Supplemental Material for 'Optimizing Model Performance and Fairness Through Evolved Sample Weights'

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Introduction

This is not intended as a stand-alone document, but as a companion to our manuscript.

1.1 Contributing authors

- Anil Kumar Saini
- Jose Guadalupe Hernandez
- Emily F. Wong
- Jason H. Moore

1.2 About our supplemental material

As you may have noticed (unless you're reading a pdf version of this), our supplemental material is hosted using GitHub pages. We compiled our data analyses and supplemental documentation into this nifty web-accessible book using bookdown.

The code used for this supplemental material can be found in this GitHub repository.

Our supplemental material includes the following:

- Metric defintions (Section ??)
- Heart disease results (Section 3)
- Student math results (Section 4)
- Student por results (Section 5)

- CreditG results (Section 6)
- Titanic results (Section 7)
- US Crime results (Section 8)
- Compas Violent results (Section 9)
- NLSY results (Section 10)
- Compas results (Section 11)
- Speed dating results (Section 12)
- PMAD EPDS results (Section 13)
- PMAD PHQ results (Section 14)

1.3 Supplemental material setup

1.3.1 Required packages and variables

Variable set up.

```
library(ggplot2)
library(cowplot)
library(dplyr)
library(PupillometryR)
NAMES <- c('Evolved','Calculated','None')</pre>
TASKS <- c('heart_disease', 'student_math', 'student_por', 'creditg', 'titanic', 'us_c:
SHAPE \leftarrow c(21,24,22)
cb_palette <- c('#D81B60','#1E88E5','#FFC107')</pre>
TSIZE <- 19
p_theme <- theme(</pre>
  plot.title = element_text( face = "bold", size = 22, hjust=0.5),
  panel.border = element_blank(),
  panel.grid.minor = element_blank(),
  legend.title=element_text(size=18),
  legend.text=element_text(size=18),
  axis.title = element_text(size=18),
  axis.text = element_text(size=14),
  legend.position="bottom",
  panel.background = element_rect(fill = "#f1f2f5",
                                   colour = "white",
                                   linewidth = 0.5, linetype = "solid")
)
testing <- read.csv(paste('./', 'hv_test.csv', sep = "", collapse = NULL), header = TR
testing$exp <- gsub('Evolved Weights', 'Evolved', testing$ex)</pre>
testing exp <- gsub('Calculated Weights', 'Calculated', testing ex)
```

```
testing$exp <- gsub('No Weights', 'None', testing$ex)
testing$exp <- factor(testing$exp, levels = NAMES)</pre>
```

1.3.2 Helper functions

Function to plot hypervolume results

```
# function to plot hyper-volume data
volume_plotter <- function(data, id)</pre>
  ggplot(data, aes(x = exp, y = hv, color = exp, fill = exp, shape = exp)) +
  geom_flat_violin(position = position_nudge(x = .1, y = 0), scale = 'width', alpha = 0.2, width
  geom_boxplot(color = 'black', width = .07, outlier.shape = NA, alpha = 0.0, size = 1.0, posit
  geom_point(position = position_jitter(width = 0.02, height = 0.0001), size = 1.5, alpha = 1.0
  scale_y_continuous(
   name="Volume",
 scale_x_discrete(
   name="Strategy"
 )+
  scale_shape_manual(values=SHAPE, name="Weight\nStrategy") +
  scale_colour_manual(values = cb_palette, name="Weight\nStrategy") +
  scale_fill_manual(values = cb_palette, name="Weight\nStrategy") +
  ggtitle(TASKS[id])+
 p_theme + coord_flip()
```

Function to summarize hypervolume results

```
# function to plot hyper-volume data
volume_summarize <- function(data)
{
    data %>%
    group_by(exp) %>%
    dplyr::summarise(
        count = n(),
        na_cnt = sum(is.na(hv)),
        min = min(hv, na.rm = TRUE),
        median = median(hv, na.rm = TRUE),
        mean = mean(hv, na.rm = TRUE),
        max = max(hv, na.rm = TRUE),
        IQR = IQR(hv, na.rm = TRUE)
    )
}
```

Bias defintions

Multiple metrics exist to measure the fairness of predictions made by a machine learning model. Each metric is defined in relation to a specific application context and attempts to quantify different properties (false negative rate, accuracy, etc.) of the predictions for people belonging to different groups. Different metrics try to quantify different properties (false negative rate, accuracy, etc.) of the predictions for people belonging to different groups. For example, 'Demographic parity' measures whether the acceptance rates (proportion of individuals belonging to the group receiving positive prediction) are the same for all groups. 'Error rate parity' measures whether the false positive and false negative rates in all groups are equal, and 'Predictive parity' ensures an equal positive prediction rate across all groups. Here, we discuss in detail two commonly used metrics to measure the fairness in the predictions of a given model: 'Subgroup False Positive Fairness', and 'Subgroup False Negative Fairness'. Before delving into the definitions of the above-mentioned metrics, we describe some terminologies here. Let $\mathcal{D}=\{(X,X',Y)_i\}_{i=1}^N$ be the dataset under consideration. For each data point $(X,X',Y),\,X\in\mathcal{X}^d$ contains values corresponding to d non-sensitive features, $X' \in \mathcal{X}'^p$ contains values corresponding to p sensitive features, and Y contains the target variables. Features deemed 'sensitive', or 'protected', such as race, sex, and gender, are classified as sensitive features (X'). Here, we would assume X' and X do not overlap, and therefore, X + X' would give us the full feature set for a particular data point. Based on the values of sensitive attributes, each data point can fall into one of the groups defined by those sensitive attributes. For example, 'Black women younger than 25' would be one of the groups when the sensitive attributes are race, gender, and age. Let $G \in \mathcal{G}$ be one such group. We show the membership to this group by $X' \in G$. Finally, let $\hat{Y} \in \{0,1\}$ be the predicted target value output by the classifier. Finally, let $R(X, X') \in [0.0, 1.0]$ be the risk score output by a given ML model, $\hat{Y} \in \{0, 1\}$ is the predicted target value, and for simplicity, also the classifier, formed by applying a threshold on R(X,X'). False Positive Subgroup Fairness and False Positive Subgroup Fairness capture the maximum deviation of a model's performance among any one group in \mathcal{G} , normalized by the probability of observing an individual from that group in the negative or positive labels, respectively. Since in most scenarios, we would want the model to perform similarly in all groups, lower values on these metrics denote more fair models. For a dataset \mathcal{D} , and risk model R(X,X'), the following are the definitions. False Positive (FP) Rate: False positive (FP) rate can be defined as

$$FP(R) = Pr[\hat{Y} = 1|Y = 0].$$

And the False Positive Rate for a group G can be defined as

$$FP(R, G) = Pr[\hat{Y} = 1|Y = 0, X' \in G].$$

False Negative (FN) Rate: False positive (FP) rate can be defined as

$$FN(R) = Pr[\hat{Y} = 0|Y = 1].$$

And the False Negative Rate for a group G can be defined as

$$FN(R,G) = Pr[\hat{Y} = 1|Y = 0, X' \in G].$$

False Positive Subgroup Fairness : Let the probability of getting negative labels in group G be

$$\alpha_{FP}(G) = Pr[X' \in G, Y = 0].$$

We also define the absolute difference in false positive rate between the whole population and for a specific group G as

$$\beta(R,G) = |FP(R) - FP(R,G)|.$$

Then the False Positive Subgroup Fairness (FPSF) is given by

$$FPSF(D,R) = \max_{G \in \mathcal{G}} \alpha_{FP}(G)\beta(R,G).$$

False Negative Subgroup Fairness : Let the probability of getting positive labels in group G be

$$\alpha_{FN}(G) = Pr[X' \in G, Y = 1].$$

We also define the absolute difference in false negative rate between the whole population and for a specific group G as

$$\beta(R,G) = |FN(R) - FN(R,G)|.$$

Then the False Positive Subgroup Fairness (FPSF) is given by

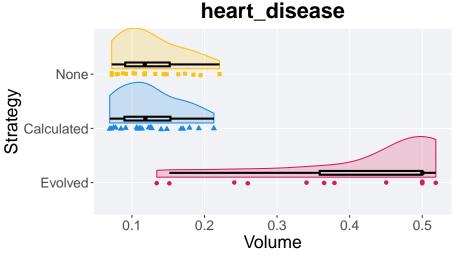
$$FNSF(D,R) = \max_{G \in \mathcal{G}} \alpha_{FN}(G)\beta(R,G).$$

Heart Disease

Here we report the **hypervolume** achived by evaluating the performance of each solution wittin the Pareto front on the test set of the **heart_disease** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "heart_disease")</pre>
```

```
volume_plotter(data,1)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
             count na_cnt
                           min median mean
                                                 IQR
    <fct>
             <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                20
                       0 0.134
                               0.5
                                    0.417 0.519 0.141
## 2 Calculated
                20
                       ## 3 None
                20
                       0 0.0722 0.118 0.126 0.221 0.0613
```

3.1.2 Kruskal-Wallis test

Detected differences between weight strategies.

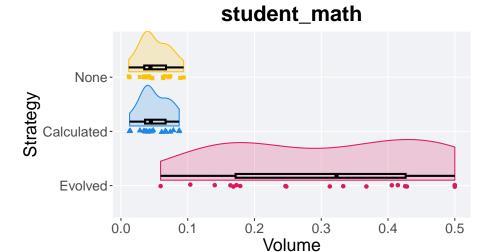
```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 34.987, df = 2, p-value = 2.528e-08
```

Student Math

Here we report the **hypervolume** achived by evaluating the performance of each solution wihtin the Pareto front on the test set of the **student_math** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "student_math")</pre>
```

```
volume_plotter(data,2)
```



Weight **□** Evolved **□** Calculated **□** None Strategy

```
volume_summarize(data)
## # A tibble: 3 x 8
                count na_cnt
                                min median
                                                            IQR
                                             mean
                                                     max
     <fct>
                <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                   20
                           0 0.0594 0.323 0.308 0.5
## 2 Calculated
                   20
                           0 0.0129 0.0448 0.0504 0.0873 0.0307
## 3 None
                   20
                           0 0.0116 0.0441 0.0503 0.0939 0.0326
```

4.1.2 Kruskal-Wallis test

 ${\bf Detected\ differences\ between\ weight\ strategies.}$

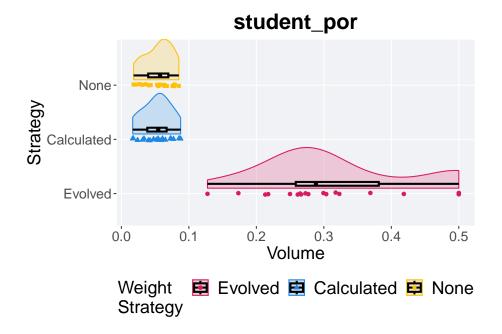
```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 36.282, df = 2, p-value = 1.323e-08
```

Student Por

Here we report the **hypervolume** achived by evaluating the performance of each solution wihtin the Pareto front on the test set of the **student_por** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "student_por")</pre>
```

```
volume_plotter(data,3)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
                count na_cnt
                                min median
                                                            IQR
                                             mean
                                                     max
     <fct>
                <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                           0 0.128  0.288  0.318  0.5
                20
## 2 Calculated
                   20
                           0 0.0168 0.0546 0.0528 0.0878 0.0286
## 3 None
                   20
                           0 0.0181 0.0573 0.0547 0.0851 0.0298
```

5.1.2 Kruskal-Wallis test

 ${\bf Detected\ differences\ between\ weight\ strategies.}$

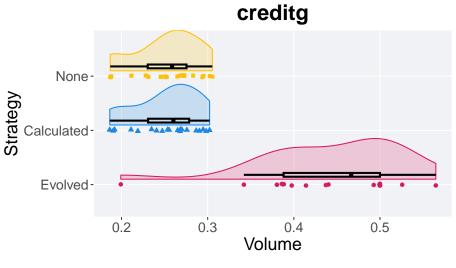
```
###
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 39.429, df = 2, p-value = 2.742e-09
```

CreditG

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the **creditg** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "creditg")</pre>
```

```
volume_plotter(data,4)
```



Weight **■** Evolved **■** Calculated **■** None Strategy

```
volume_summarize(data)
## # A tibble: 3 x 8
                count na_cnt
                               min median mean
                                                         IQR
     <fct>
                <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <
## 1 Evolved
                           0 0.199  0.467  0.443  0.565  0.112
                20
                           0 0.186  0.260  0.252  0.302  0.0477
## 2 Calculated
                   20
## 3 None
                   20
                           0 0.187 0.259 0.253 0.305 0.0450
```

6.1.2 Kruskal-Wallis test

 ${\bf Detected\ differences\ between\ weight\ strategies.}$

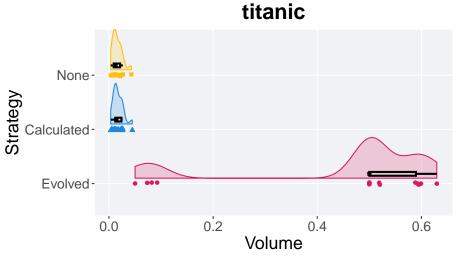
```
###
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 32.972, df = 2, p-value = 6.922e-08
```

Titanic

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the **titanic** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "titanic")</pre>
```

```
volume_plotter(data,5)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
    exp
               count na_cnt
                                min median
                                                            IQR
                                             mean
     <fct>
               <int> <int>
                              <dbl> <dbl> <dbl> <dbl> <dbl> <
## 1 Evolved
                          0 0.0502 0.5
                                           0.447 0.629 0.0894
                20
## 2 Calculated
                  20
                          0 0.00334 0.0143 0.0171 0.0448 0.0119
## 3 None
                  20
                          0 0.00340 0.0126 0.0157 0.0430 0.0125
```

7.1.2 Kruskal-Wallis test

 ${\bf Detected\ differences\ between\ weight\ strategies.}$

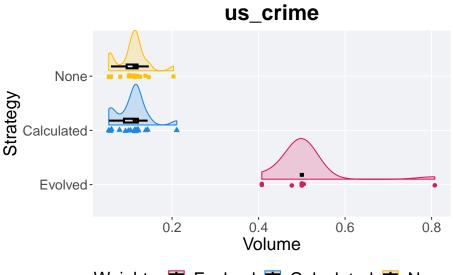
```
###
## Kruskal-Wallis rank sum test
###
## data: hv by exp
## Kruskal-Wallis chi-squared = 39.658, df = 2, p-value = 2.445e-09
```

US Crime

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the us_crime dataset.

```
# heart-disease data
data <- filter(testing, dataset == "us_crime")</pre>
```

```
volume_plotter(data,6)
```



8.1.1 Summary stats

```
volume_summarize(data)
## # A tibble: 3 x 8
             count na_cnt
                           min median mean
                                                  IQR
    <fct>
             <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
              20
                       0 0.407
                                0.5 0.505 0.807 0
## 2 Calculated
                20
                       ## 3 None
                20
                       0 0.0534 0.113 0.107 0.203 0.0252
```

8.1.2 Kruskal-Wallis test

Detected differences between weight strategies.

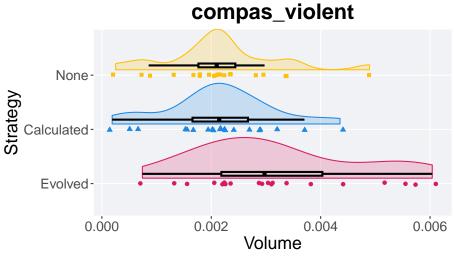
```
###
## Kruskal-Wallis rank sum test
###
## data: hv by exp
## Kruskal-Wallis chi-squared = 39.978, df = 2, p-value = 2.084e-09
```

Compas Violent

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the **compas_violent** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "compas_violent")</pre>
```

```
volume_plotter(data,7)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
                count na_cnt
                                  min median
                                                                    IQR
                                                 mean
                                                           max
     <fct>
                <int> <int>
                                <dbl>
                                        <dbl>
                                                         <dbl>
                                                 <dbl>
                           0 0.000741 0.00297 0.00319 0.00604 0.00185
## 1 Evolved
                   20
## 2 Calculated
                   20
                           0 0.000188 0.00215 0.00215 0.00435 0.00101
## 3 None
                   20
                           0 0.000251 0.00210 0.00217 0.00489 0.000675
```

9.1.2 Kruskal-Wallis test

Detected differences between weight strategies.

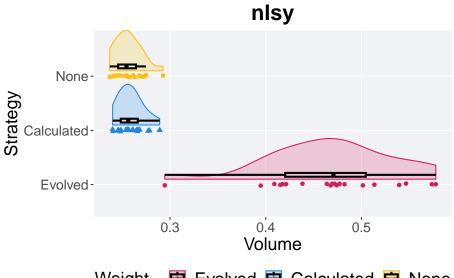
```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 6.7764, df = 2, p-value = 0.03377
```

NLSY

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the nlsy dataset.

```
# heart-disease data
data <- filter(testing, dataset == "nlsy")</pre>
```

```
volume_plotter(data,8)
```



Weight **□** Evolved **□** Calculated **□** None Strategy

```
volume_summarize(data)
## # A tibble: 3 x 8
    exp
               count na_cnt
                              min median mean
                                                        IQR
                                                 max
    <fct>
               <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                          0 0.294 0.471 0.468 0.578 0.0843
                20
## 2 Calculated
                  20
                          0 0.240 0.256 0.259 0.289 0.0177
## 3 None
                  20
                          0 0.237 0.254 0.256 0.293 0.0186
```

10.1.2 Kruskal-Wallis test

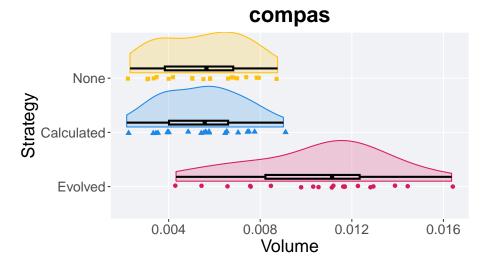
```
###
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 39.518, df = 2, p-value = 2.623e-09
```

Compas

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the **compas** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "compas")</pre>
```

```
volume_plotter(data,9)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
     exp
                count na_cnt
                                 min median
                                                                 IQR
                                                mean
                                                         max
     <fct>
                <int> <int>
                               <dbl>
                                       <dbl>
                                               <dbl>
                                                        <dbl>
## 1 Evolved
                           0 0.00432 0.0111 0.0105 0.0164 0.00411
                   20
## 2 Calculated
                   20
                           0 0.00217 0.00558 0.00546 0.00901 0.00258
## 3 None
                   20
                           0 0.00231 0.00565 0.00548 0.00876 0.00299
```

11.1.2 Kruskal-Wallis test

```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 26.298, df = 2, p-value = 1.947e-06
```

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Speeddating

Here we report the **hypervolume** achived by evaluating the performance of each solution wihtin the Pareto front on the test set of the **speeddating** dataset.

```
# heart-disease data
data <- filter(testing, dataset == "speeddating")</pre>
```

```
volume_plotter(data,10)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
                                                                       IQR
               count na_cnt
                                         median
                                   min
                                                    mean
                                                              max
     <fct>
                <int> <int>
                                 <dbl>
                                          <dbl>
                                                            <dbl>
## 1 Evolved
                           0 0.229
                                       0.5
                                                0.486
                                                         0.5
                20
## 2 Calculated
                   20
                           0 0.0000388 0.000102 0.000114 0.000239 0.000121
## 3 None
                   20
                           0 0.0000297 0.000109 0.000124 0.000255 0.000122
```

12.1.2 Kruskal-Wallis test

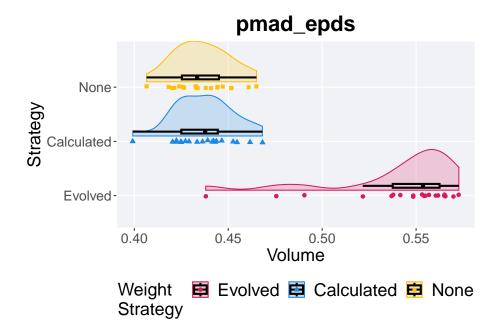
```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 40.672, df = 2, p-value = 1.473e-09
```

PMAD EPDS

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the pmad_epds dataset.

```
# heart-disease data
data <- filter(testing, dataset == "pmad_epds")</pre>
```

```
volume_plotter(data,11)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
             count na_cnt
                           min median mean
                                                  IQR
    <fct>
              <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                       0 0.438 0.554 0.541 0.573 0.0249
              20
                       ## 2 Calculated
                20
## 3 None
                20
                       0 0.407 0.433 0.436 0.465 0.0197
```

13.1.2 Kruskal-Wallis test

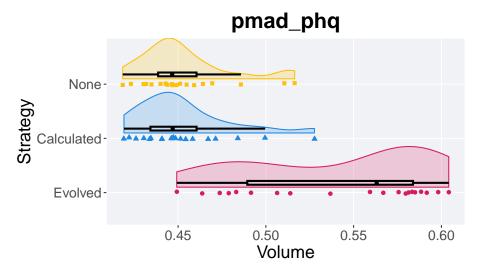
```
##
##
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 35.731, df = 2, p-value = 1.742e-08
```

PMAD PHQ

Here we report the **hypervolume** achived by evaluating the performance of each solution within the Pareto front on the test set of the <code>pmad_phq</code> dataset.

```
# heart-disease data
data <- filter(testing, dataset == "pmad_phq")</pre>
```

```
volume_plotter(data,13)
```



```
volume_summarize(data)
## # A tibble: 3 x 8
             count na_cnt
                          min median mean
                                                  IQR
    <fct>
              <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Evolved
                       0 0.449 0.563 0.541 0.604 0.0944
              20
## 2 Calculated
                20
                       0 0.419 0.447 0.452 0.528 0.0263
## 3 None
                20
```

14.1.2 Kruskal-Wallis test

```
###
## Kruskal-Wallis rank sum test
##
## data: hv by exp
## Kruskal-Wallis chi-squared = 29.615, df = 2, p-value = 3.708e-07
```