

tidyposterior

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February 22, 2019

Intro

Bayesian analysis is used here to answer the question: “When looking at resampling results, are the differences between models ‘real’?” To answer this, a model can be created where the outcome is the resampling statistics (e.g. accuracy or RMSE). These values are explained by the model types. In doing this, we can get parameter estimates for each model’s effect on performance and make statistical and practical comparisons between models.

function summaries

perf_mod() - Bayesian analysis of resampling statistics

tidy(perf_mod) - Extract posterior distributions for models

contrast_models() - Estimate the difference between models

summary(posterior) - Summarize the posterior distributions of model statistics

summary(posterior_diff) - Summarize posterior differences of model differences

ggplot(posterior) - Visualize the posterior distributions of model statistics

ggplot(posterior_diff) - Visualize the posterior distributions of model differences

no_trans, logit_trans, Fisher_trans, ln_trans, inv_trans - simple transformations

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This package can be used to conduct post hoc analyses of resampling results generated by models.

For example, if two models are evaluated with the root mean squared error (RMSE) using 10-fold cross-validation, there are 10 paired statistics. These can be used to make comparisons between models without involving a test set.

There is a rich literature on the analysis of model resampling results such as McLachlan’s Discriminant Analysis and Statistical Pattern Recognition and the references therein. This package follows the spirit of Benavoli et al (2017).

tidyposterior uses Bayesian generalized linear models for this purpose and can be considered an upgraded version of the caret::resamples function. The package works with rsample objects natively but any results in a data frame can be used.

Summary of Time for a Change: a Tutorial for Comparing Multiple Classifiers Through Bayesian Analysis

Abstract

The machine learning community adopted the use of null hypothesis significance testing (NHST) in order to ensure the statistical validity of results. Many scientific fields however realized the shortcomings of frequentist reasoning and in the most radical cases even banned its use in publications. We should do the same: just as we have embraced the Bayesian paradigm in the development of new machine learning methods, so we should also use it in the analysis of our own results. We argue for abandonment of NHST by exposing its fallacies and, more importantly, offer better—more sound and useful—alternatives for it.

Pitfalls with Frequentist Analysis of Experimental Results

- Due to the overlapping nature of cross validation, we can not consider each fold to be independent from each other. Therefore when comparing results across many data sets we shouldn't use the t-test, but instead use the correlation t-test:

$$t(x, \mu) = \frac{\bar{x} - \mu}{\sqrt{\hat{\sigma}^2 (\frac{1}{n} + \frac{\rho}{1 - \rho})}}$$

given the heuristic correlation parameter $\rho = \frac{n_{te}}{n_{tot}}$ where $n_{tot} = n_{te} + n_{tr}$

TODO:

- Figure out why tek isn't running properly
- summarize the rest of the paper
- get the Gamma family performance model working

Example 1

```
# load library
library(tidyverse)
library(tidytext)

## -- Attaching packages -----
## v ggplot2 3.1.0      v purrr  0.3.0
## v tibble  2.0.1      v dplyr  0.8.0.1
## v tidyr   0.8.2      v stringr 1.4.0
## v readr   1.3.1      v forcats 0.4.0

## -- Conflicts -----
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()     masks stats::lag()

# attach data
data("precise_example")

# look at data
precise_example %>% head()

## # A tibble: 6 x 29
##   splits id glm_Accuracy glm_Kappa glm_ROC glm_Sens glm_Spec glm_PRAUC
## * <lgl> <chr>      <dbl>      <dbl> <dbl> <dbl> <dbl> <dbl>
```

```
## 1 NA Fold~ 0.722 0.328 0.798 0.729 0.720 0.489
## 2 NA Fold~ 0.696 0.290 0.778 0.720 0.691 0.456
## 3 NA Fold~ 0.701 0.297 0.790 0.723 0.696 0.486
## 4 NA Fold~ 0.704 0.316 0.795 0.763 0.691 0.497
## 5 NA Fold~ 0.721 0.324 0.797 0.722 0.721 0.481
## 6 NA Fold~ 0.711 0.303 0.780 0.706 0.712 0.484
## # ... with 21 more variables: glm_Precision <dbl>, glm_Recall <dbl>,
## # glm_F <dbl>, knn_Accuracy <dbl>, knn_Kappa <dbl>, knn_ROC <dbl>,
## # knn_Sens <dbl>, knn_Spec <dbl>, knn_PRAUC <dbl>, knn_Precision <dbl>,
## # knn_Recall <dbl>, knn_F <dbl>, nnet_Accuracy <dbl>, nnet_Kappa <dbl>,
## # nnet_ROC <dbl>, nnet_Sens <dbl>, nnet_Spec <dbl>, nnet_PRAUC <dbl>,
## # nnet_Precision <dbl>, nnet_Recall <dbl>, nnet_F <dbl>
```

```
# get classification accuracy results for each cross validated fold
```

```
accuracy <- precise_example %>%
  select(id, contains("Accuracy")) %>%
  setNames(tolower(gsub("_Accuracy$", "", names(.))))
```

```
accuracy
```

```
## # A tibble: 10 x 4
##   id      glm knn nnet
##   <chr> <dbl> <dbl> <dbl>
## 1 Fold01 0.722 0.478 0.783
## 2 Fold02 0.696 0.492 0.766
## 3 Fold03 0.701 0.459 0.781
## 4 Fold04 0.704 0.454 0.783
## 5 Fold05 0.721 0.468 0.789
## 6 Fold06 0.711 0.474 0.776
## 7 Fold07 0.702 0.489 0.775
## 8 Fold08 0.718 0.458 0.785
## 9 Fold09 0.720 0.508 0.786
## 10 Fold10 0.719 0.440 0.777
```

```
# model accuracy results
```

```
acc_model <- perf_mod(accuracy, seed = 13311, verbose = FALSE)
```

```
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 1).
## Chain 1:
## Chain 1: Gradient evaluation took 6.4e-05 seconds
## Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.64 seconds.
## Chain 1: Adjust your expectations accordingly!
## Chain 1:
## Chain 1:
## Chain 1: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 1: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 1: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 1: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 1: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 1: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 1: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 1: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 1: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 1: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 1: Iteration: 1800 / 2000 [ 90%] (Sampling)
```

```

## Chain 1: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 1:
## Chain 1: Elapsed Time: 2.53189 seconds (Warm-up)
## Chain 1: 0.460603 seconds (Sampling)
## Chain 1: 2.99249 seconds (Total)
## Chain 1:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 2).
## Chain 2:
## Chain 2: Gradient evaluation took 4.5e-05 seconds
## Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.45 seconds.
## Chain 2: Adjust your expectations accordingly!
## Chain 2:
## Chain 2:
## Chain 2: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 2: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 2: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 2: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 2: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 2: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 2: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 2: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 2: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 2: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 2: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 2: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 2:
## Chain 2: Elapsed Time: 2.53882 seconds (Warm-up)
## Chain 2: 0.428695 seconds (Sampling)
## Chain 2: 2.96752 seconds (Total)
## Chain 2:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 3).
## Chain 3:
## Chain 3: Gradient evaluation took 3.9e-05 seconds
## Chain 3: 1000 transitions using 10 leapfrog steps per transition would take 0.39 seconds.
## Chain 3: Adjust your expectations accordingly!
## Chain 3:
## Chain 3:
## Chain 3: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 3: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 3: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 3: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 3: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 3: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 3: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 3: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 3: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 3: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 3: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 3: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 3:
## Chain 3: Elapsed Time: 2.346 seconds (Warm-up)
## Chain 3: 0.356749 seconds (Sampling)

```

```
## Chain 3:                2.70275 seconds (Total)
## Chain 3:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 4).
## Chain 4:
## Chain 4: Gradient evaluation took 3.5e-05 seconds
## Chain 4: 1000 transitions using 10 leapfrog steps per transition would take 0.35 seconds.
## Chain 4: Adjust your expectations accordingly!
## Chain 4:
## Chain 4:
## Chain 4: Iteration:    1 / 2000 [ 0%] (Warmup)
## Chain 4: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 4: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 4: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 4: Iteration:   800 / 2000 [ 40%] (Warmup)
## Chain 4: Iteration:  1000 / 2000 [ 50%] (Warmup)
## Chain 4: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 4: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 4: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 4: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 4: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 4: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 4:
## Chain 4: Elapsed Time: 2.55038 seconds (Warm-up)
## Chain 4:                0.256164 seconds (Sampling)
## Chain 4:                2.80654 seconds (Total)
## Chain 4:
```

```
# extract posterior distributions
accuracy_dists <- tidy(acc_model)

# credible intervals for accuracy per model
summary(accuracy_dists)
```

```
## # A tibble: 3 x 4
##   model mean lower upper
##   <chr> <dbl> <dbl> <dbl>
## 1 glm   0.711 0.704 0.719
## 2 knn   0.472 0.464 0.480
## 3 nnet  0.780 0.772 0.788
```

Plotting

```
# create plot function
plot_model_posteriors <- function(data, model_chosen, geom_chosen = geom_point){
  data %>%
    filter(model %in% model_chosen) %>%
    ggplot(aes(x = model, y = posterior)) +
    geom_chosen(alpha = 0.5, col = "#4B0082") +
    scale_y_continuous(limits = c(0.4, 1))
}

# generate mapper
pmp <- as_mapper(partial(plot_model_posteriors, accuracy_dists))
```

```

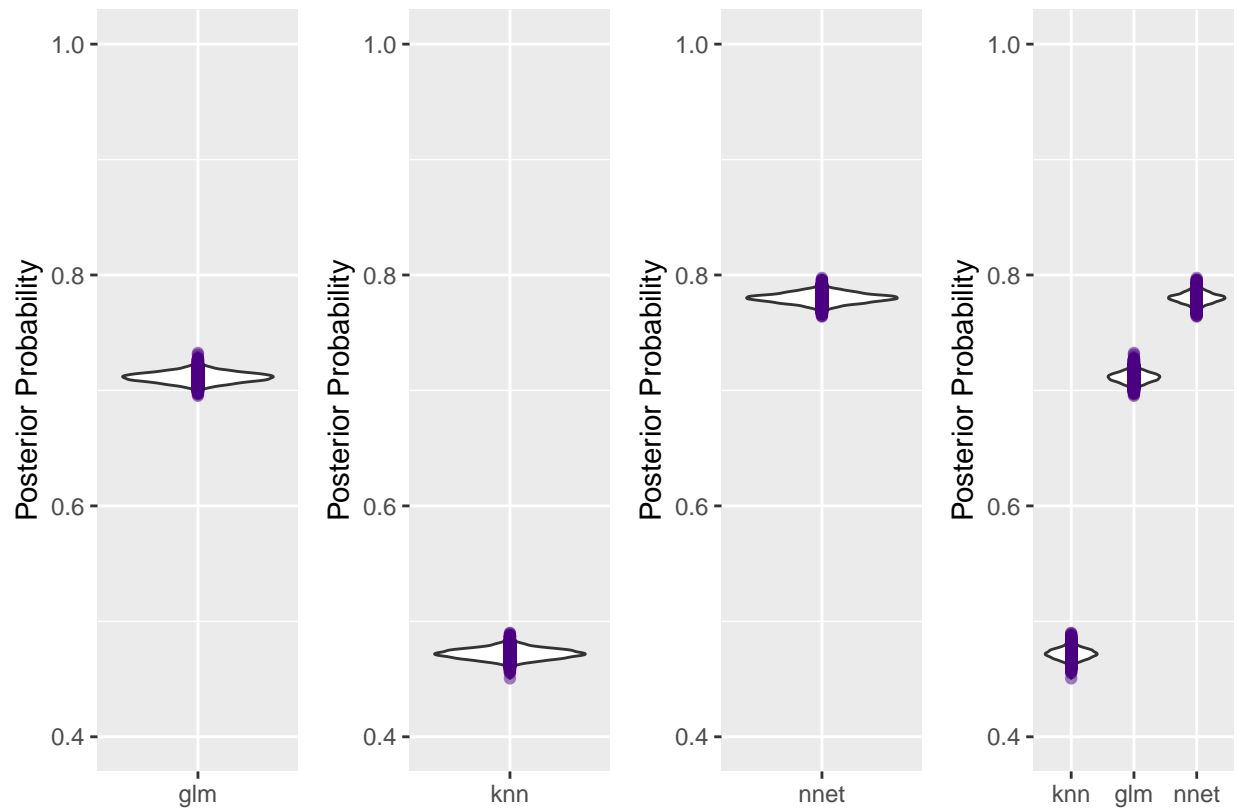
# grab model list
model_list <- unique(accuracy_dists$model)

# map
posterior_plots <- map(model_list, pmp)

# create all together
all_together <- accuracy_dists %>% plot_model_posteriors(model_list)

gridExtra::grid.arrange(posterior_plots[[1]], posterior_plots[[2]], posterior_plots[[3]], all_together,

```



Getting Started

The example that will be used is from the analysis of a fairly large classification data set using 10 fold cross validation with three models.

```

# check area under ROC curve
rocs <- precise_example %>%
  select(id, contains("ROC")) %>%
  set_names(tolower(gsub("_ROC$", "", names(.))))

rocs

## # A tibble: 10 x 4

```

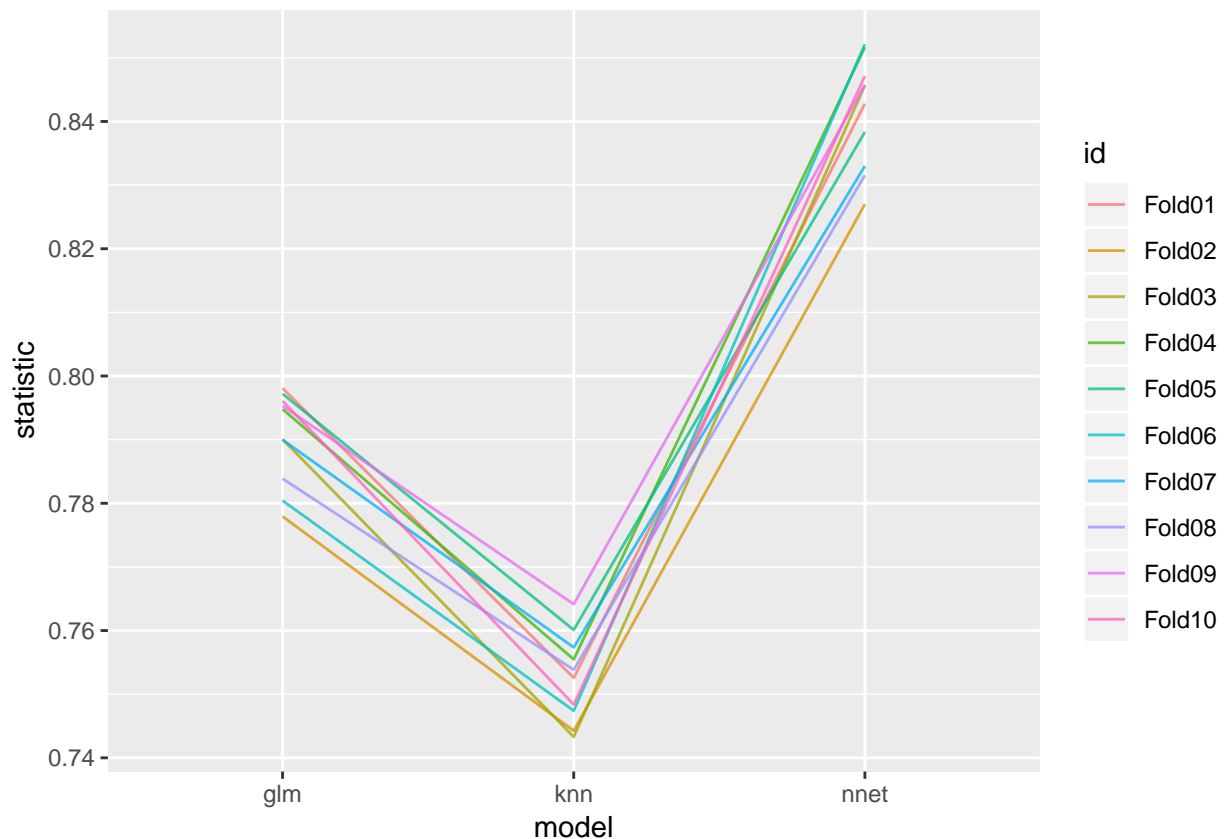
```
##   id      glm   knn  nnet
##   <chr> <dbl> <dbl> <dbl>
## 1 Fold01 0.798 0.753 0.843
## 2 Fold02 0.778 0.744 0.827
## 3 Fold03 0.790 0.743 0.846
## 4 Fold04 0.795 0.755 0.852
## 5 Fold05 0.797 0.760 0.838
## 6 Fold06 0.780 0.747 0.852
## 7 Fold07 0.790 0.757 0.833
## 8 Fold08 0.784 0.754 0.832
## 9 Fold09 0.795 0.764 0.846
## 10 Fold10 0.796 0.748 0.847
```

```
# gather ROCs for plotting comparison
```

```
rocs_stacked <- gather(rocs, key = model, value = statistic, -id)
```

```
# plot
```

```
ggplot(rocs_stacked, aes(x = model, y = statistic, group = id, col = id)) +
  geom_line(alpha = 0.75)
```



Since the lines are fairly parallel, there is likely to be a strong resample-to-resample effect. Note that the variation is fairly small; the within-model results don't vary a lot and are not near the ceiling of performance (i.e. an AUC of one). It also seems pretty clear that the models are producing different levels of performance. There also seems to be roughly equal variation for each model despite the difference in performance.

A Basic Linear Model

When looking at resampling results, are the differences between models “real”?

To answer this, a model can be created where the outcome is the resampling statistics (area under the ROC curve). These values are explained by the model types. In doing this, we can get the parameter estimates for each model’s effect on the resampled ROC values and make statistical and practical comparisons between models.

We will try a simple linear model with Gaussian errors that has a random effect for the resamples so that the within resample correlation can be estimated. Although the outcome is bounded in the interval $[0, 1]$, the variability of these estimates might be precise enough to achieve a well fitting model.

To fit the model, `perf_mod` will be used to fit a model using the `stan_glmer` function in the `rstanarm` package:

```
# fit model
roc_model <- perf_mod(rocs, seed = 2824)

##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 1).
## Chain 1:
## Chain 1: Gradient evaluation took 4.5e-05 seconds
## Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.45 seconds.
## Chain 1: Adjust your expectations accordingly!
## Chain 1:
## Chain 1:
## Chain 1: Iteration:    1 / 2000 [  0%] (Warmup)
## Chain 1: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 1: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 1: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 1: Iteration:   800 / 2000 [ 40%] (Warmup)
## Chain 1: Iteration:  1000 / 2000 [ 50%] (Warmup)
## Chain 1: Iteration:  1001 / 2000 [ 50%] (Sampling)
## Chain 1: Iteration:  1200 / 2000 [ 60%] (Sampling)
## Chain 1: Iteration:  1400 / 2000 [ 70%] (Sampling)
## Chain 1: Iteration:  1600 / 2000 [ 80%] (Sampling)
## Chain 1: Iteration:  1800 / 2000 [ 90%] (Sampling)
## Chain 1: Iteration:  2000 / 2000 [100%] (Sampling)
## Chain 1:
## Chain 1: Elapsed Time: 4.7853 seconds (Warm-up)
## Chain 1:                0.501577 seconds (Sampling)
## Chain 1:                5.28687 seconds (Total)
## Chain 1:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 2).
## Chain 2:
## Chain 2: Gradient evaluation took 5.6e-05 seconds
## Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.56 seconds.
## Chain 2: Adjust your expectations accordingly!
## Chain 2:
## Chain 2:
## Chain 2: Iteration:    1 / 2000 [  0%] (Warmup)
## Chain 2: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 2: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 2: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 2: Iteration:   800 / 2000 [ 40%] (Warmup)
```



```

## Chain 2: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 2: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 2: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 2: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 2: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 2: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 2: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 2:
## Chain 2: Elapsed Time: 4.27489 seconds (Warm-up)
## Chain 2: 0.413705 seconds (Sampling)
## Chain 2: 4.6886 seconds (Total)
## Chain 2:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 3).
## Chain 3:
## Chain 3: Gradient evaluation took 4.4e-05 seconds
## Chain 3: 1000 transitions using 10 leapfrog steps per transition would take 0.44 seconds.
## Chain 3: Adjust your expectations accordingly!
## Chain 3:
## Chain 3:
## Chain 3: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 3: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 3: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 3: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 3: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 3: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 3: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 3: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 3: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 3: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 3: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 3: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 3:
## Chain 3: Elapsed Time: 5.3229 seconds (Warm-up)
## Chain 3: 0.441724 seconds (Sampling)
## Chain 3: 5.76462 seconds (Total)
## Chain 3:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 4).
## Chain 4:
## Chain 4: Gradient evaluation took 3.3e-05 seconds
## Chain 4: 1000 transitions using 10 leapfrog steps per transition would take 0.33 seconds.
## Chain 4: Adjust your expectations accordingly!
## Chain 4:
## Chain 4:
## Chain 4: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 4: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 4: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 4: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 4: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 4: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 4: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 4: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 4: Iteration: 1400 / 2000 [ 70%] (Sampling)

```

```
## Chain 4: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 4: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 4: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 4:
## Chain 4: Elapsed Time: 4.08531 seconds (Warm-up)
## Chain 4: 0.266426 seconds (Sampling)
## Chain 4: 4.35173 seconds (Total)
## Chain 4:

# The `stan_glmer` model is contained in the element `roc_model$stan`
roc_model$stan
```

```
## stan_glmer
## family:      gaussian [identity]
## formula:     statistic ~ model + (1 | id)
## observations: 30
## -----
##              Median MAD_SD
## (Intercept) 0.8      0.0
## modelknn    0.0      0.0
## modelnnet   0.1      0.0
##
## Auxiliary parameter(s):
##              Median MAD_SD
## sigma 0.0      0.0
##
## Error terms:
## Groups   Name      Std.Dev.
## id       (Intercept) 0.0044
## Residual                0.0069
## Num. levels: id 10
##
## Sample avg. posterior predictive distribution of y:
##              Median MAD_SD
## mean_PPD 0.8      0.0
##
## -----
## * For help interpreting the printed output see ?print.stanreg
## * For info on the priors used see ?prior_summary.stanreg
```

To ensure the validity of this fit, the `shinystan` package can be used to generate an interactive assessment of the model results. One other thing that we can do is to examine the posterior distributions to see if they make sense in terms of the range of values.

Getting the Posterior Distributions

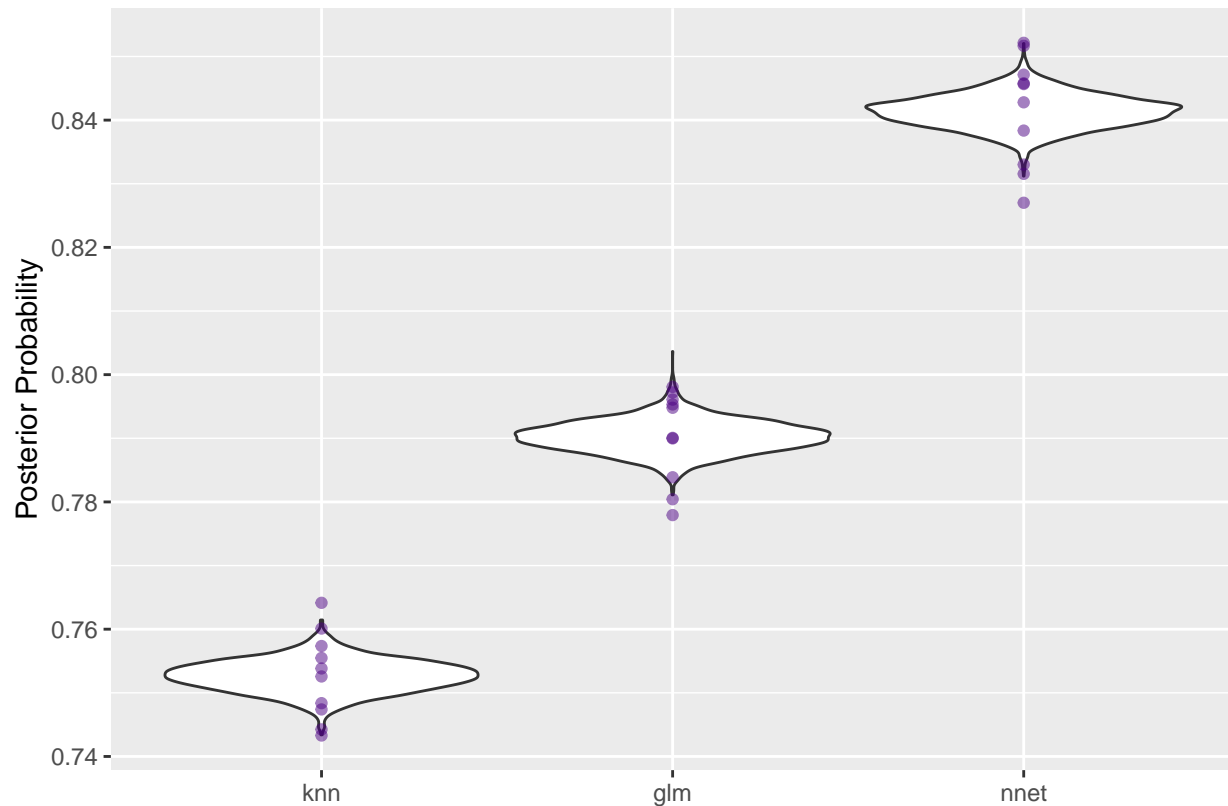
```
# the tidy function can be used to extract the distributions into a simple data frame
roc_post <- tidy(roc_model)

# plot
ggplot(roc_post) +
  # add the observed data to check for consistency
  geom_point(
    data = rocs_stacked,
```

```

aes(x = model, y = statistic),
alpha = 0.5, col = "#4B0082"
)

```



These results look fairly reasonable given that we estimated a common variance for each of the models.

Comparing Models

We will compare the generalized linear model with the neural network. Before doing so, it helps to specify what a real difference between models would be. Suppose that a 2% increase in accuracy was considered to be substantive results. We can add this into the analysis.

```

# compute the posterior for the difference in RMSE for the two models
glm_v_nnet <- contrast_models(roc_model, "nnet", "glm")

```

```

# look at data
head(glm_v_nnet)

```

```

##   difference model_1 model_2
## 1 0.05353329   nnet    glm
## 2 0.04916246   nnet    glm
## 3 0.05211164   nnet    glm
## 4 0.05317553   nnet    glm
## 5 0.05411325   nnet    glm
## 6 0.05102618   nnet    glm

```

The summary function can be used to quantify this difference. It has an argument called size where we can add our belief about the size of a true difference.

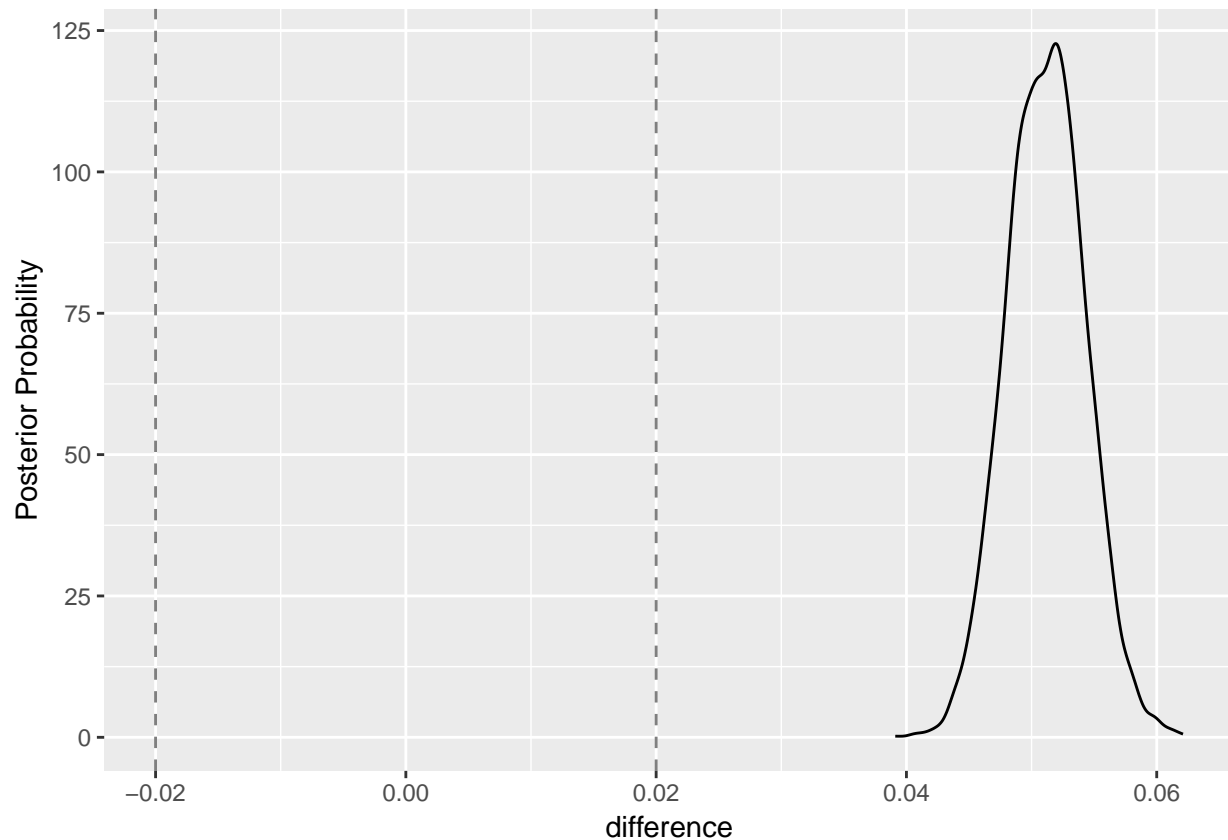
```
summary(glm_v_nnet, size = 0.02)
```

```
## # A tibble: 1 x 9
##   contrast probability    mean lower upper size pract_neg pract_equiv
##   <chr>          <dbl> <dbl> <dbl> <dbl> <dbl>      <dbl>      <dbl>
## 1 nnet vs~          1 0.0511 0.0461 0.0562 0.02          0          0
## # ... with 1 more variable: pract_pos <dbl>
```

The probability column indicates the proportion of the posterior distribution that is greater than 0. This result indicates that the entire distribution is larger than one. The credible intervals reflect the large difference in the area under the ROC curves for these models. The column pract_neg reflects the area where the posterior distribution is *less* than -2% (i.e. practically negative). Similarly, the pract_pos column shows that most of the area is greater than 2% which leads us to believe that this is truly a substantial difference in performance. The pract_equiv reflects how much of the posterior is in [-2%, 2%]. If this were near one, it might indicate that the models are not practically different based on the yardstick of 2%.

```
# plot posterior of the differences
```

```
ggplot(glm_v_nnet, size = 0.02)
```



Different Bayesian Models

The dataset `noisy_example` contains the results of a series of regression models that were created from a small dataset with considerable variability. For resampling, 10 repeats of 10-fold cross validation were used

to estimate performance. We will compare models using the root mean squared error.

```
# load data
data("noisy_example")

# look at data
noisy_example %>% head()

## # A tibble: 6 x 15
##   splits id    id2    bag_RMSE bag_Rsquared bag_MAE cubist_RMSE
## * <lgl> <chr> <chr>    <dbl>         <dbl>    <dbl>    <dbl>
## 1 NA     Repe~ Fold~    27.7         0.0205    22.6     14.0
## 2 NA     Repe~ Fold~    16.3         0.105     12.3      9.74
## 3 NA     Repe~ Fold~    21.6         0.224     18.2     12.7
## 4 NA     Repe~ Fold~    17.7         0.117     16.9     16.5
## 5 NA     Repe~ Fold~    14.0         0.101     12.6     19.0
## 6 NA     Repe~ Fold~    27.8         0.728     18.4     23.6
## # ... with 8 more variables: cubist_Rsquared <dbl>, cubist_MAE <dbl>,
## #   mars_RMSE <dbl>, mars_Rsquared <dbl>, mars_MAE <dbl>, nnet_RMSE <dbl>,
## #   nnet_Rsquared <dbl>, nnet_MAE <dbl>

# grab RMSEs
rmses <- noisy_example %>%
  select(id, id2, contains("RMSE")) %>%
  set_names(tolower(gsub("_RMSE$", "", names(.))))

rmses %>% head()

## # A tibble: 6 x 6
##   id    id2    bag cubist  mars  nnet
##   <chr>  <chr> <dbl> <dbl> <dbl> <dbl>
## 1 Repeat01 Fold01 27.7 14.0 25.3 24.4
## 2 Repeat02 Fold01 16.3 9.74 13.1 13.4
## 3 Repeat03 Fold01 21.6 12.7 12.7 15.1
## 4 Repeat04 Fold01 17.7 16.5 19.8 15.4
## 5 Repeat05 Fold01 14.0 19.0 17.2 14.9
## 6 Repeat06 Fold01 27.8 23.6 26.9 29.7

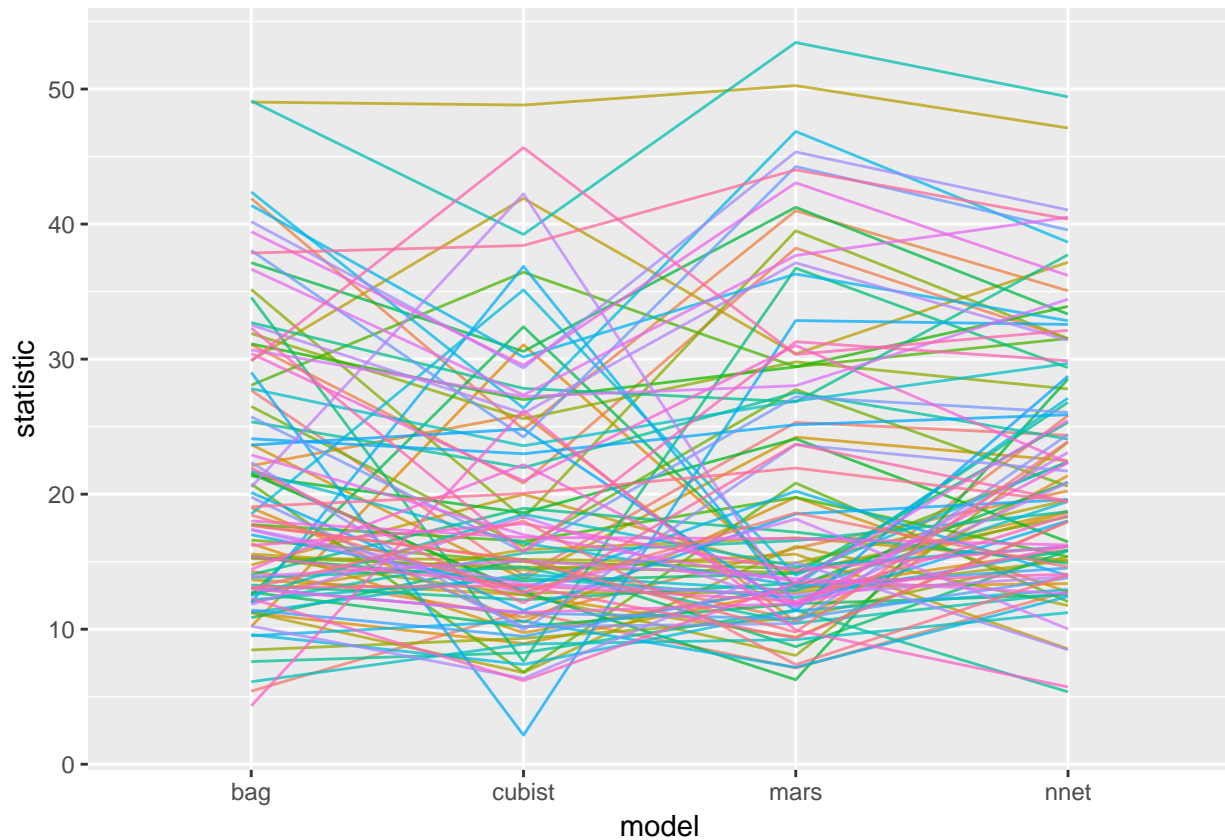
# gather RMSE for comparison
stacked_rmse <- gather(rmses, key = model, value = statistic, -c(id, id2))

# summarize
mean_rmse <- stacked_rmse %>%
  group_by(model) %>%
  summarise(statistic = mean(statistic))

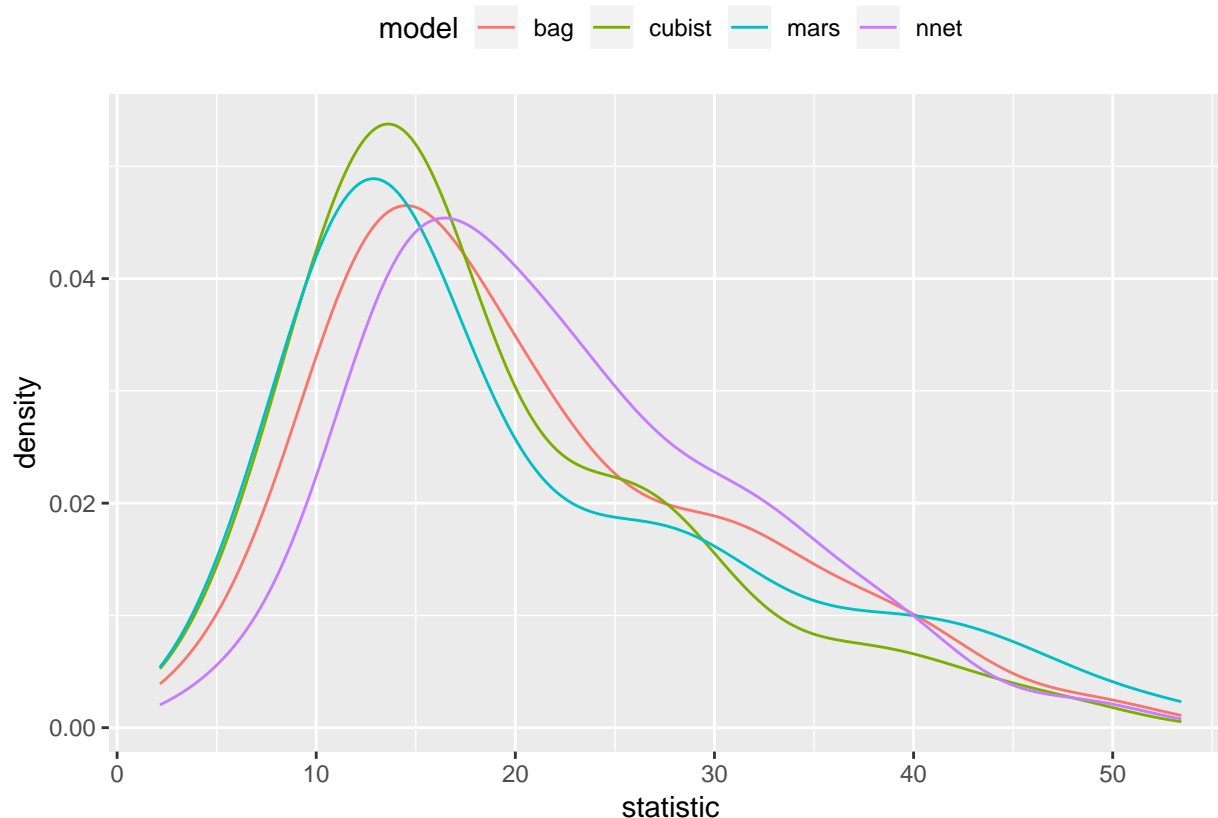
mean_rmse %>% head()

## # A tibble: 4 x 2
##   model statistic
##   <chr>    <dbl>
## 1 bag      21.0
## 2 cubist   18.7
## 3 mars     20.5
## 4 nnet     22.3
```

```
# plot RMSE across different runs
ggplot(stacked_rmse, aes(
  x = model, y = statistic,
  group = paste(id, id2),
  col = paste(id, id2))) +
  geom_line(alpha = 0.75) +
  theme(legend.position = "none")
```



```
# plot RMSE densities across runs
ggplot(stacked_rmse, aes(col = model, x = statistic)) +
  geom_line(stat = "density", trim = FALSE) +
  theme(legend.position = "top")
```



A few observations: - The RMSE values vary 5-fold over the resampling results - Many of the lines cross, indicating that the resample-to-resample variability might be larger than the model-to-model variability - The violin plots show right skewed distributions that, given the variability, are approaching the asymptote of 0.

A First Model

It makes sense to use a probability model that is consistent with the characteristics of the data (in terms of skewness). Instead of using a symmetric distribution for the data (such as a Gaussian), a potentially right skewed probability model might make more sense. A gamma distribution is a reasonable choice and can be fit using the generalized linear model embedded in `perf_mod`. This also requires a link function to be chosen to model the data. The canonical link for this distribution is the inverse transformation and this will be our choice.

```
# fit model using family arg. The default link is the inverse and no transformation is used
# gamma_model <- perf_mod(rmses[, -2], family = Gamma(), seed = 74)
```

```
# get the posterior distributions of the mean parameters
# gamma_post <- tidy(gamma_model, seed = 3750)
# gamma_mean <- summary(gamma_post)
# gamma_mean
```

Are these values consistent with the data? Let's look at the posterior distribution and overlay the observed and predicted mean RMSE values

```
# ggplot(gamma_post) +
#   geom_point(data = gamma_mean, aes(y = mean), alpha = 0.5) +
#   geom_point(data = mean_rmse, aes(y = statistic),
```

```
# col = "red", pch = 4, cex = 3)
```

The observed mean is not close to the center of the skewed posterior distributions. Let's try something else.

Transforming the Data

Another approach is to transform the RMSE values to something model symmetric and model the data on a different scale. A log transform will be used here using the built-in object `ln_trans`. In using this option, the posterior distributions are computed on the log scale and is automatically back-transformed into the original units. By not passing family to the function, we are using a Gaussian model.

```
log_linear_model <- perf_mod(rmses, transform = ln_trans, seed = 74)
```

```
## Warning: Since no specific resampling method is known,the ID variables are
## collapsed into one column.

##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 1).
## Chain 1:
## Chain 1: Gradient evaluation took 0.000113 seconds
## Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 1.13 seconds.
## Chain 1: Adjust your expectations accordingly!
## Chain 1:
## Chain 1:
## Chain 1: Iteration:    1 / 2000 [ 0%] (Warmup)
## Chain 1: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 1: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 1: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 1: Iteration:   800 / 2000 [ 40%] (Warmup)
## Chain 1: Iteration:  1000 / 2000 [ 50%] (Warmup)
## Chain 1: Iteration:  1001 / 2000 [ 50%] (Sampling)
## Chain 1: Iteration:  1200 / 2000 [ 60%] (Sampling)
## Chain 1: Iteration:  1400 / 2000 [ 70%] (Sampling)
## Chain 1: Iteration:  1600 / 2000 [ 80%] (Sampling)
## Chain 1: Iteration:  1800 / 2000 [ 90%] (Sampling)
## Chain 1: Iteration:  2000 / 2000 [100%] (Sampling)
## Chain 1:
## Chain 1: Elapsed Time: 2.68949 seconds (Warm-up)
## Chain 1:                2.21535 seconds (Sampling)
## Chain 1:                4.90484 seconds (Total)
## Chain 1:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 2).
## Chain 2:
## Chain 2: Gradient evaluation took 0.000101 seconds
## Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 1.01 seconds.
## Chain 2: Adjust your expectations accordingly!
## Chain 2:
## Chain 2:
## Chain 2: Iteration:    1 / 2000 [ 0%] (Warmup)
## Chain 2: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 2: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 2: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 2: Iteration:   800 / 2000 [ 40%] (Warmup)
```



```

## Chain 2: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 2: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 2: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 2: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 2: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 2: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 2: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 2:
## Chain 2: Elapsed Time: 2.51509 seconds (Warm-up)
## Chain 2: 2.09119 seconds (Sampling)
## Chain 2: 4.60629 seconds (Total)
## Chain 2:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 3).
## Chain 3:
## Chain 3: Gradient evaluation took 0.0001 seconds
## Chain 3: 1000 transitions using 10 leapfrog steps per transition would take 1 seconds.
## Chain 3: Adjust your expectations accordingly!
## Chain 3:
## Chain 3:
## Chain 3: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 3: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 3: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 3: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 3: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 3: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 3: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 3: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 3: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 3: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 3: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 3: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 3:
## Chain 3: Elapsed Time: 2.60272 seconds (Warm-up)
## Chain 3: 1.24672 seconds (Sampling)
## Chain 3: 3.84944 seconds (Total)
## Chain 3:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 4).
## Chain 4:
## Chain 4: Gradient evaluation took 0.000108 seconds
## Chain 4: 1000 transitions using 10 leapfrog steps per transition would take 1.08 seconds.
## Chain 4: Adjust your expectations accordingly!
## Chain 4:
## Chain 4:
## Chain 4: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 4: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 4: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 4: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 4: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 4: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 4: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 4: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 4: Iteration: 1400 / 2000 [ 70%] (Sampling)

```

```
## Chain 4: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 4: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 4: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 4:
## Chain 4: Elapsed Time: 2.35595 seconds (Warm-up)
## Chain 4: 2.02654 seconds (Sampling)
## Chain 4: 4.38249 seconds (Total)
## Chain 4:
```

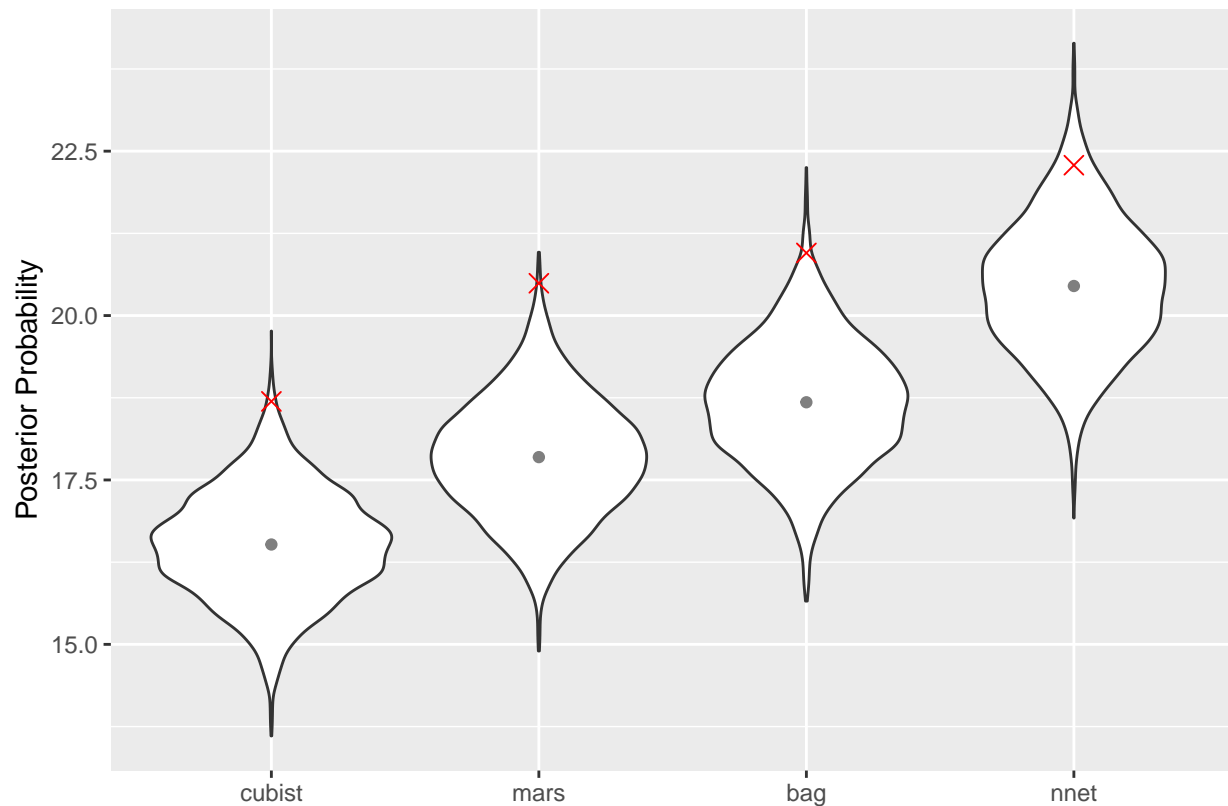
```
# look at posterior and means
```

```
log_linear_post <- tidy(log_linear_model, seed = 3750)
log_linear_mean <- summary(log_linear_post)
log_linear_mean
```

```
## # A tibble: 4 x 4
##   model mean lower upper
##   <chr> <dbl> <dbl> <dbl>
## 1 bag    18.7  17.2  20.3
## 2 cubist 16.5  15.2  17.9
## 3 mars   17.8  16.4  19.4
## 4 nnet   20.4  18.8  22.2
```

```
# plot
```

```
ggplot(log_linear_post) +
  geom_point(data = log_linear_mean, aes(y = mean), alpha = 0.5) +
  geom_point(data = mean_rmse, aes(y = statistic),
            col = "red", pch = 4, cex = 3)
```



The posteriors are a lot less skewed by the observed and estimated means are still fairly far away from one another. Since these differences are in the same direction, this would not appear to be related to the shrinkage properties of Bayesian models.

A Simple Gaussian Model

```
# fit a gaussian model for rmse estimates
linear_model <- perf_mod(rmses, seed = 74)
```

```
## Warning: Since no specific resampling method is known,the ID variables are
## collapsed into one column.
```

```
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 1).
## Chain 1:
## Chain 1: Gradient evaluation took 0.000108 seconds
## Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 1.08 seconds.
## Chain 1: Adjust your expectations accordingly!
## Chain 1:
## Chain 1:
## Chain 1: Iteration:    1 / 2000 [  0%] (Warmup)
## Chain 1: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 1: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 1: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 1: Iteration:   800 / 2000 [ 40%] (Warmup)
## Chain 1: Iteration:  1000 / 2000 [ 50%] (Warmup)
## Chain 1: Iteration:  1001 / 2000 [ 50%] (Sampling)
## Chain 1: Iteration:  1200 / 2000 [ 60%] (Sampling)
## Chain 1: Iteration:  1400 / 2000 [ 70%] (Sampling)
## Chain 1: Iteration:  1600 / 2000 [ 80%] (Sampling)
## Chain 1: Iteration:  1800 / 2000 [ 90%] (Sampling)
## Chain 1: Iteration:  2000 / 2000 [100%] (Sampling)
## Chain 1:
## Chain 1: Elapsed Time: 2.56404 seconds (Warm-up)
## Chain 1:                2.21455 seconds (Sampling)
## Chain 1:                4.77859 seconds (Total)
## Chain 1:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 2).
## Chain 2:
## Chain 2: Gradient evaluation took 0.000111 seconds
## Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 1.11 seconds.
## Chain 2: Adjust your expectations accordingly!
## Chain 2:
## Chain 2:
## Chain 2: Iteration:    1 / 2000 [  0%] (Warmup)
## Chain 2: Iteration:   200 / 2000 [ 10%] (Warmup)
## Chain 2: Iteration:   400 / 2000 [ 20%] (Warmup)
## Chain 2: Iteration:   600 / 2000 [ 30%] (Warmup)
## Chain 2: Iteration:   800 / 2000 [ 40%] (Warmup)
## Chain 2: Iteration:  1000 / 2000 [ 50%] (Warmup)
## Chain 2: Iteration:  1001 / 2000 [ 50%] (Sampling)
## Chain 2: Iteration:  1200 / 2000 [ 60%] (Sampling)
```

```

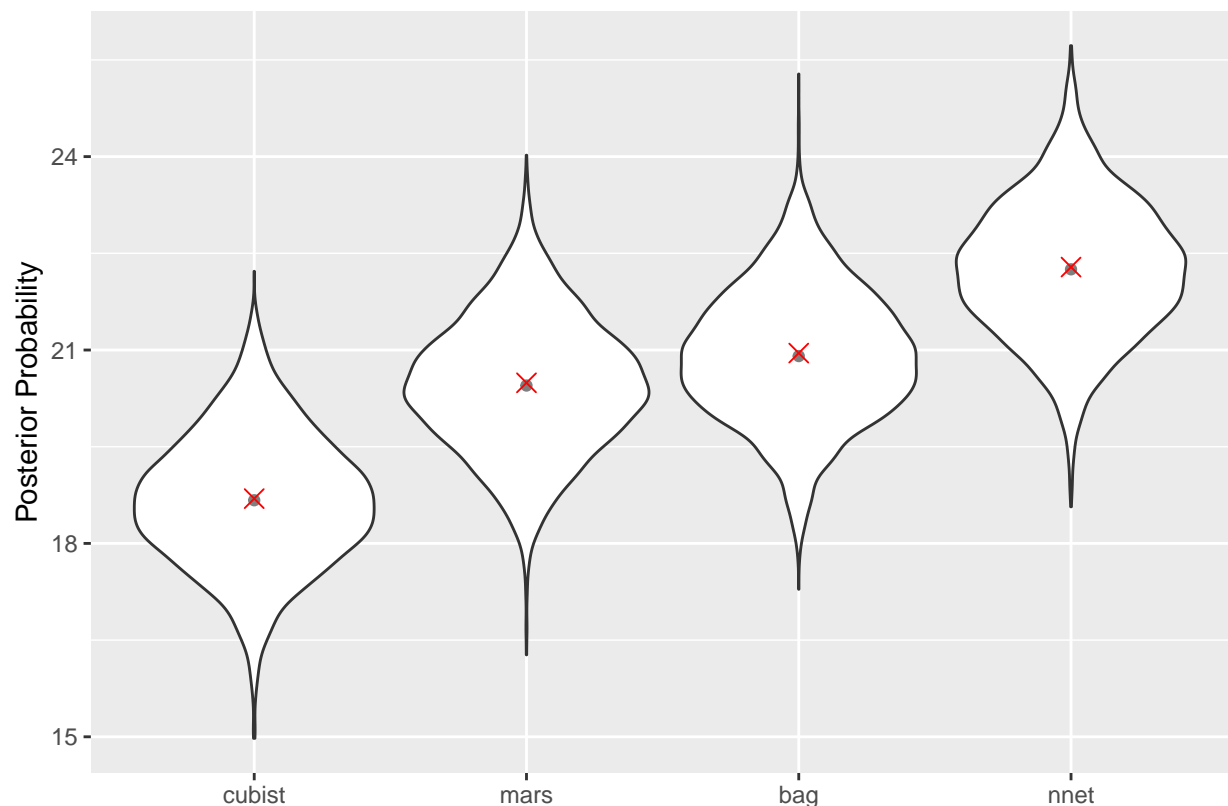
## Chain 2: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 2: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 2: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 2: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 2:
## Chain 2: Elapsed Time: 2.50453 seconds (Warm-up)
## Chain 2: 2.03775 seconds (Sampling)
## Chain 2: 4.54228 seconds (Total)
## Chain 2:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 3).
## Chain 3:
## Chain 3: Gradient evaluation took 0.000106 seconds
## Chain 3: 1000 transitions using 10 leapfrog steps per transition would take 1.06 seconds.
## Chain 3: Adjust your expectations accordingly!
## Chain 3:
## Chain 3:
## Chain 3: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 3: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 3: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 3: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 3: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 3: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 3: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 3: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 3: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 3: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 3: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 3: Iteration: 2000 / 2000 [100%] (Sampling)
## Chain 3:
## Chain 3: Elapsed Time: 2.81841 seconds (Warm-up)
## Chain 3: 2.31637 seconds (Sampling)
## Chain 3: 5.13478 seconds (Total)
## Chain 3:
##
## SAMPLING FOR MODEL 'continuous' NOW (CHAIN 4).
## Chain 4:
## Chain 4: Gradient evaluation took 0.000104 seconds
## Chain 4: 1000 transitions using 10 leapfrog steps per transition would take 1.04 seconds.
## Chain 4: Adjust your expectations accordingly!
## Chain 4:
## Chain 4:
## Chain 4: Iteration: 1 / 2000 [ 0%] (Warmup)
## Chain 4: Iteration: 200 / 2000 [ 10%] (Warmup)
## Chain 4: Iteration: 400 / 2000 [ 20%] (Warmup)
## Chain 4: Iteration: 600 / 2000 [ 30%] (Warmup)
## Chain 4: Iteration: 800 / 2000 [ 40%] (Warmup)
## Chain 4: Iteration: 1000 / 2000 [ 50%] (Warmup)
## Chain 4: Iteration: 1001 / 2000 [ 50%] (Sampling)
## Chain 4: Iteration: 1200 / 2000 [ 60%] (Sampling)
## Chain 4: Iteration: 1400 / 2000 [ 70%] (Sampling)
## Chain 4: Iteration: 1600 / 2000 [ 80%] (Sampling)
## Chain 4: Iteration: 1800 / 2000 [ 90%] (Sampling)
## Chain 4: Iteration: 2000 / 2000 [100%] (Sampling)

```

```
## Chain 4:
## Chain 4: Elapsed Time: 2.37352 seconds (Warm-up)
## Chain 4: 2.16289 seconds (Sampling)
## Chain 4: 4.53641 seconds (Total)
## Chain 4:
```

```
# get posterior and derive means
linear_post <- tidy(linear_model, seed = 3750)
linear_mean <- summary(linear_post)

# plot
ggplot(linear_post) +
  geom_point(data = linear_mean, aes(y = mean), alpha = 0.5) +
  geom_point(data = mean_rmse, aes(y = statistic),
            col = "red", pch = 4, cex = 3)
```

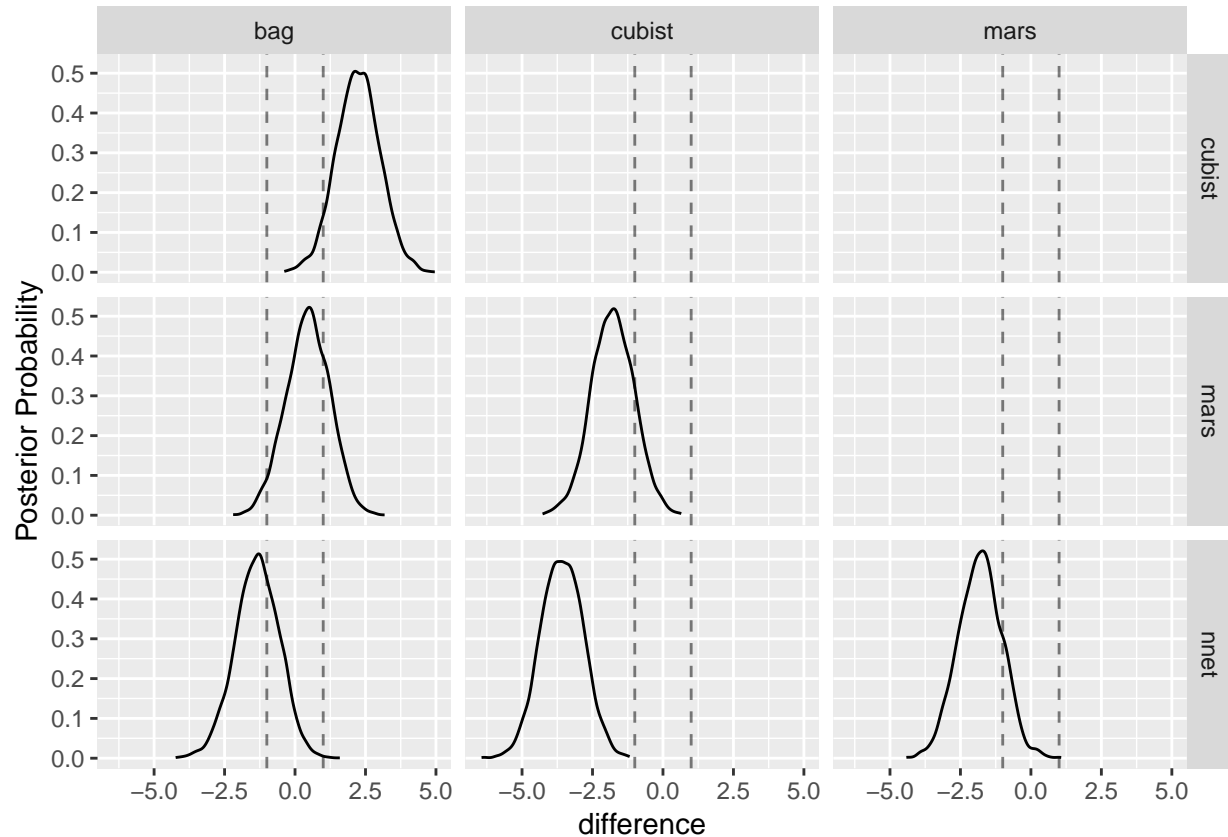


These are right on target. Despite the skewness of the original data, a simple linear model did best here. In hindsight, this makes sense since we are modeling *summary statistics* as our outcome. Even if we believe these to be potentially skewed distributions, the central limit theorem is kicking in here and the estimates are trending to normality.

We can compare models using the `contrast_models` function. The function has arguments for two sets of models to compare but if these are left to their default (NULL), all pair wise combinations are used. Let's say that an RMSE difference of 1 unit is important.

```
# get contrasts
all_contrasts <- contrast_models(linear_model, seed = 8967)
```

```
# plot
ggplot(all_contrasts, size = 1)
```



```
# get summary
summary(all_contrasts, size = 1)
```

```
## # A tibble: 6 x 9
##   contrast probability    mean lower  upper  size pract_neg pract_equiv
##   <chr>          <dbl> <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
## 1 bag vs ~      0.998   2.24  0.967  3.52     1      0      0.0555
## 2 bag vs ~      0.728   0.457 -0.823  1.71     1    0.0342   0.716
## 3 bag vs ~      0.0382  -1.35 -2.66 -0.0947    1    0.668    0.330
## 4 cubist ~      0.00925 -1.78 -3.02 -0.516     1    0.847    0.153
## 5 cubist ~      0      -3.58 -4.82 -2.35     1      1      0
## 6 mars vs~      0.0115  -1.80 -3.08 -0.577     1    0.846    0.154
## # ... with 1 more variable: pract_pos <dbl>
```

Based on our effect size of a single unit, the only pair that are practically equivalent are MARS and bagged trees. Since cubist has the smallest RMSE, it is not unreasonable to say that this model provides uniformly better results than the others shown here.

One Final Note

The Bayesian models have population parameters for the model effects (akin to “fixed” effects in mixed models) as well as variance parameter(s) related to the resamples. The posteriors computed by this package only reflect the mean parameters and should only be used to make inferences about this data set generally.

This posterior calculation could not be used to predict the level of performance for a model a new *resample* of the data. In this case, the variance paramaters come into play and the posterior would be much wider. In essence, the posteriors shown here are measuring the average performance value instead of a resample-specific value.