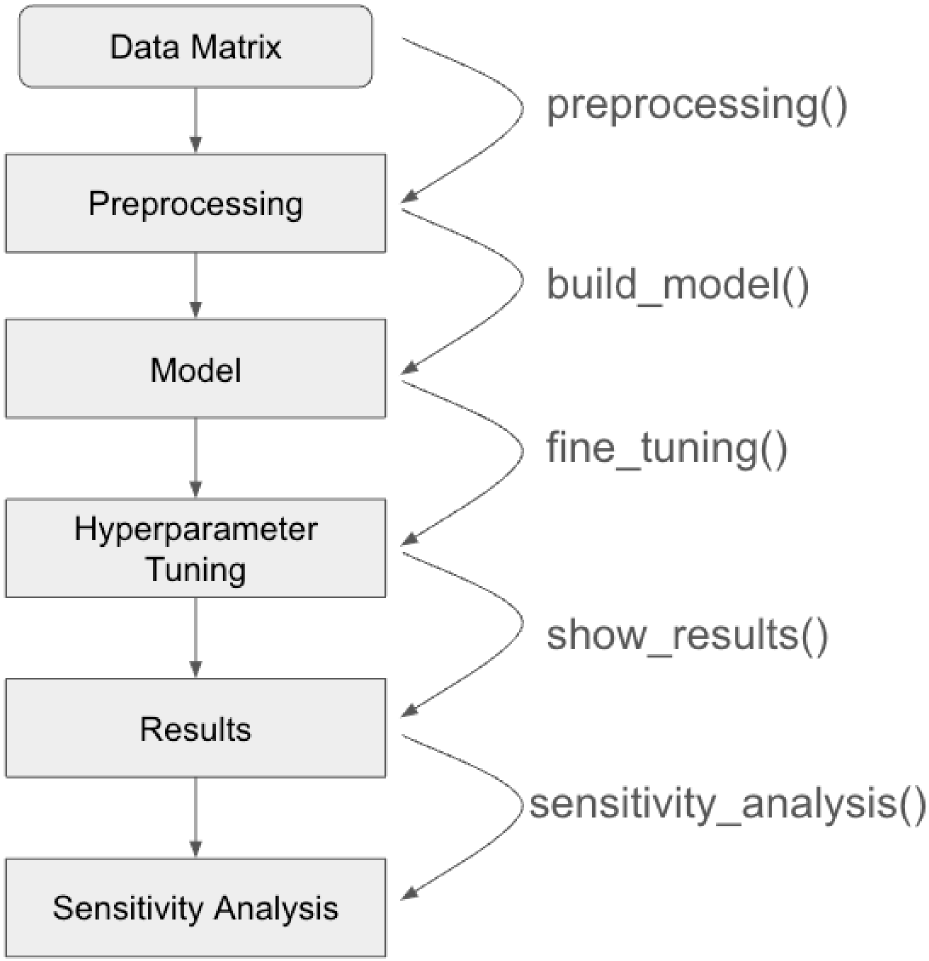
Tutorial TidyML

Introduction

TidyML is a minimal library focused on providing all the essential tools for the workflow of a machine learning modelling process. It divides the whole process into 5 sequential steps:

1. Preprocessing
2. Model Building
3. Fine Tuning
4. Computing Performance Metrics
5. Sensitivity Analysis / Interpretable ML



Internally, due to the sequential nature of the workflow, each step stores new information of the analysis on an object called "tidy_object". At any time during the process, the internal information of the analysis can be retrieved from the tidy_object using the "$" operator. The implemented fields are:

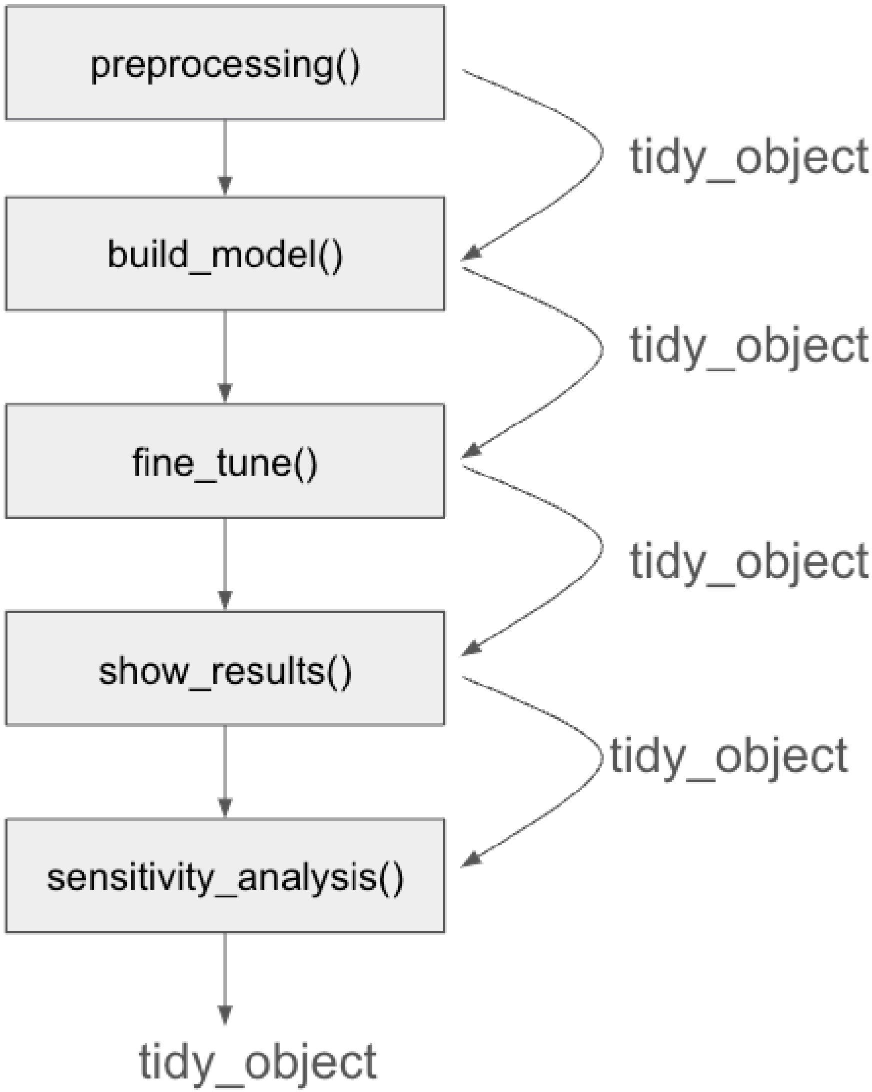
```r
devtools::load_all()
```

```
i Loading TidyML
Loading required package: tidyverse

-- Attaching core tidyverse packages ------------------------ tidyverse 2.0.0 --
v dplyr     1.1.4     v readr     2.1.5
v forcats   1.0.0     v stringr   1.5.1
v ggplot2   3.5.2     v tibble    3.2.1
```

```
v lubridate 1.9.4     v tidyr     1.3.1
v purrr     1.0.4
-- Conflicts ------------------------------------------ tidyverse_conflicts() --
x dplyr::filter() masks stats::filter()
x dplyr::lag()    masks stats::lag()
i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to becom

Warning: Objects listed as exports, but not present in namespace:
* create_models
* create_recipe
* transformer
```

```r
library(dplyr)

tidy_object = TidyMLObject$new(0, 0, 0, 0,0)

names(tidy_object)
```

```
 [1] ".__enclos_env__"      "sensitivity_analysis" "outcome_levels"
 [4] "predictions"          "fit_summary"          "formula"
 [7] "final_models"         "tuner_fit"            "tuner"
[10] "metrics"              "workflow"             "models_names"
[13] "models"               "hyperparameters"      "task"
[16] "transformer"          "validation_data"      "test_data"
[19] "train_data"           "full_data"            "clone"
[22] "modify"               "initialize"
```



Binary Classification Example

We will start by creating a small binary classification dataset using the palmerpenguins data.

Create Dataset

```r
df <- palmerpenguins::penguins %>%
  na.omit() %>%
  dplyr::select(-year) %>%
  dplyr::filter(species == "Adelie" | species == "Gentoo") %>%
  dplyr::mutate(species = droplevels(species))
```

Preprocessing Step

We will first preprocess the data set using the ***preprocessing()*** function. We will pass the dataset along with the formula for our problem. The preprocessing step requires to specify which columns are going to be preprocessed:

- Numerical columns will be normalized by z-score
- Categorical columns will be one-hot encoded

As well as the task to be performed: "regression" or "classification".

In our case, we will preprocess all numerical columns and all categorical columns using the **all** keyword (by default):

```r
formula = "species ~ ."

tidy_object = preprocessing(df,
                            formula = formula,
                            norm_num_vars = "all",
                            encode_cat_vars = "all",
                            task = "classification"
                            )
```

Model Definition

The function ***build_model()*** allows to create a ML model. Each model has it's own set of hyperparameters which we can choose to fine_tune by passing a range of values or to set to a specific value. By default each hyperparameter will be tuned within a given range. The The ML models implemented are:

1. **Neural Network**:

    1. *hidden_units* : number of hidden_units
    2. *activation* : activation functions ("relu", "sigmoid", "tanh")

    3. *learn_rate* : learning rate

2. **Support Vector Machine ("SVM")**:

    1. *cost* : regularization penalty
    2. *margin* : margin of classifier
    3. *type* : type of kernel ("linear", "rbf", "polynomial")
    4. *rbf_sigma* (rbf kernel only) : rbf kernel sigma
    5. *degree* (polynomial kernel only) : polynomial kernel degree
    6. *scale_factor* (polynomial kernel only) : polynomial kernel scale factor

3. **Random Forest**:

    1. *mtry* : Size of feature sampling
    2. *trees* : Number of trees
    3. *min_n* : Minimum number of samples for splitting

4. **XGBoost**:

    1. *mtry* : Size of feature sampling
    2. *trees* : Number of trees
    3. *min_n* : Minimum number of samples for splitting
    4. *tree_depth* : Maximum tree depth
    5. *learn_rate* : Learning rate
    6. *loss_reduction* : Loss reduction

```
tidy_object <- build_model(tidy_object,
                           model_names = "Random Forest",
                           hyperparameters =
                             list(
                                  mtry = c(2,3),
                                  trees = 15
                                  )
                           )
```

Hyperparameter Tuning

Once the model has been defined, we can fine tune the hyperparameters using the ***fine_tune()*** function. There are 2 different hyperparameter tuning strategies:

1. *Bayesian Optimization*
2. *Grid Search CV*

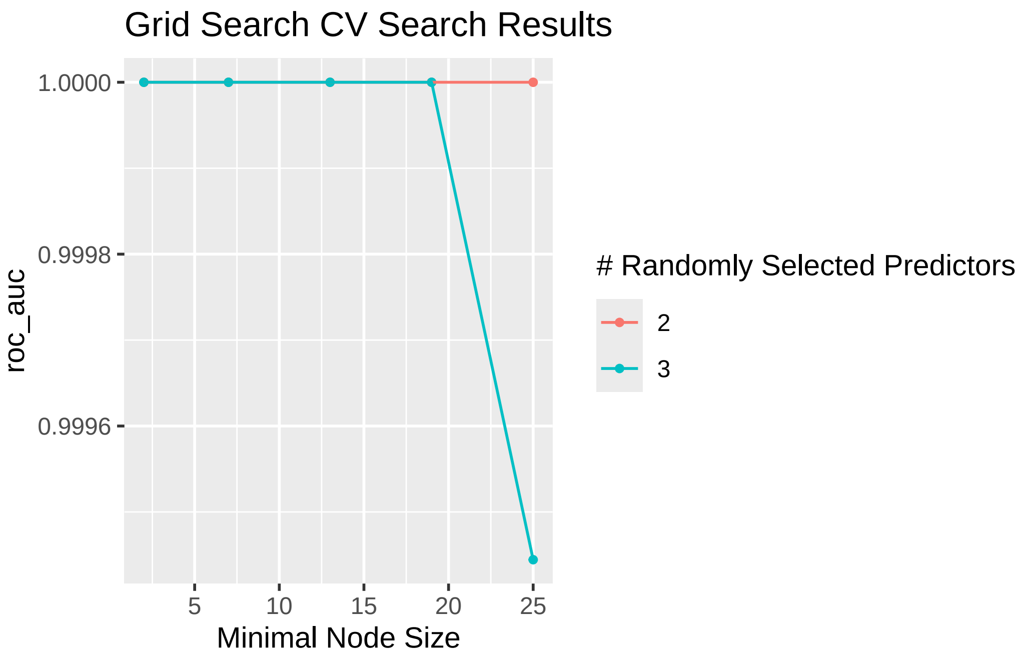
Additionally, we will specify the metric used to select the best performing hyperparameters:

Regression	Classification
rmse	accuracy
mae	bal_accuracy
mpe	precision
mape	recall
ccc	specificity
smape	sensitivity
rpiq	kap
rsq	f_meas
	mcc
	detection_prevalence
	j_index
	roc_auc
	pr_auc
	gain_capture
	brier_class
	roc_aunp

We can visualize the tuning results by setting the *plot_results* parameter to TRUE:

```
tidy_object <- fine_tuning(tidy_object,
                           tuner = "Grid Search CV",
                           metrics = "roc_auc",
                           plot_results = T
                           )
```

```
[1] "Commencing Tuning..."
[1] "Tuning Finalized"
[1] "############# Hyperparameter Tuning Results"
```




```
[1] "############# Best Hyperparameters Found:"
# A tibble: 1 x 8
   mtry min_n .metric .estimator  mean     n std_err .config
  <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1     2     2 roc_auc binary         1     5       0 Preprocessor1_Model01
```

Results

Once we have found the best hyperparameter configuration we can compute the performance metrics of our model based on the test data using the ***show_results()*** function. There are different options for the results depending on whether we are doing a regression task or a classification task:

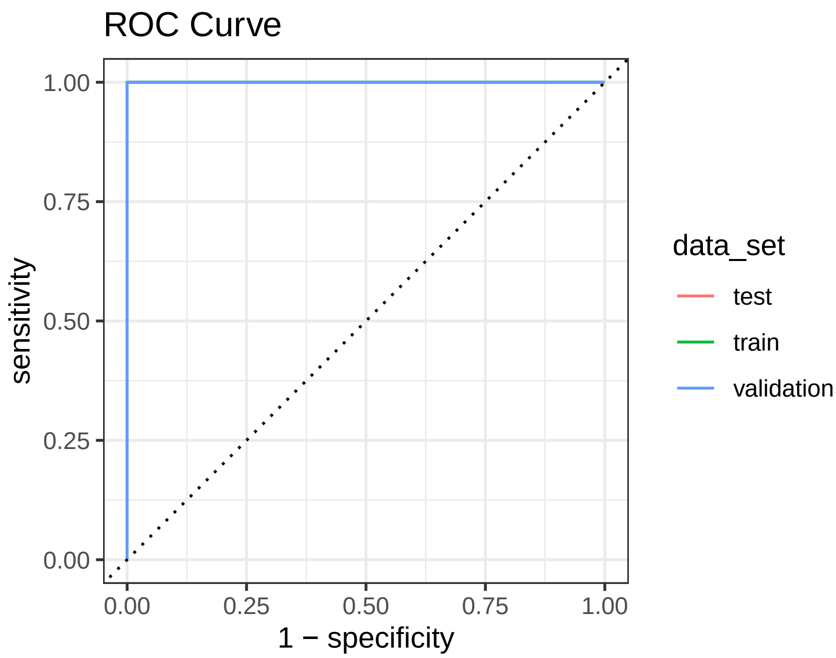
- **Regression**:
  - *summary*
  - *scatter_residuals*
  - *scatter_predictions*
  - *residuals_dist*
- **Classification**:

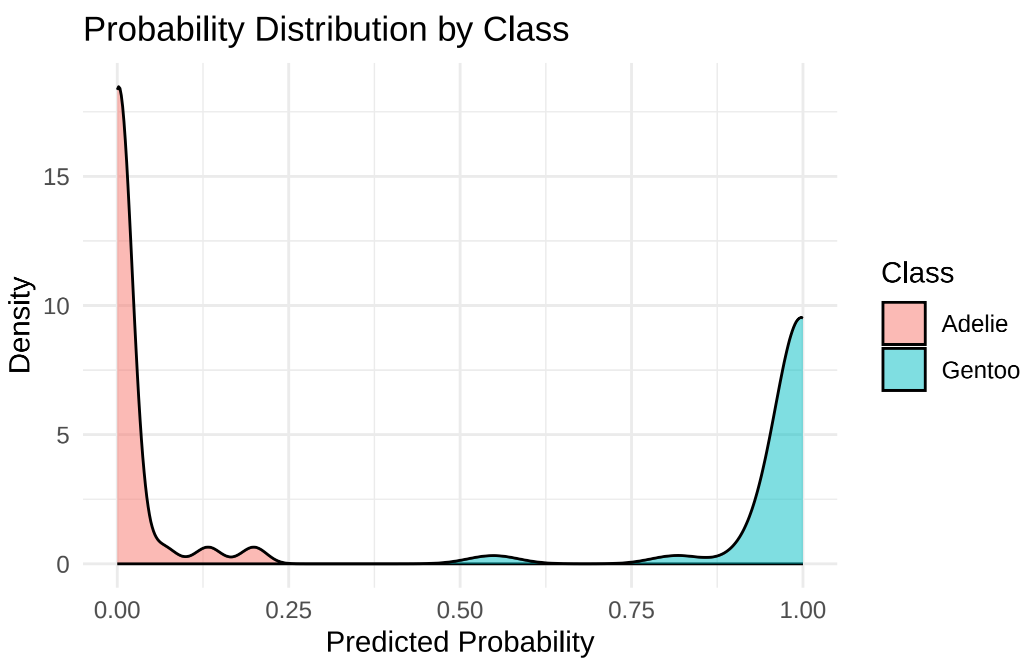
- *summary*
- *roc_curve*
- *pr_curve*
- *gain_curve*
- *lift_curve*
- *dist_by_class*
- *reliability_plot*
- *confusion_matrix*

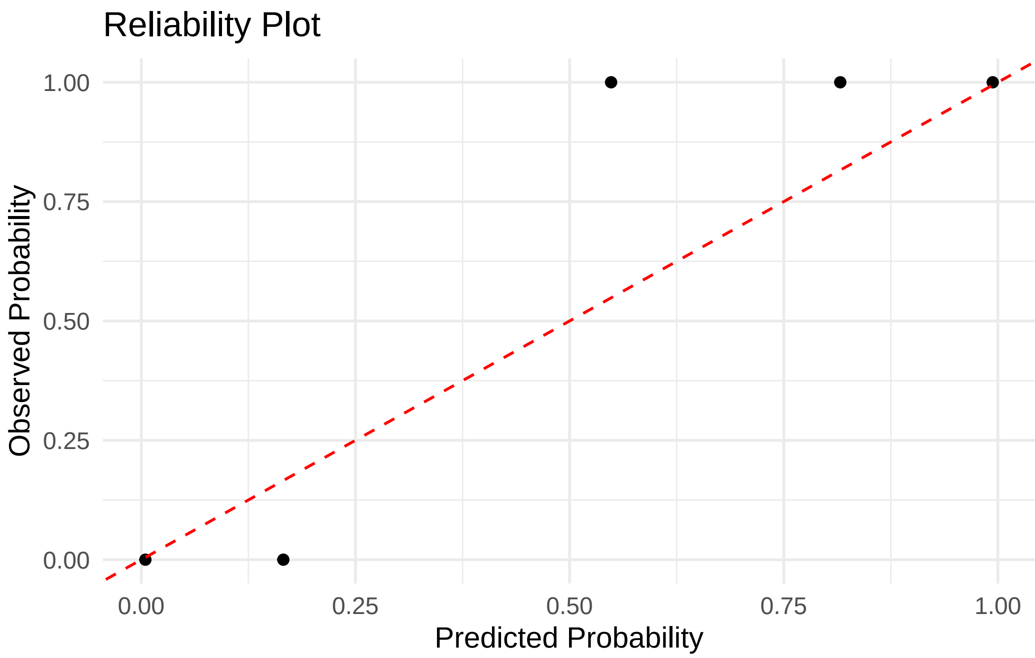
```
tidy_object <- show_results(tidy_object,
                            summary = TRUE,
                            roc_curve = TRUE,
                            confusion_matrix = TRUE,
                            reliability_plot = TRUE,
                            dist_by_class = TRUE)
```

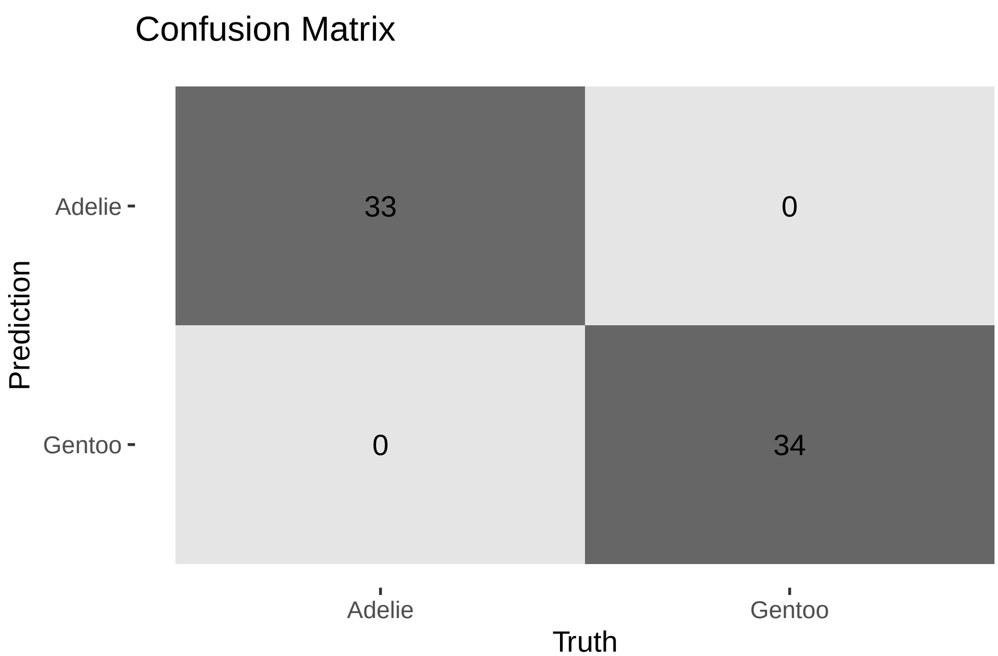
```
[1] "############# Showing Results"
```

Accuracy	1.000
Balanced_Accuracy	1.000
Precision	1.000
Recall	1.000
Specificity	1.000
Sensitivity	1.000
Kappa	1.000
F1_score	1.000
MCC	1.000
J_index	1.000
Detection_Prevalence	0.507
AUC_ROC	1.000
AUC_PR	1.000
Gain_Capture	1.000


ROC Curve
1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 − specificity
data_set
test
train
validation


Probability Distribution by Class
15
10
5
0
Density
0.00
0.25
0.50
0.75
1.00
Predicted Probability
Class
Adelie
Gentoo



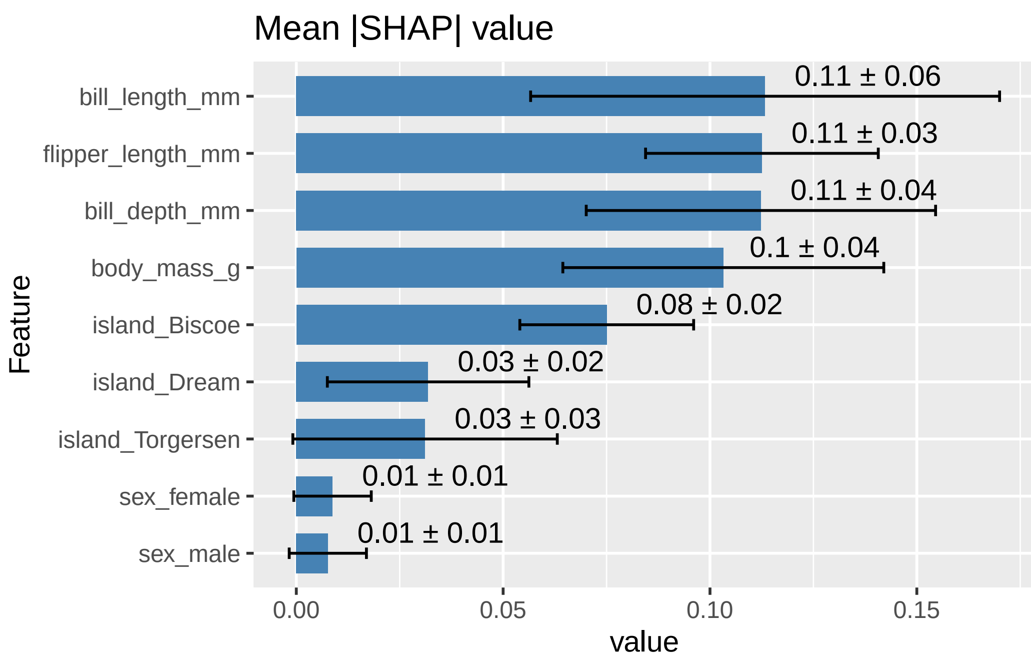


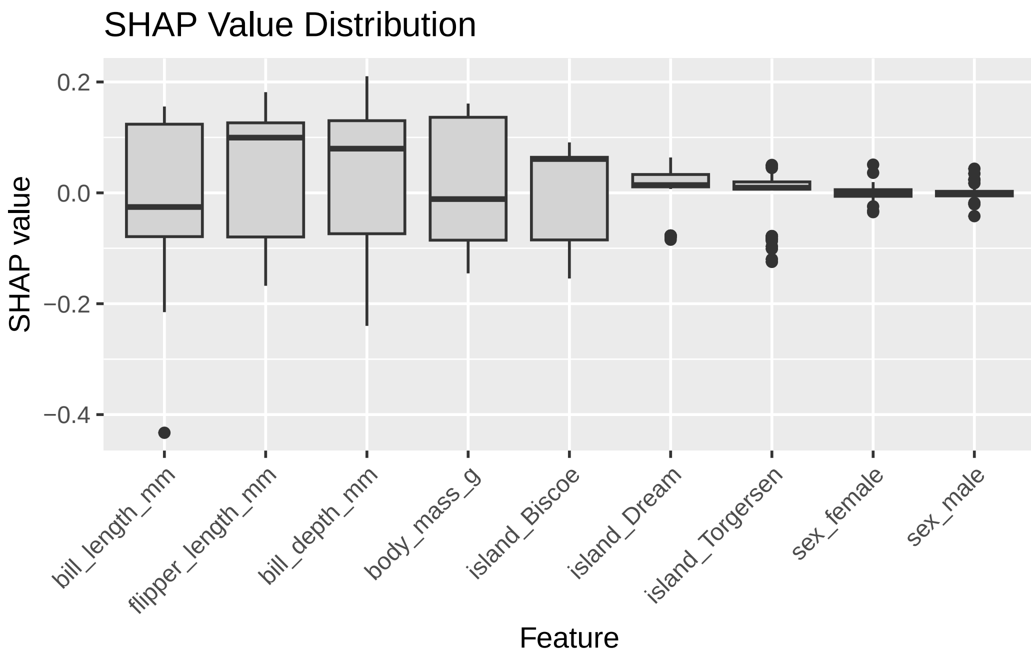
Sensitivity Analysis

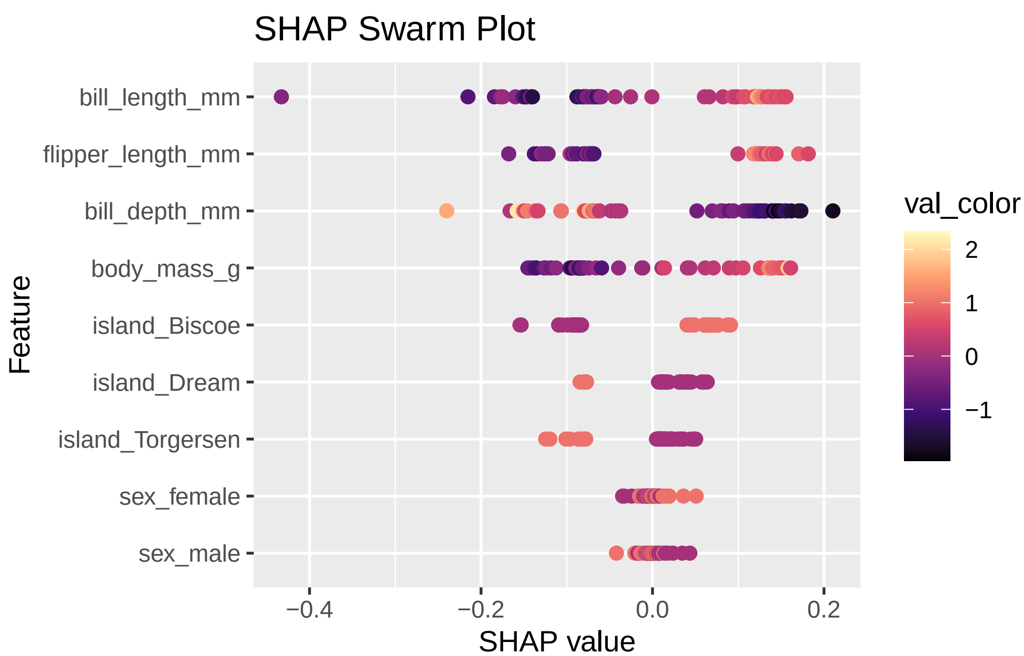
We can also perform sensitivity analysis for our fitted model using the ***sensitivity_analysis()*** function. There are currently different methods implemented, some of these methods only work for particular models:

1. Permutation Feature Importance ("PFI")
2. SHAP
3. Integrated Gradients (Neural Network only)
4. Olden method (Neural Network only)
5. **TO DO**: SOBOL? Shapley Effects?:

```
tidy_object <- sensitivity_analysis(tidy_object, type = "SHAP")
```




SHAP Value Distribution
SHAP value
0.2
0.0
−0.2
−0.4
bill_length_mm
flipper_length_mm
bill_depth_mm
body_mass_g
island_Biscoe
island_Dream
island_Torgersen
sex_female
sex_male
Feature


SHAP Swarm Plot
Feature
bill_length_mm
flipper_length_mm
bill_depth_mm
body_mass_g
island_Biscoe
island_Dream
island_Torgersen
sex_female
sex_male
−0.4
−0.2
0.0
0.2
SHAP value
val_color
2
1
0
−1

Regression Example

Create Dataset

We will again use the palmerpenguins dataset but choose a different formula for a regression task:

```
df <- palmerpenguins::penguins %>%
  na.omit() %>%
  dplyr::select(-year)
```

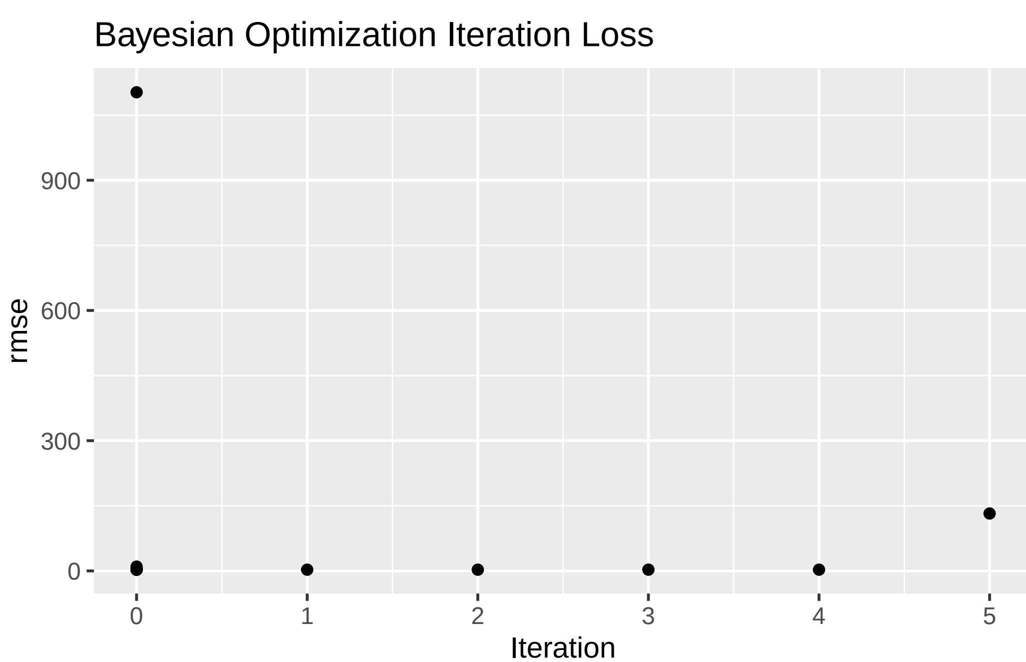
The Pipe (%>%) Operator

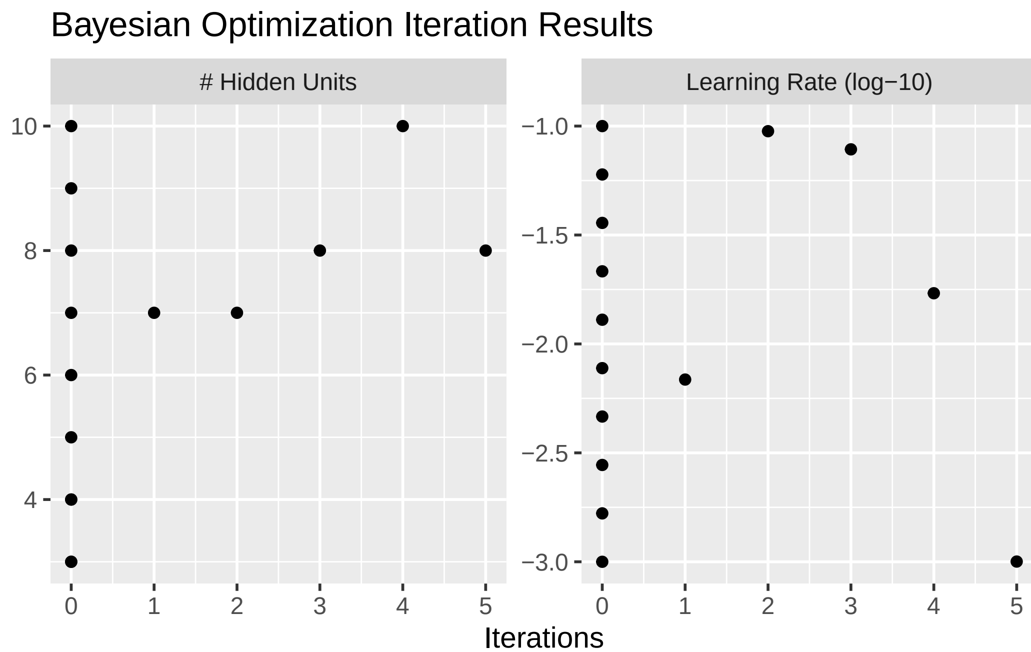
Due to the sequential nature of the processing, we can concatenate all the modelling steps using the %>% (pipe) operator without expliciting passing the tidy_object each time:

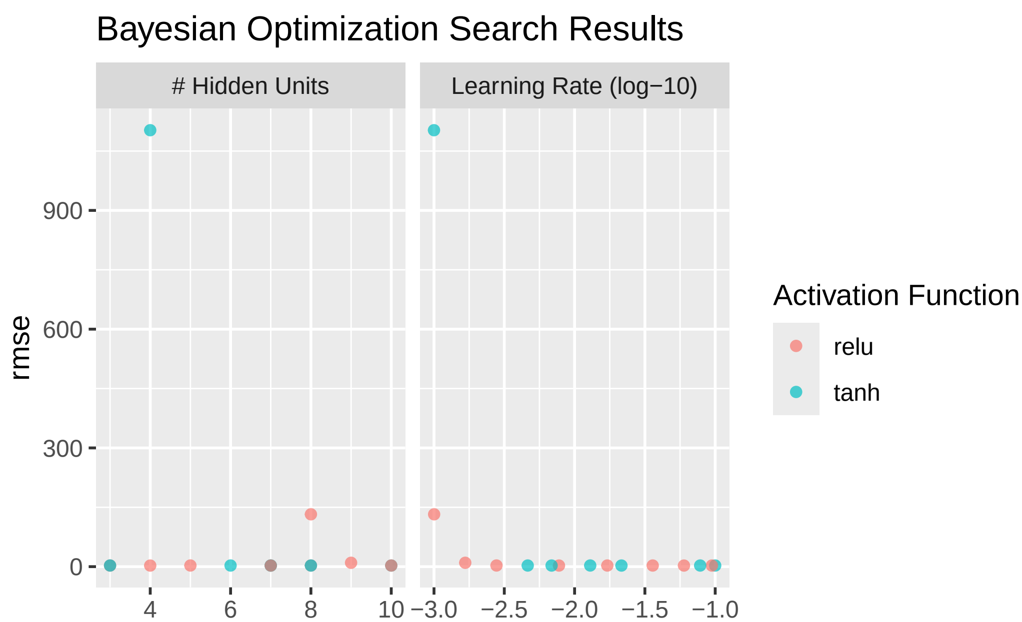
```
formula = "bill_length_mm ~ ."

tidy_object =  preprocessing(
                              df,
                              formula = formula,
                              norm_num_vars = "all",
                              encode_cat_vars = "all",
                              task = "regression"
                          ) %>%

               build_model(
                              model_names = "Neural Network",
                              hyperparameters =
                                list(
                                    hidden_units = c(3,10),
                                    activation = c("relu", "tanh")
                                    )
                          ) %>%

              fine_tuning(
                              tuner = "Bayesian Optimization",
                              metrics = "rmse",
                              plot_results = T
                         ) %>%
```

```
            show_results(
                        summary = TRUE,
                        scatter_residuals = TRUE,
                        scatter_predictions = TRUE
                ) %>%

            sensitivity_analysis(
                        type = "Integrated Gradients"
                ) %>%

            sensitivity_analysis(
                        type = "Olden"
            )
```

```
[1] "Commencing Tuning..."

! No improvement for 5 iterations; returning current results.

[1] "Tuning Finalized"
[1] "############# Hyperparameter Tuning Results"
```

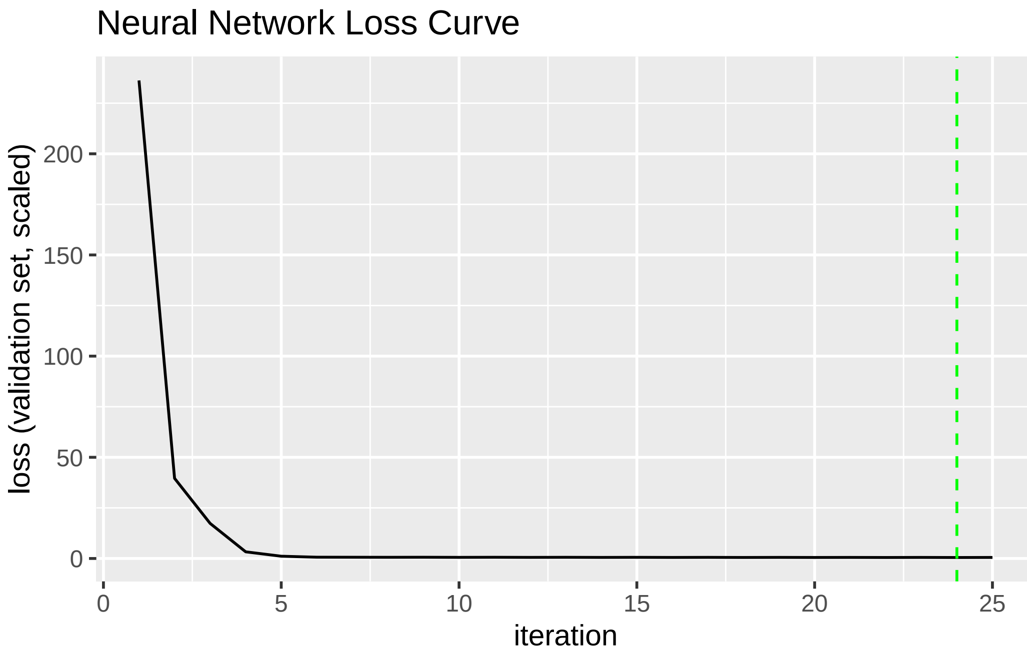






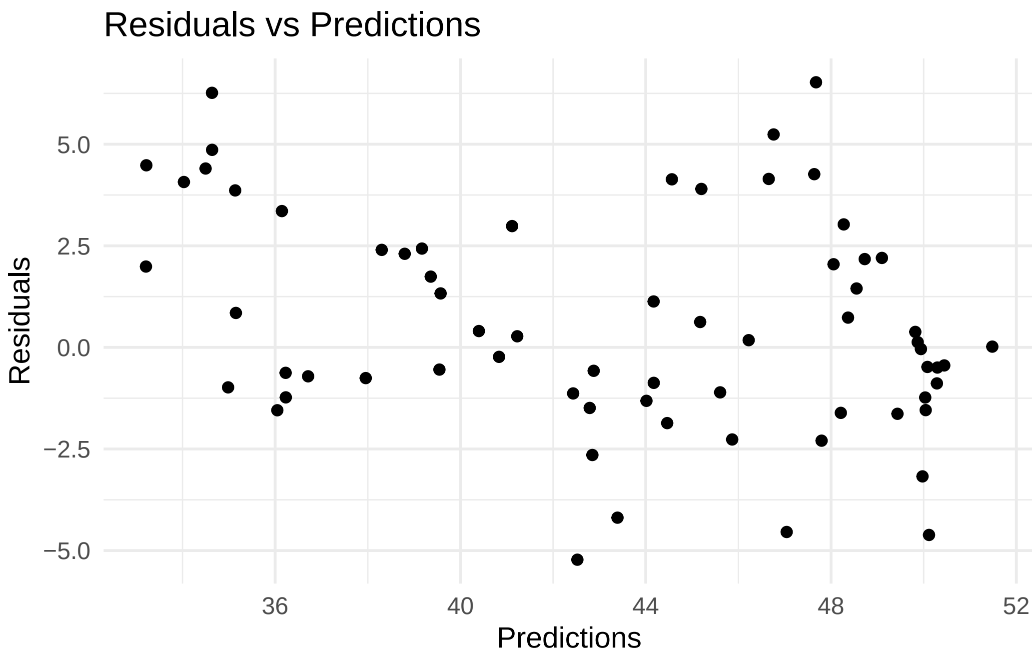

```
[1] "############# Best Hyperparameters Found:"
# A tibble: 1 x 10
  hidden_units activation learn_rate .metric .estimator  mean     n std_err
         <int> <chr>           <dbl> <chr>   <chr>      <dbl> <int>   <dbl>
1            4 relu           0.0599 rmse    standard    2.76     1      NA
# i 2 more variables: .config <chr>, .iter <int>
```

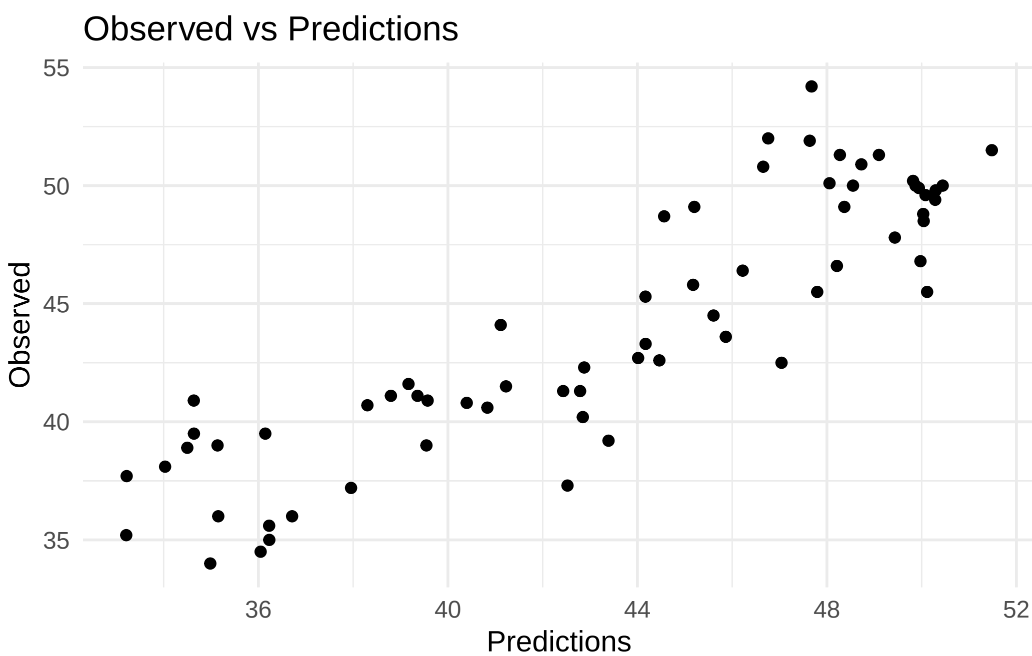
```
[1] "############# Loss Curve"
```

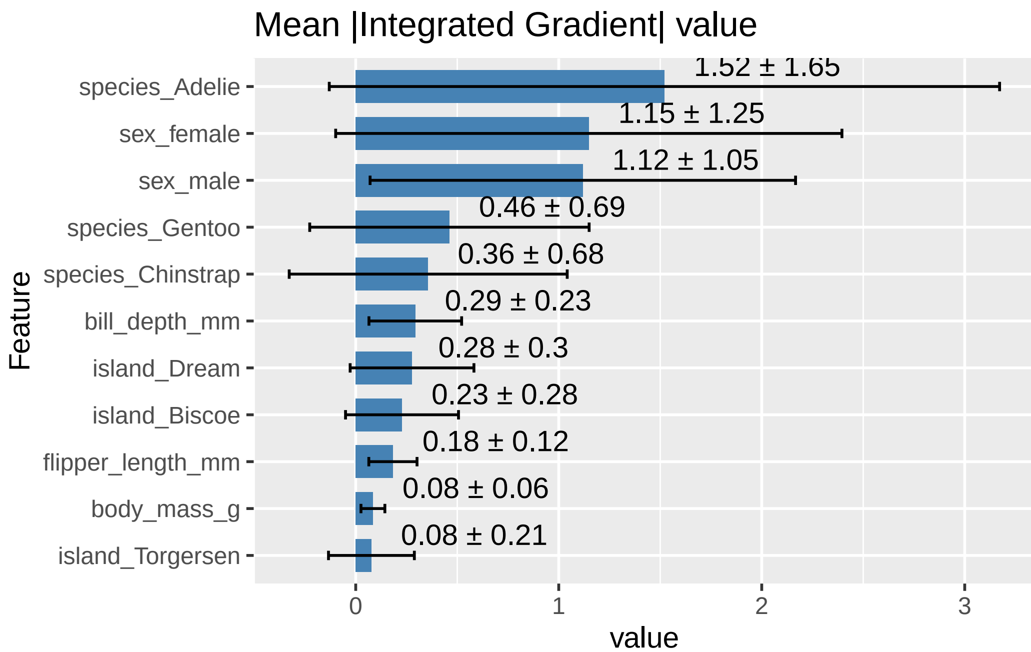



```
[1] "############# Showing Results"
```

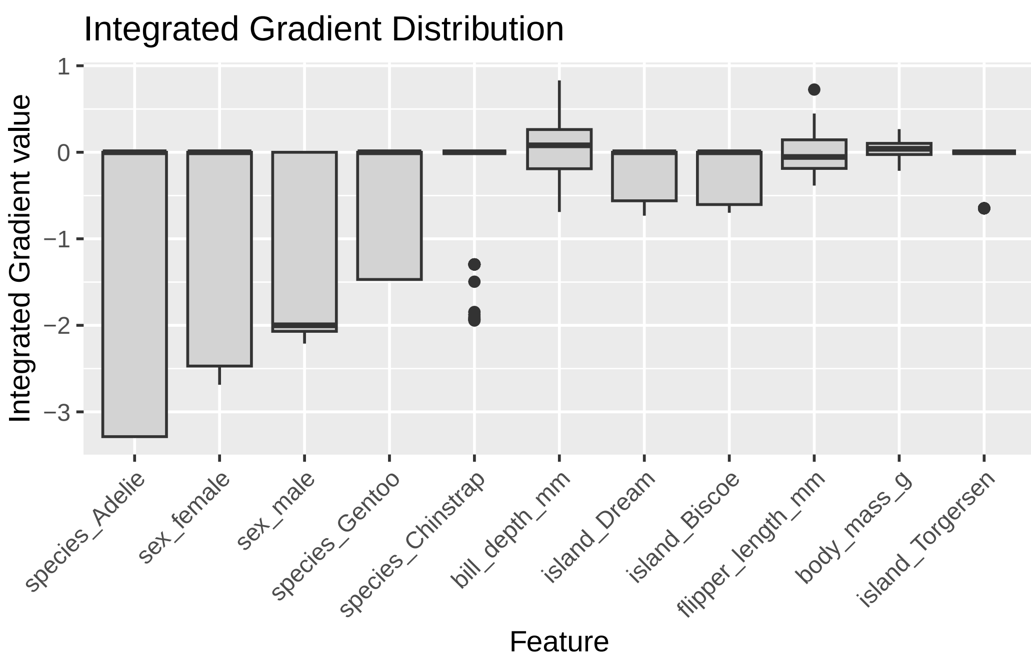
Metric	Value
RMSE	2.700
MAE	2.130
MAPE	4.910
MPE	1.190
CCC	0.878
SMAPE	4.990
RPIQ	3.480
RSQ	0.780


Residuals vs Predictions
5.0
2.5
0.0
−2.5
−5.0
Residuals
36
40
44
48
52
Predictions

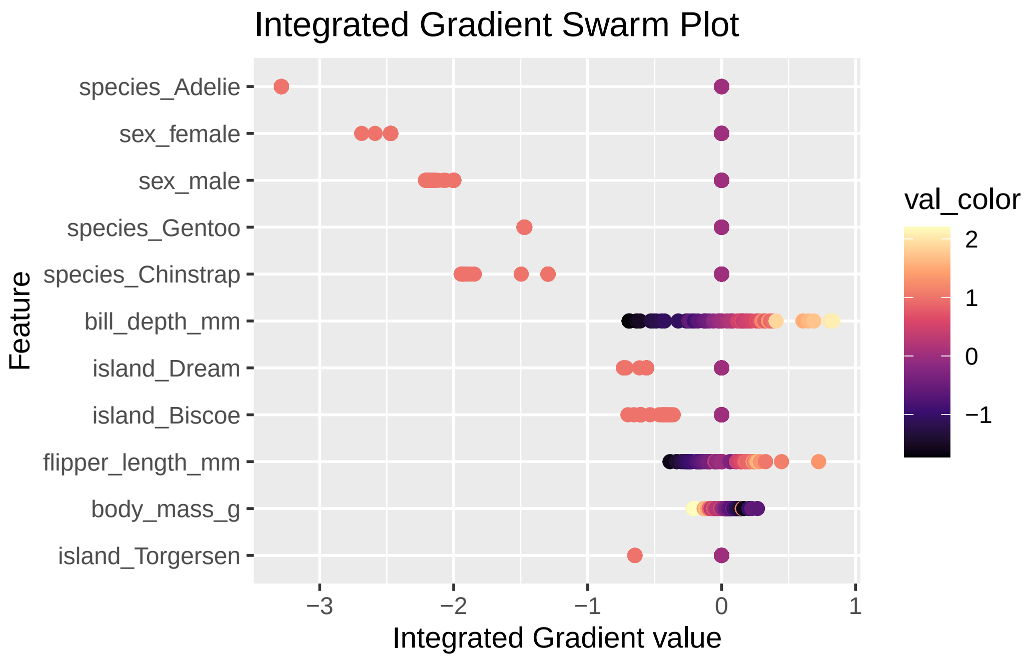

Observed vs Predictions
55
50
45
40
35
Observed
36
40
44
48
52
Predictions



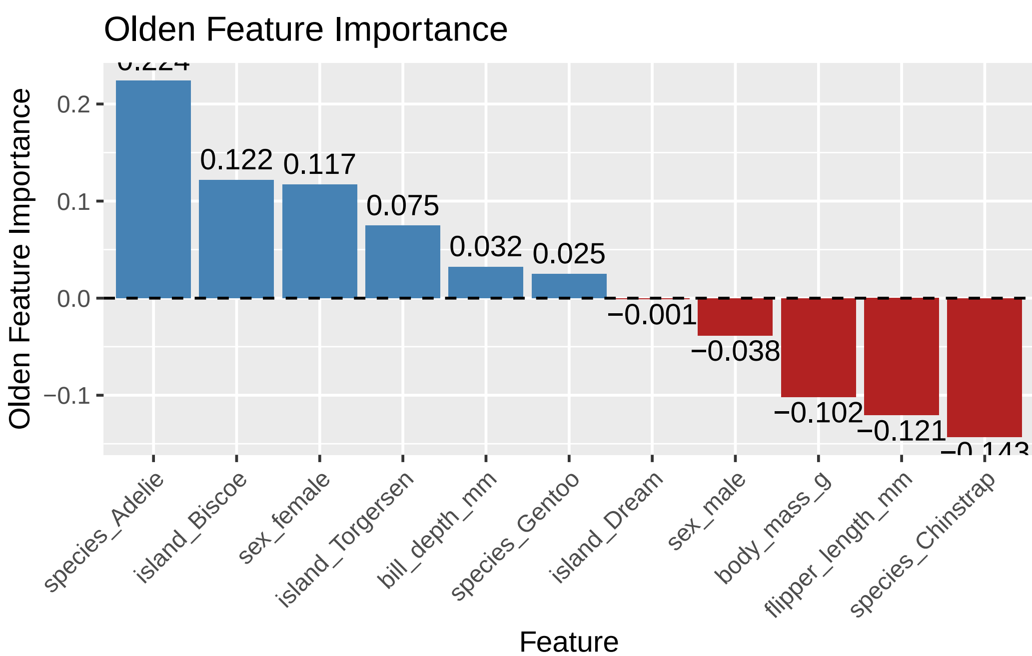
Mean |Integrated Gradient| value
species_Adelie
sex_female
sex_male
species_Gentoo
species_Chinstrap
bill_depth_mm
island_Dream
island_Biscoe
flipper_length_mm
body_mass_g
island_Torgersen
1.52 ± 1.65
1.15 ± 1.25
1.12 ± 1.05
0.46 ± 0.69
0.36 ± 0.68
0.29 ± 0.23
0.28 ± 0.3
0.23 ± 0.28
0.18 ± 0.12
0.08 ± 0.06
0.08 ± 0.21
Feature
0
1
2
3
value



Integrated Gradient Distribution
Integrated Gradient value
1
0
−1
−2
−3
species_Adelie
sex_female
sex_male
species_Gentoo
species_Chinstrap
bill_depth_mm
island_Dream
island_Biscoe
flipper_length_mm
body_mass_g
island_Torgersen
Feature



Integrated Gradient Swarm Plot
species_Adelie
sex_female
sex_male
species_Gentoo
species_Chinstrap
bill_depth_mm
island_Dream
island_Biscoe
flipper_length_mm
body_mass_g
island_Torgersen
Feature
−3
−2
−1
0
1
Integrated Gradient value
val_color
2
1
0
−1



Olden Feature Importance
0.224
0.122
0.117
0.075
0.032
0.025
−0.001
−0.038
−0.102
−0.121
−0.143
0.2
0.1
0.0
−0.1
Olden Feature Importance
species_Adelie
island_Biscoe
sex_female
island_Torgersen
bill_depth_mm
species_Gentoo
island_Dream
sex_male
body_mass_g
flipper_length_mm
species_Chinstrap
Feature