(y),
    R2_bayes   = var(y_hat) / (var(y_hat) + var(resid))
  )
## # A tibble: 1 × 2
##   R2_classic R2_bayes
##        <dbl>    <dbl>
## 1      0.627    0.627
```

Some problems with R^2

Some new issues,

- R^2 doesn't really make sense in the Bayesian context
  - multiple possible definitions with different properties
  - fundamental equality doesn't hold anymore
  - Possible to have $R^2 > 1$

Some old issues,

- R^2 always increases (or stays the same) when adding a predictor
- R^2 is highly susceptible to over fitting
- R^2 is sensitive to outliers
- R^2 depends heavily on values of y (can differ for two equivalent models)

Some Other Metrics

Root Mean Square Error

The traditional definition of rmse is as follows

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2}$$

In the bayesian context, we have posterior samples from each parameter / prediction of interest so we can express this as

$$\frac{1}{m}\sum_{s=1}^{m}\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_{i,s}\right)^2}$$

where m is the number of iterations and $\hat{Y}_i^s$ is the prediction for Y_i at iteration s.

Continuous Rank Probability Score

Another approach is the continuous rank probability score which comes from the probabilistic forecasting literature, it compares the full posterior predictive distribution to the observation / truth.

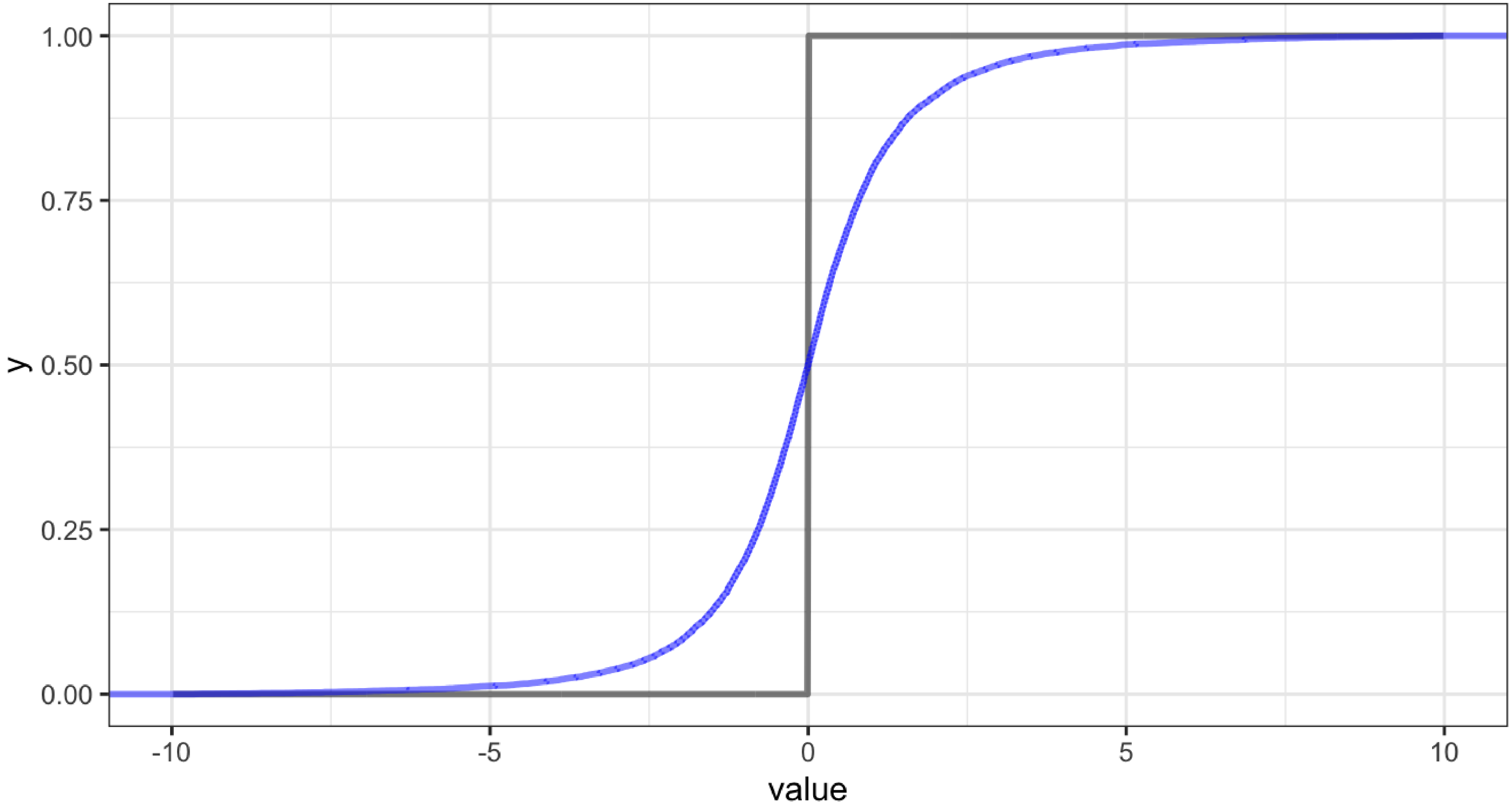
$$\text{CRPS} = \int_{-\infty}^{\infty} \left(F_{\hat{y}}(z) - 1_{z \geq y}\right)^2 dz$$

where $F_{\hat{y}}$ is the CDF of $\hat{y}$ (the posterior predictive distribution for y) and $1_{z \geq Y}$ is an indicator function which equals 1 when $z \geq y$, the true/observed value of y.

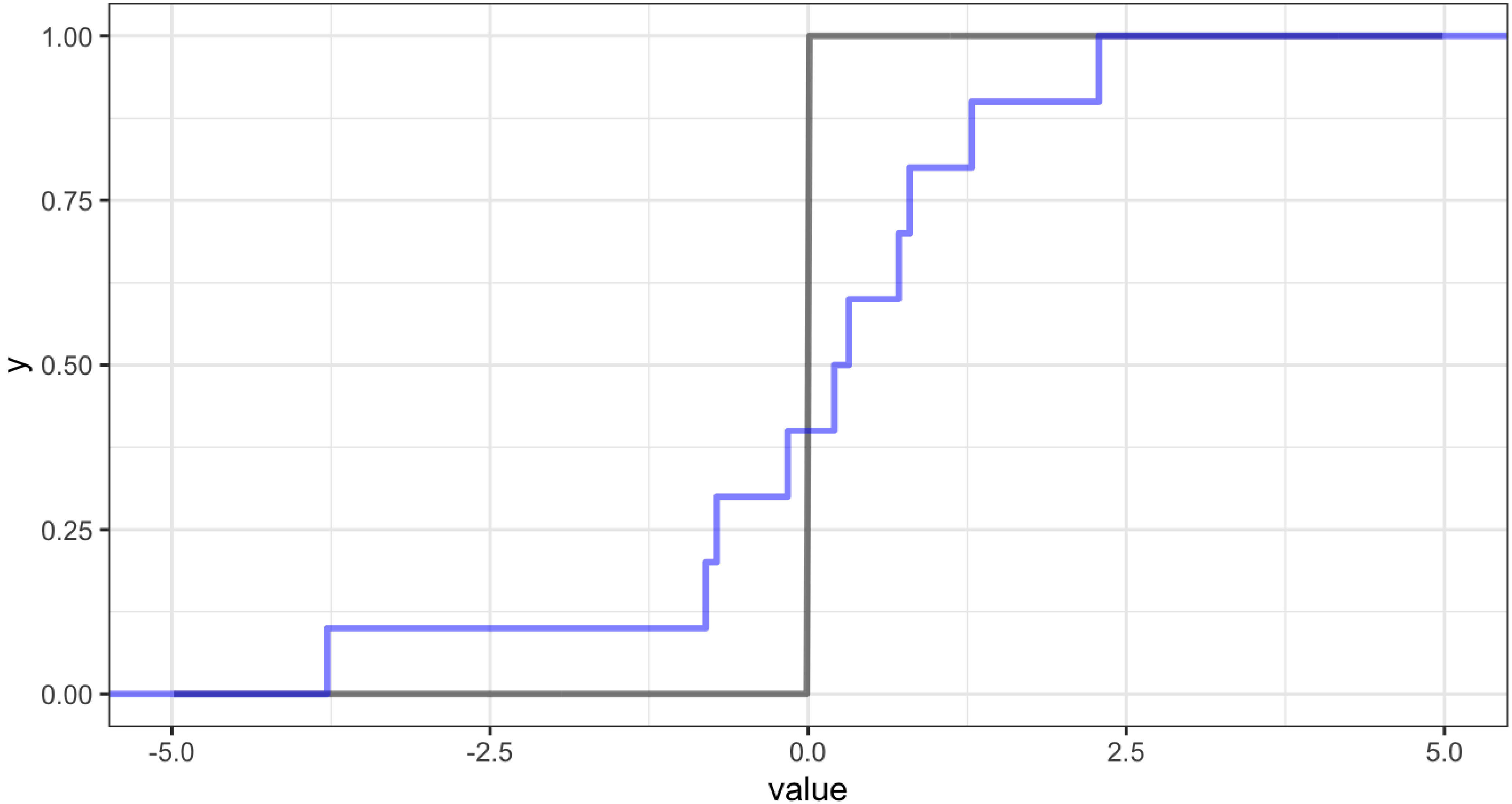
Since this calculates a score for a single probabilistic prediction we can naturally extend it to multiple predictions by calculating an average CRPS

$$\frac{1}{n} \sum_{i=1}^{n} \int_{-\infty}^{\infty} \left(F_{\hat{y}_i}(z) - 1_{z \geq y_i}\right)^2 dz$$

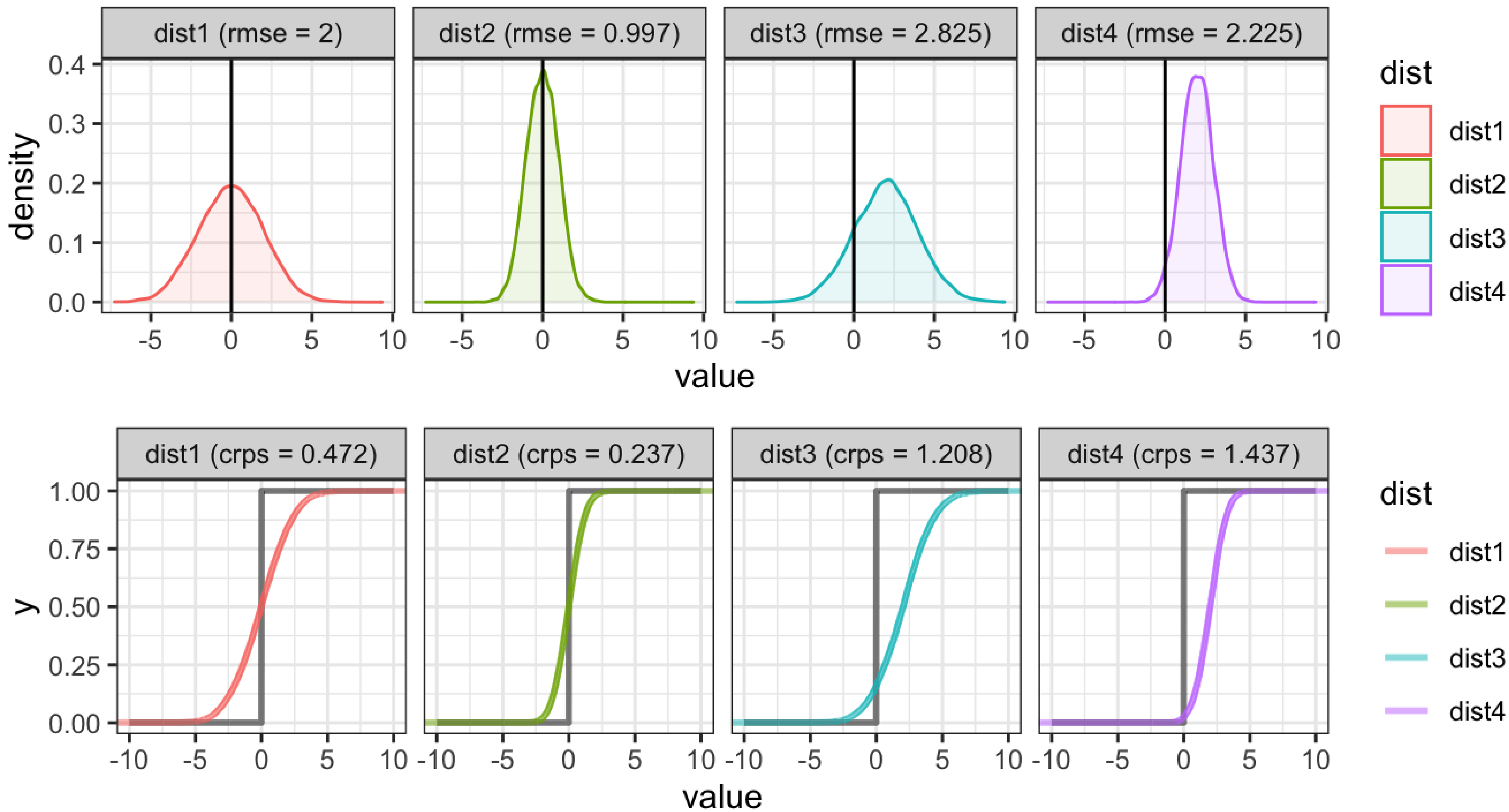
CDF vs Indicator



Empirical CDF vs Indicator

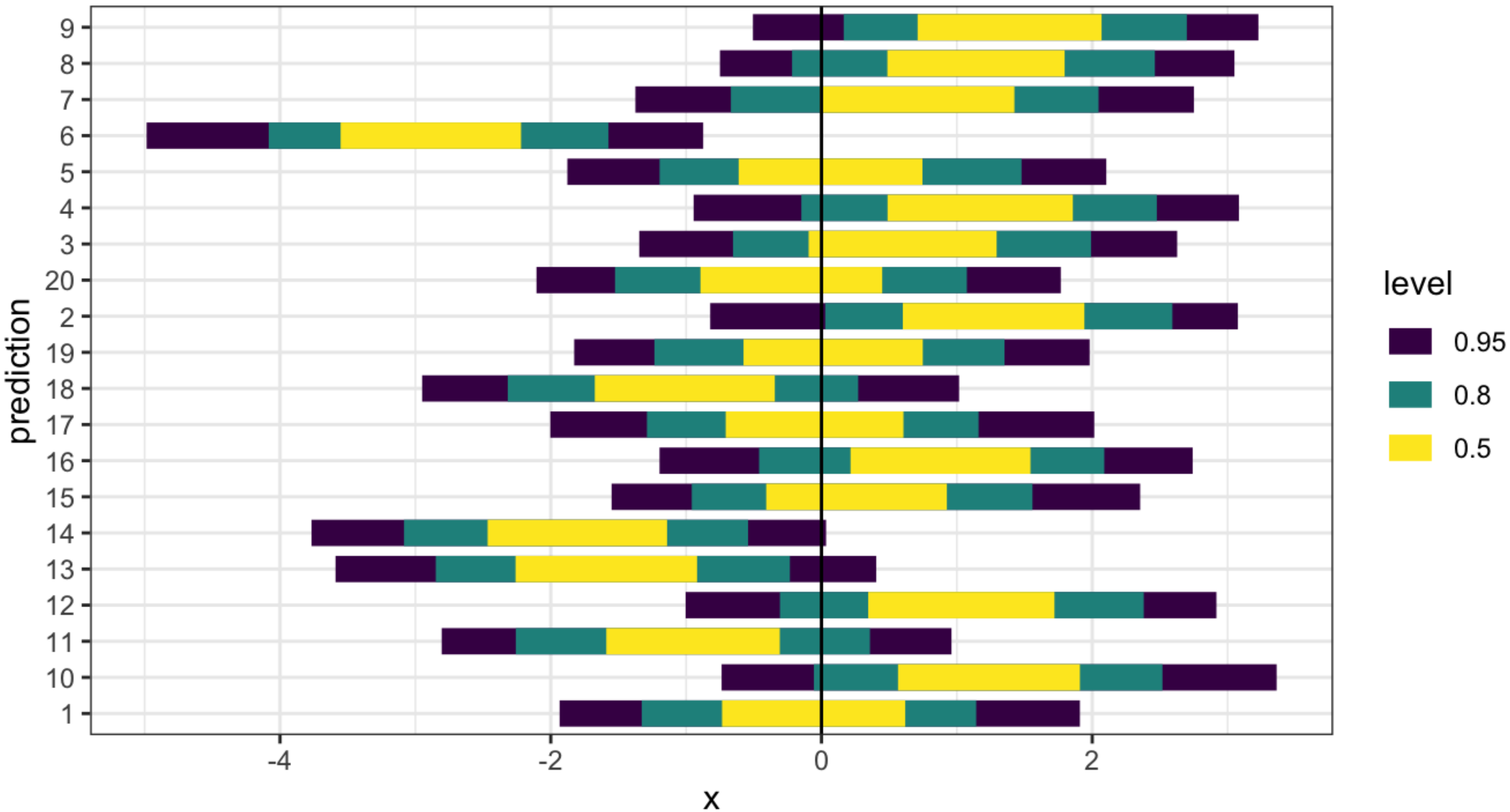


Accuracy vs. Precision



Empirical Coverage

One final method, which assesses model calibration is to examine how well credible intervals, derived from the posterior predictive distributions of the ys, capture the true/observed values.



Back to our example

RMSE - $\hat{y}$

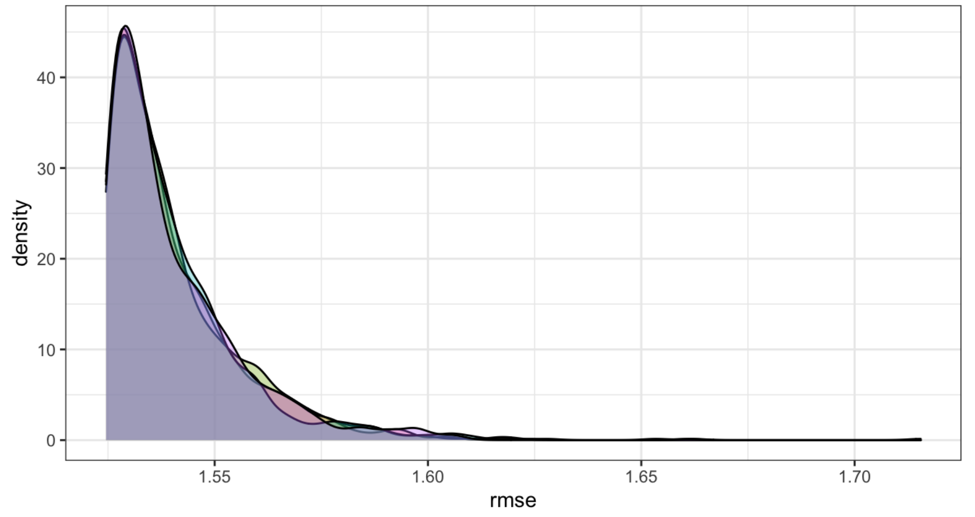
```
broom::augment(l) |>
  yardstick::rmse(y, .fitted)
## # A tibble: 1 × 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard        1.52

( b_rmse = b_post_full %>%
    group_by(.chain, .iteration) %>%
    summarize(
      rmse = sqrt( sum( (y - y_hat)^2 ) / n())
    )
)
## # A tibble: 4,000 × 3
## # Groups:   .chain [4]
##    .chain .iteration  rmse
```

RMSE - $\hat{y}$ - Results

```r
b_rmse |>
  group_by(.chain) |>
  summarize(post_mean = mean(rmse))
## # A tibble: 4 × 2
##   .chain post_mean
##    <int>     <dbl>
## 1      1      1.54
## 2      2      1.54
## 3      3      1.54
## 4      4      1.54
```

```r
ggplot(b_rmse) +
  geom_density(
    aes(x=rmse, fill=as.factor(.chain
    alpha=0.33
  ) +
  guides(fill="none")
```



CRPS - $\hat{y}$

```r
( b_crps = b_post_full |>
    group_by(.chain, x) |>
    summarise(
      crps = calc_crps(y_hat, y)
    )
)
## # A tibble: 400 × 3
## # Groups:   .chain [4]
##     .chain     x  crps
##      <int> <int> <dbl>
##   1      1     1 2.10
##   2      1     2 0.934
##   3      1     3 1.60
##   4      1     4 2.14
##   5      1     5 1.03
##   6      1     6 0.113
##   7      1     7 1.38
##   8      1     8 0.156
```

```r
b_crps |>
  group_by(.chain) |>
  summarize(
    avg_crps = mean(crps)
  )
## # A tibble: 4 × 2
##   .chain avg_crps
##    <int>    <dbl>
## 1      1     1.19
## 2      2     1.19
## 3      3     1.19
## 4      4     1.19
```

Empirical Coverage - $\hat{y}$

```
( b_cover = b_post_full %>%
    group_by(x, y) %>%
    tidybayes::mean_hdi(
      y_hat, .prob = c(0.5,0.9,0.95)
    )
)
## # A tibble: 300 × 8
##         x       y   y_hat .lower .upper .width .point .interval
##     <int>   <dbl>   <dbl>  <dbl>  <dbl>  <dbl> <chr>  <chr>
##   1     1 -3.24   -0.963 -1.14  -0.735    0.5 mean   hdi
##   2     2 -2.00   -0.894 -1.07  -0.669    0.5 mean   hdi
##   3     3 -2.59   -0.826 -1.02  -0.630    0.5 mean   hdi
##   4     4 -3.07   -0.758 -0.947 -0.562    0.5 mean   hdi
##   5     5 -1.88   -0.689 -0.847 -0.467    0.5 mean   hdi
##   6     6 -0.807  -0.621 -0.771 -0.398    0.5 mean   hdi
##   7     7 -2.09   -0.552 -0.745 -0.378    0.5 mean   hdi
##   8     8 -0.227  -0.484 -0.667 -0.306    0.5 mean   hdi
##   9     9  0.333  -0.415 -0.594 -0.240    0.5 mean   hdi
```

Empirical Coverage - $\hat{y}$ - Results

```
b_cover %>%
  mutate(contains = y >= .lower & y <= .upper) %>%
  group_by(prob = .width) %>%
  summarize(
    emp_cov = sum(contains)/n()
  )
## # A tibble: 3 × 2
##    prob emp_cov
##   <dbl>   <dbl>
## 1  0.5     0.02
## 2  0.9     0.11
## 3  0.95    0.14
```

What went wrong now?