Explore data

The
Datasaurus Dozen dataset is a collection of 13 sets of `x`/`y` data that have very similar summary statistics but look very different when plotted. Our modeling goal is to predict which member of the "dozen" each point belongs to.

Let's start by reading in the data from the
datasauRus package.

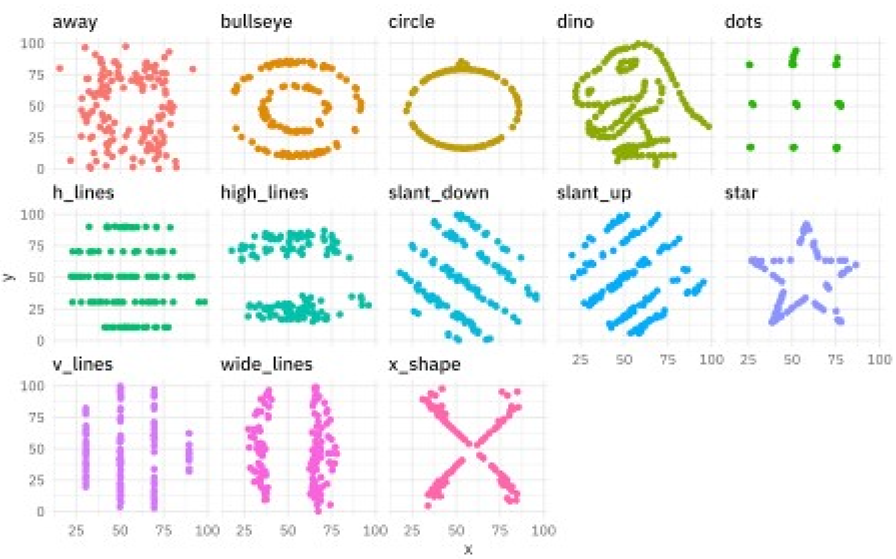
```
library(tidyverse)
library(datasauRus)

datasaurus_dozen
```

```
## # A tibble: 1,846 x 3
##    dataset     x     y
##
##  1 dino     55.4  97.2
##  2 dino     51.5  96.0
##  3 dino     46.2  94.5
##  4 dino     42.8  91.4
##  5 dino     40.8  88.3
##  6 dino     38.7  84.9
##  7 dino     35.6  79.9
##  8 dino     33.1  77.6
##  9 dino     29.0  74.5
## 10 dino     26.2  71.4
## # … with 1,836 more rows
```

These datasets are very different from each other!

```
datasaurus_dozen %>%
  ggplot(aes(x, y, color = dataset)) +
  geom_point(show.legend = FALSE) +
  facet_wrap(~dataset, ncol = 5)
```



But their summary statistics are so similar.

```
datasaurus_dozen %>%
  group_by(dataset) %>%
  summarise(across(c(x, y), list(mean = mean, sd = sd)),
    x_y_cor = cor(x, y)
  )

## # A tibble: 13 x 6
##    dataset    x_mean  x_sd y_mean  y_sd x_y_cor
##
##  1 away         54.3  16.8   47.8  26.9 -0.0641
##  2 bullseye     54.3  16.8   47.8  26.9 -0.0686
##  3 circle       54.3  16.8   47.8  26.9 -0.0683
##  4 dino         54.3  16.8   47.8  26.9 -0.0645
##  5 dots         54.3  16.8   47.8  26.9 -0.0603
##  6 h_lines      54.3  16.8   47.8  26.9 -0.0617
##  7 high_lines   54.3  16.8   47.8  26.9 -0.0685
##  8 slant_down   54.3  16.8   47.8  26.9 -0.0690
##  9 slant_up     54.3  16.8   47.8  26.9 -0.0686
## 10 star         54.3  16.8   47.8  26.9 -0.0630
## 11 v_lines      54.3  16.8   47.8  26.9 -0.0694
## 12 wide_lines   54.3  16.8   47.8  26.9 -0.0666
## 13 x_shape      54.3  16.8   47.8  26.9 -0.0656
```

Let’s explore whether we can use modeling to predict which dataset a point belongs to. This is not a large dataset compared to the number of classes (13!) so this isn’t a tutorial that shows best practices for a predictive modeling workflow overall, but it *does* demonstrate how to evaluate a multiclass model, as well as a bit about how random forest models work.

```
datasaurus_dozen %>%
  count(dataset)

## # A tibble: 13 x 2
##    dataset        n
##
##  1 away         142
##  2 bullseye     142
##  3 circle       142
##  4 dino         142
##  5 dots         142
##  6 h_lines      142
##  7 high_lines   142
##  8 slant_down   142
##  9 slant_up     142
## 10 star         142
## 11 v_lines      142
## 12 wide_lines   142
## 13 x_shape      142
```

Build a model

Let’s start out by creating bootstrap resamples of the Datasaurus Dozen. Notice that we aren’t splitting into testing and training sets, so we won't have an unbiased estimate of performance on new data. Instead, we will use these resamples to understand the dataset and multiclass models better.

```
library(tidymodels)

set.seed(123)
dino_folds <- datasaurus_dozen %>%
  mutate(dataset = factor(dataset)) %>%
  bootstraps()

dino_folds

## # Bootstrap sampling
## # A tibble: 25 x 2
##    splits             id
##
##  1  Bootstrap01
##  2  Bootstrap02
##  3  Bootstrap03
##  4  Bootstrap04
##  5  Bootstrap05
##  6  Bootstrap06
##  7  Bootstrap07
##  8  Bootstrap08
##  9  Bootstrap09
## 10  Bootstrap10
## # … with 15 more rows
```

Let's create a random forest model and set up a model workflow with the model and a formula preprocessor. We are predicting the `dataset` class (dino vs. circle vs. bullseye vs. …) from `x` and `y`. A random forest model can often do a good job of learning complex interactions in predictors.

```
rf_spec <- rand_forest(trees = 1000) %>%
  set_mode("classification") %>%
  set_engine("ranger")

dino_wf <- workflow() %>%
  add_formula(dataset ~ x + y) %>%
  add_model(rf_spec)

dino_wf

## ══ Workflow ════════════════════════════════
════════════════════════════════════════
## Preprocessor: Formula
## Model: rand_forest()
##
## ── Preprocessor ──────────────────────────────
──────────────────────────────────────
## dataset ~ x + y
```

```
##
## ── Model ──────────────────────────────
──────────────────────────────────────────
## Random Forest Model Specification (classification)
##
## Main Arguments:
##   trees = 1000
##
## Computational engine: ranger
```

Let's fit the random forest model to the bootstrap resamples.

```
doParallel::registerDoParallel()
dino_rs <- fit_resamples(
  dino_wf,
  resamples = dino_folds,
  control = control_resamples(save_pred = TRUE)
)

dino_rs

## # Resampling results
## # Bootstrap sampling
## # A tibble: 25 x 5
##    splits            id          .metrics       .notes
.predictions
##
##  1
```

We did it!

Evaluate model

How did these models do overall?

```
collect_metrics(dino_rs)

## # A tibble: 2 x 5
##   .metric  .estimator  mean     n std_err
##
## 1 accuracy multiclass 0.449    25 0.00337
## 2 roc_auc  hand_till  0.846    25 0.00128
```

The accuracy is not great; a multiclass problem like this, especially one with so many classes, is harder than a binary classification problem. There are so many possible wrong answers!

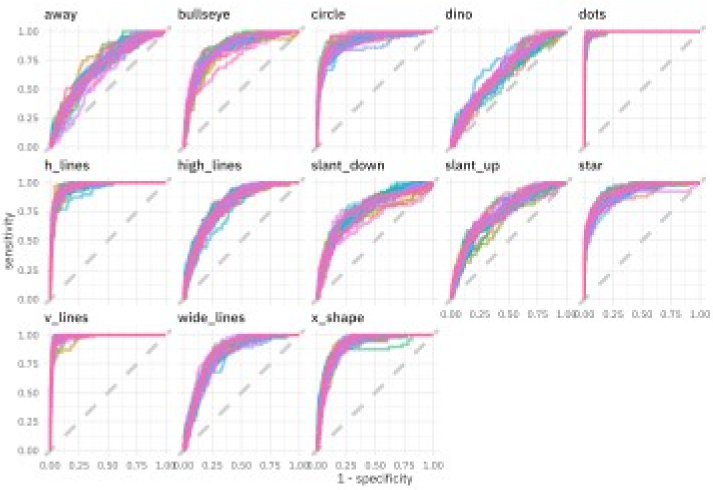
Since we saved the predictions with `save_pred = TRUE` we can compute other performance metrics. Notice that by default the positive predictive value (like accuracy) is macro-weighted for multiclass problems.

```
dino_rs %>%
  collect_predictions() %>%
  group_by(id) %>%
  ppv(dataset, .pred_class)
```

```
## # A tibble: 25 x 4
##    id          .metric .estimator .estimate
##
##  1 Bootstrap01 ppv     macro          0.428
##  2 Bootstrap02 ppv     macro          0.431
##  3 Bootstrap03 ppv     macro          0.436
##  4 Bootstrap04 ppv     macro          0.418
##  5 Bootstrap05 ppv     macro          0.445
##  6 Bootstrap06 ppv     macro          0.413
##  7 Bootstrap07 ppv     macro          0.420
##  8 Bootstrap08 ppv     macro          0.423
##  9 Bootstrap09 ppv     macro          0.393
## 10 Bootstrap10 ppv     macro          0.429
## # … with 15 more rows
```

Next, let’s compute ROC curves for each class.

```
dino_rs %>%
  collect_predictions() %>%
  group_by(id) %>%
  roc_curve(dataset, .pred_away:.pred_x_shape) %>%
  ggplot(aes(1 - specificity, sensitivity, color = id)) +
  geom_abline(lty = 2, color = "gray80", size = 1.5) +
  geom_path(show.legend = FALSE, alpha = 0.6, size = 1.2) +
  facet_wrap(~.level, ncol = 5) +
  coord_equal()
```



We have an ROC curve for each class and each resample in this plot. Notice that the points dataset was easy for the model to identify while the dino dataset was very difficult. The model barely did better than guessing for the dino!

We can also compute a confusion matrix. We could use `tune::conf_mat_resampled()` but since there are so few examples per class and the classes were balanced, let's just look at all the resamples together.

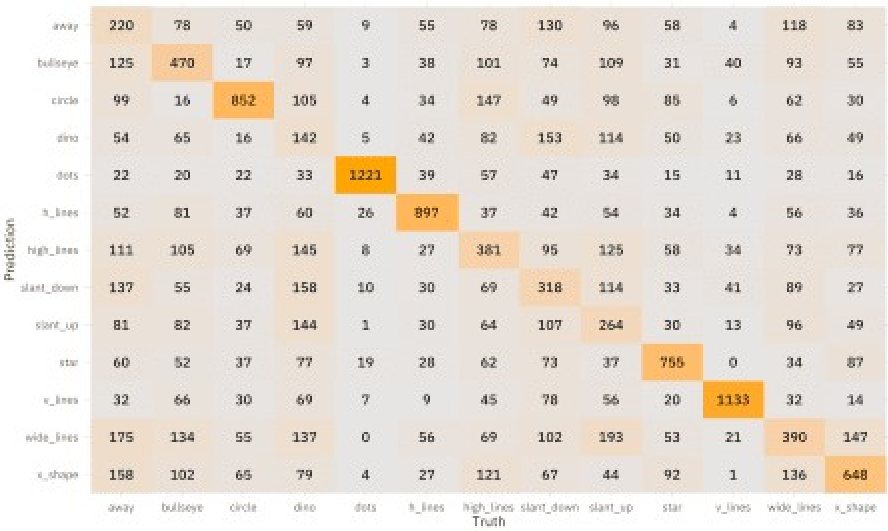
```
dino_rs %>%
  collect_predictions() %>%
  conf_mat(dataset, .pred_class)
```

```
##              Truth
## Prediction    away bullseye circle dino dots h_lines high_lines
slant_down slant_up star v_lines wide_lines x_shape
##   away         220       78     50   59    9      55         78
130        96   58        4        118       83
##   bullseye     125      470     17   97    3      38        101
74       109   31       40         93       55
##   circle        99       16    852  105    4      34        147
49        98   85        6         62       30
##   dino          54       65     16  142    5      42         82
153       114   50       23         66       49
##   dots          22       20     22   33 1221      39         57
47        34   15       11         28       16
##   h_lines       52       81     37   60   26     897         37
42        54   34        4         56       36
##   high_lines   111      105     69  145    8      27        381
95       125   58       34         73       77
##   slant_down   137       55     24  158   10      30         69
318       114   33       41         89       27
##   slant_up      81       82     37  144    1      30         64
107       264   30       13         96       49
```

```
## star 60 52 37 77 19 28 62
73 37 755 0 34 87
## v_lines 32 66 30 69 7 9 45
78 56 20 1133 32 14
## wide_lines 175 134 55 137 0 56 69
102 193 53 21 390 147
## x_shape 158 102 65 79 4 27 121
67 44 92 1 136 648
```

These counts are can be easier to understand in a visualization.

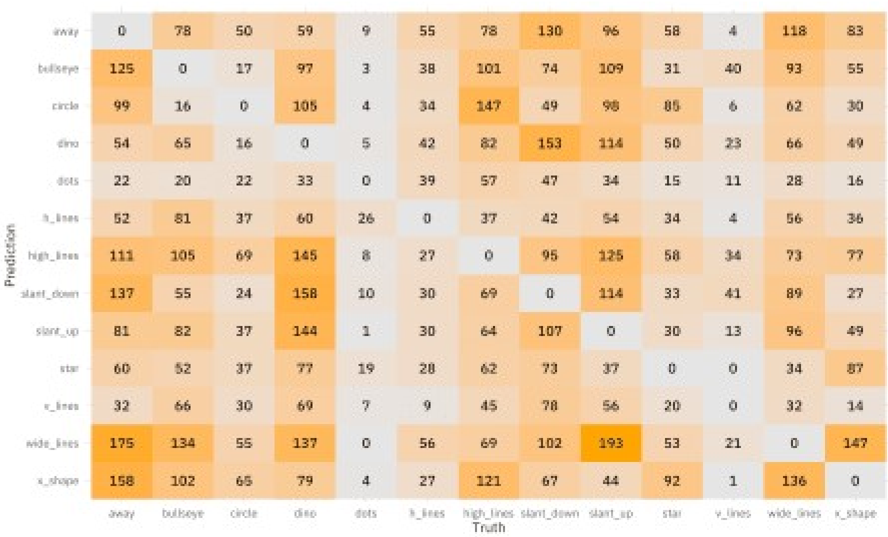
```
dino_rs %>%
  collect_predictions() %>%
  conf_mat(dataset, .pred_class) %>%
  autoplot(type = "heatmap")
```



There is some real variability on the diagonal, with a factor of 10 difference from dinos to dots.

If we set the diagonal to all zeroes, we can see which classes were most likely to be confused for each other.

```
dino_rs %>%
  collect_predictions() %>%
  filter(.pred_class != dataset) %>%
  conf_mat(dataset, .pred_class) %>%
  autoplot(type = "heatmap")
```



The dino dataset was confused with many of the other datasets, and `wide_lines` was often confused with `slant_up`.