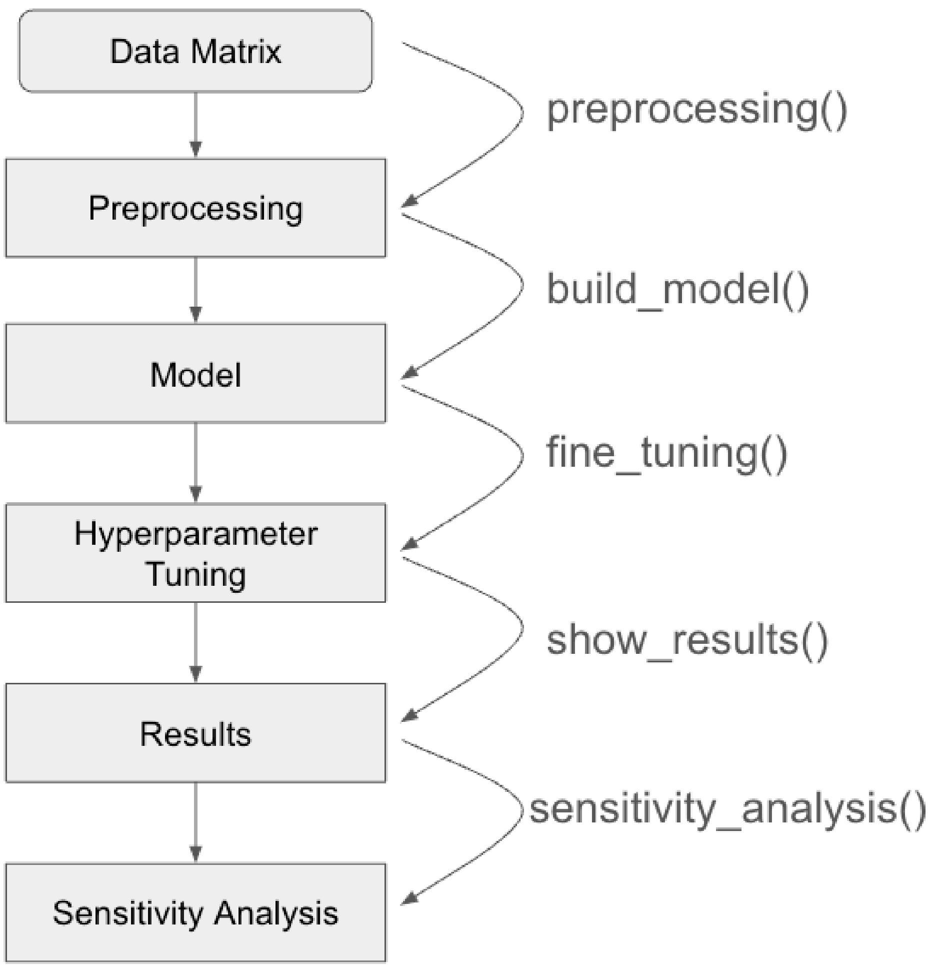
Tutorial TidyML

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



TidyML can be downloaded from github using the ***devtools::install_github()*** function.

```
#install.packages("devtools")
#devtools::install_github("JMartinezGarcia/TidyML")

library(dplyr)
```

```
Attaching package: 'dplyr'

The following objects are masked from 'package:stats':

    filter, lag
```

```
The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

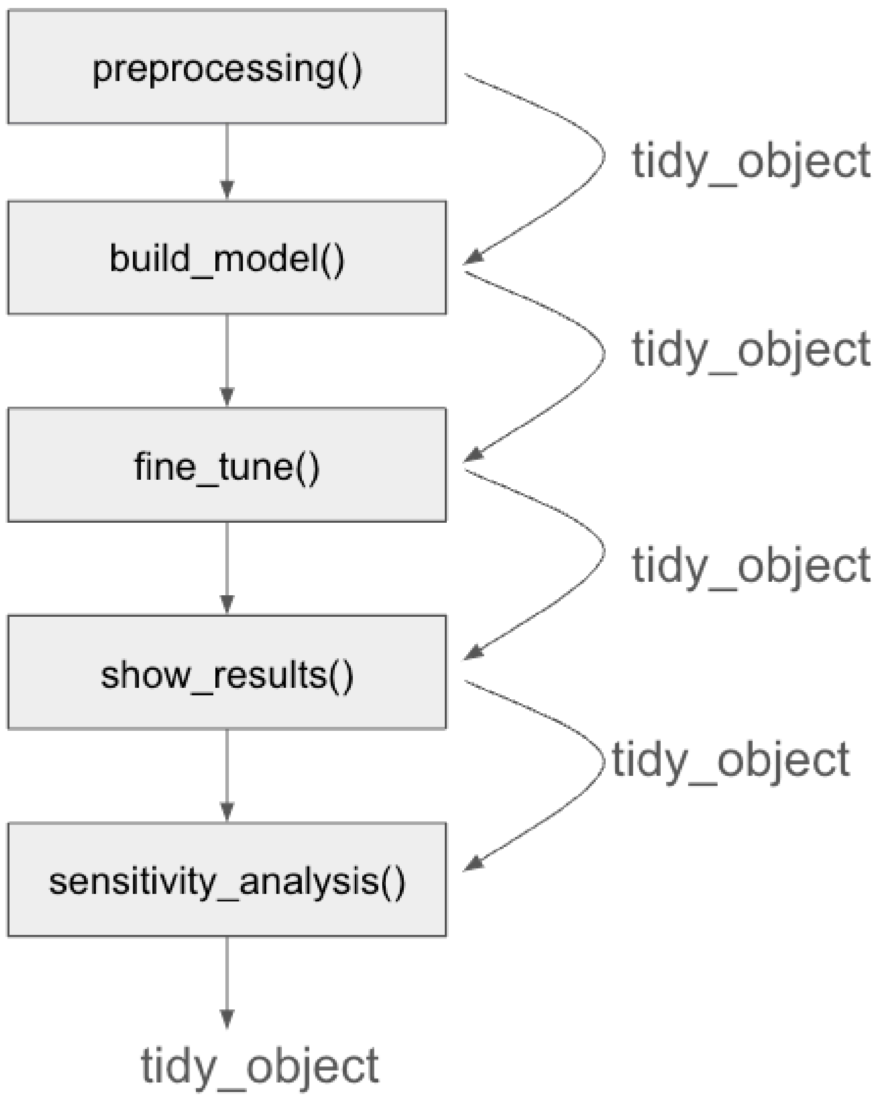
```
library(TidyML)
```

```
Loading required package: tidyverse

-- Attaching core tidyverse packages ------------------------ tidyverse 2.0.0 --
v forcats   1.0.0     v readr     2.1.5
v ggplot2   3.5.2     v stringr   1.5.1
v lubridate 1.9.4     v tibble    3.2.1
v purrr     1.0.4     v tidyr     1.3.1
-- 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
```

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:

- *formula*: Modelling formula
- *task*: task of analysis ("regression" or "classification")
- *full_data*: Full data matrix
- *train_data*: Training data matrix
- *validation_data*: Validation data matrix (with Grid Search CV there is no validation data)
- *test_data*: Testing data matrix
- *outcome_levels*: Levels of target feature if task is classification
- *transformer*: Preprocessor object (recipe from recipe library)
- *models_names*: Name of model
- *models*: Model before fitting (from parsnip library)
- *hyperparameters*: Hyperparameters for tuning
- *metrics*: Metric used for tuning

- *tuner*: Name of tuner
- *tuner_fit*: Results from tuner search
- *workflow*: Whole workflow (from workflow library)
- *final_models*: Final trained model (from parsnip library)
- *fit_summary*: Performance summary results
- *predictions*: Predictions of the model
- *sensitivity_analysis*: Sensitivity analysis results



Binary Classification Example

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

Create Dataset

```
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):

```
formula = "species ~ ."

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

```
Registered S3 method overwritten by 'future':
  method               from
  all.equal.connection parallelly
```

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

```r
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*

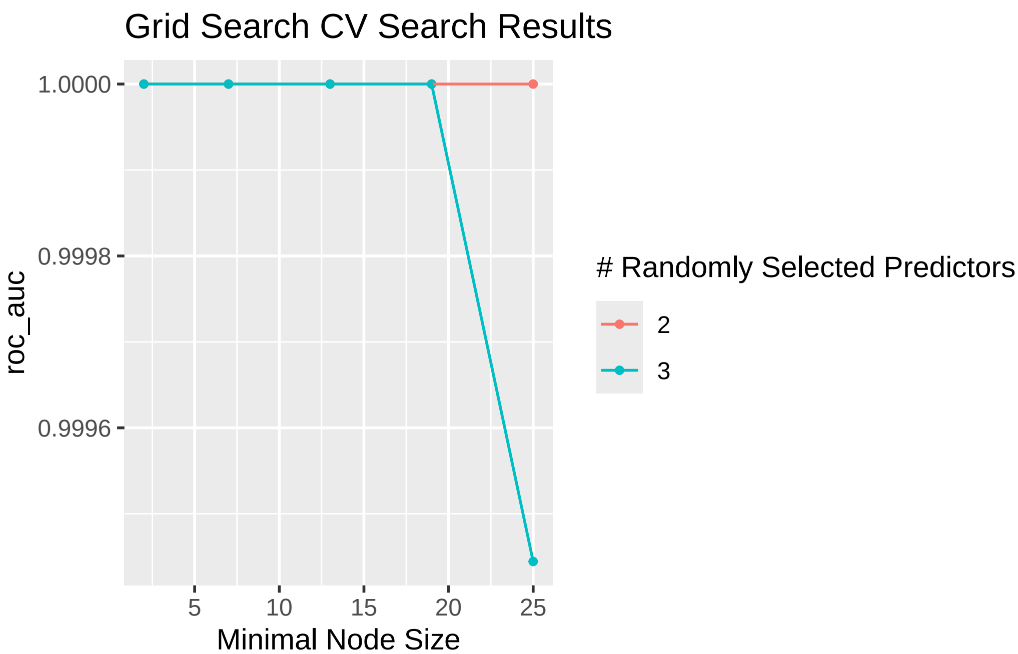
Additionally, we will specify the metric used to select the best performing hyperparameters:

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:

```r
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

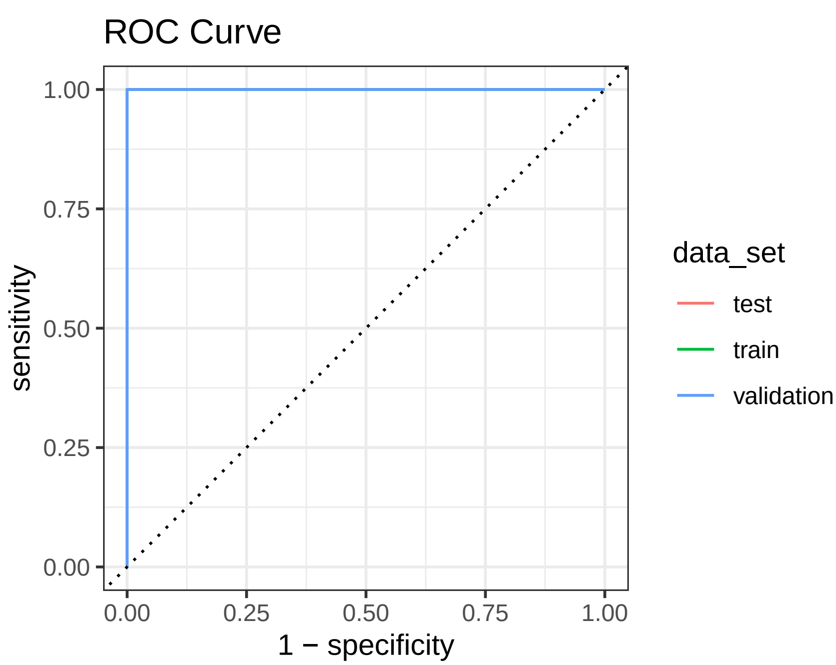
Once we have found the best hyperparameter configuration we can compute the performance metrics of our model based on the test data using the ***show_results()*** function. There are different options for the results depending on whether we are doing a regression task or a classification task:

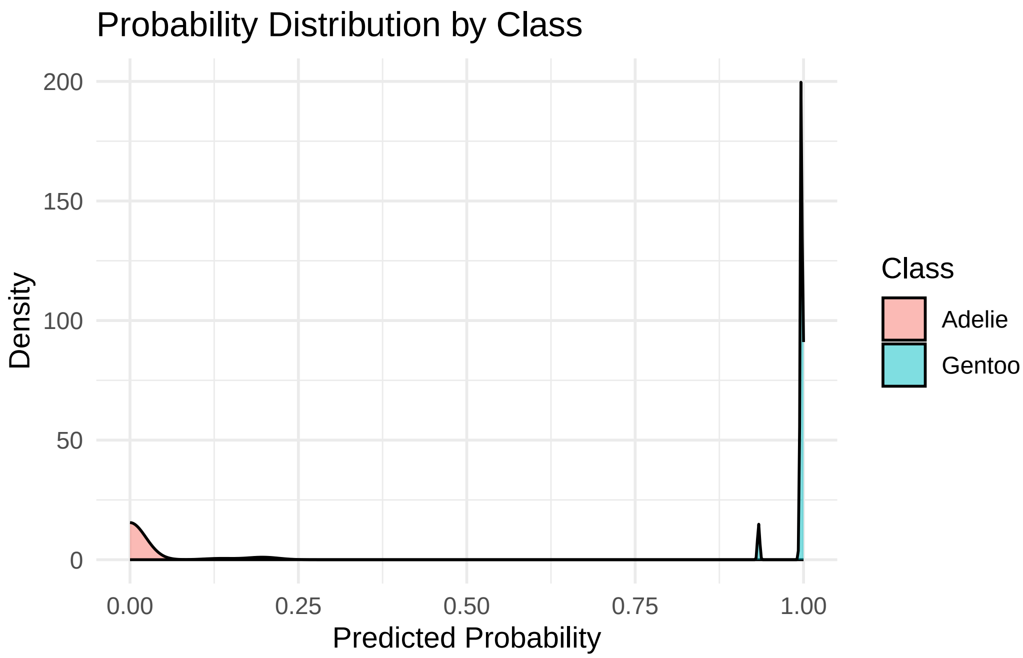
- **Regression**:
  - *summary*
  - *scatter_residuals*
  - *scatter_predictions*
  - *residuals_dist*
- **Classification**:
  - *summary*
  - *roc_curve*
  - *pr_curve*
  - *gain_curve*
  - *lift_curve*
  - *dist_by_class*
  - *reliability_plot*
  - *confusion_matrix*

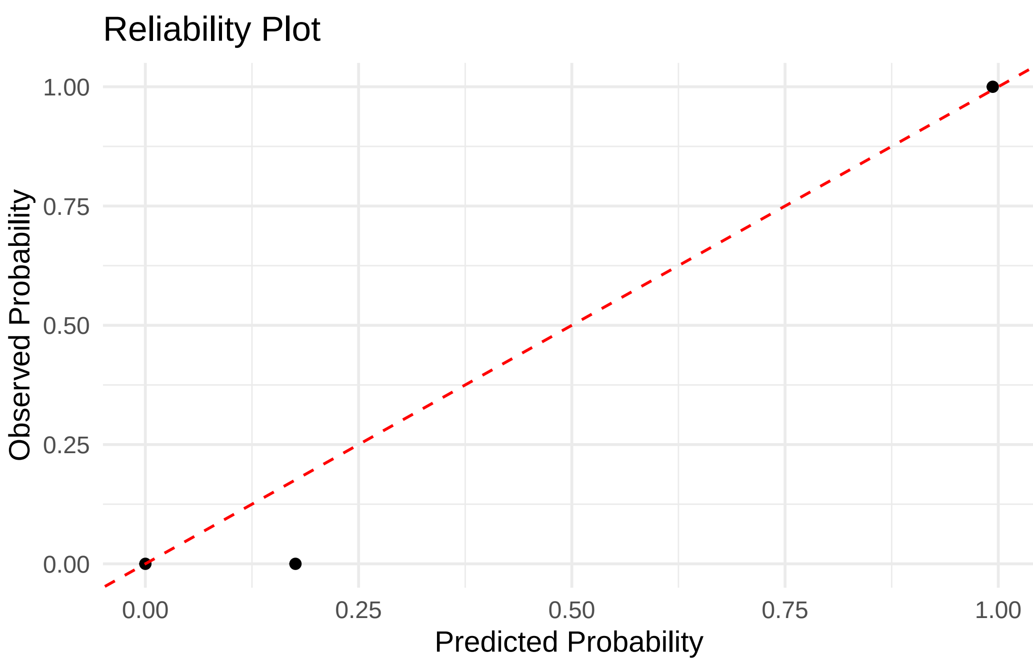
```
tidy_object <- show_results(tidy_object,
                            summary = TRUE,
                            roc_curve = TRUE,
                            confusion_matrix = TRUE,
                            reliability_plot = TRUE,
                            dist_by_class = TRUE)
```

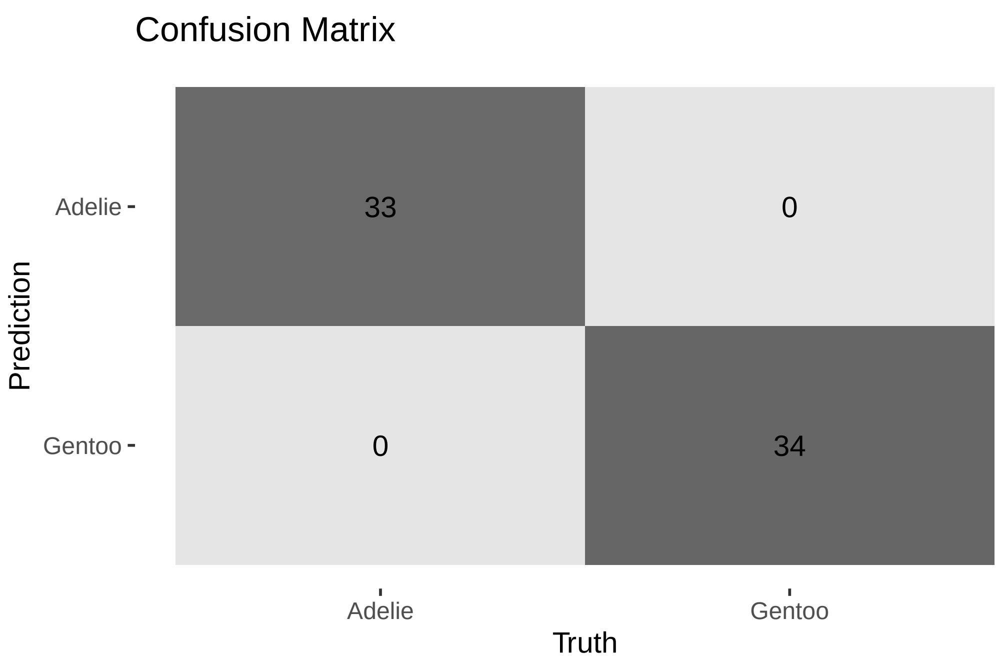
```
[1] "############# Showing Results"
```

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




Probability Distribution by Class
200
150
100
50
0
Density
0.00
0.25
0.50
0.75
1.00
Predicted Probability
Class
Adelie
Gentoo


Reliability Plot
1.00
0.75
0.50
0.25
0.00
Observed Probability
0.00
0.25
0.50
0.75
1.00
Predicted Probability

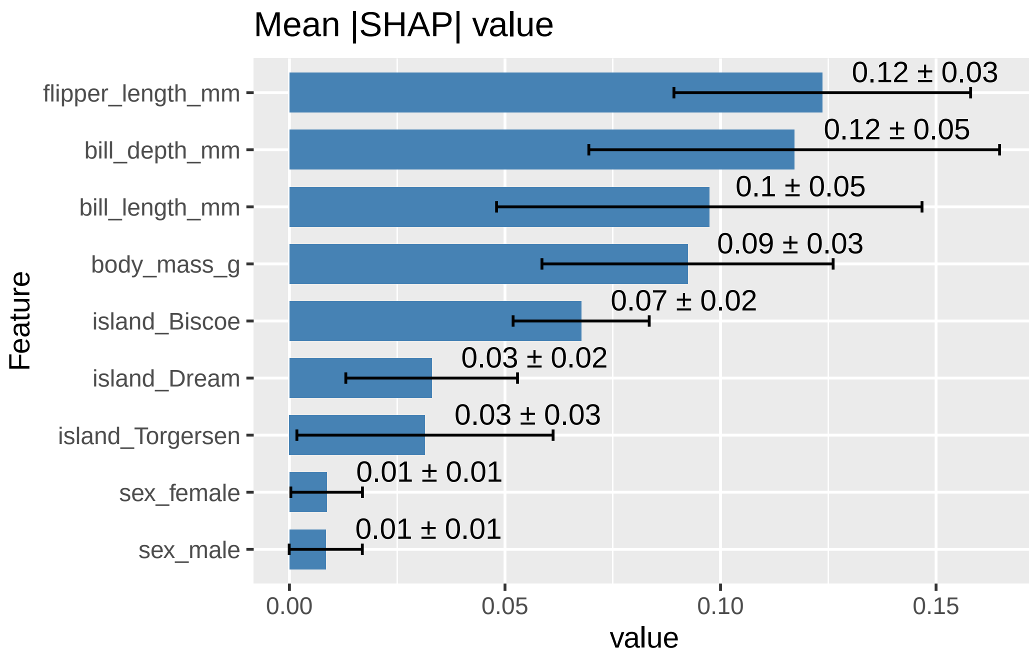


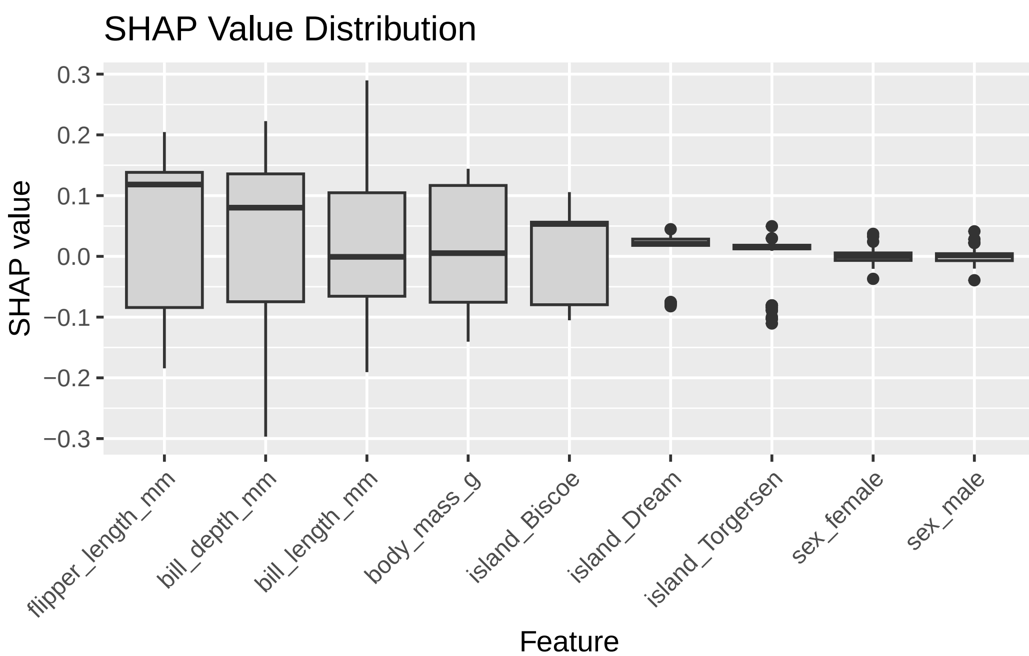
Sensitivity Analysis

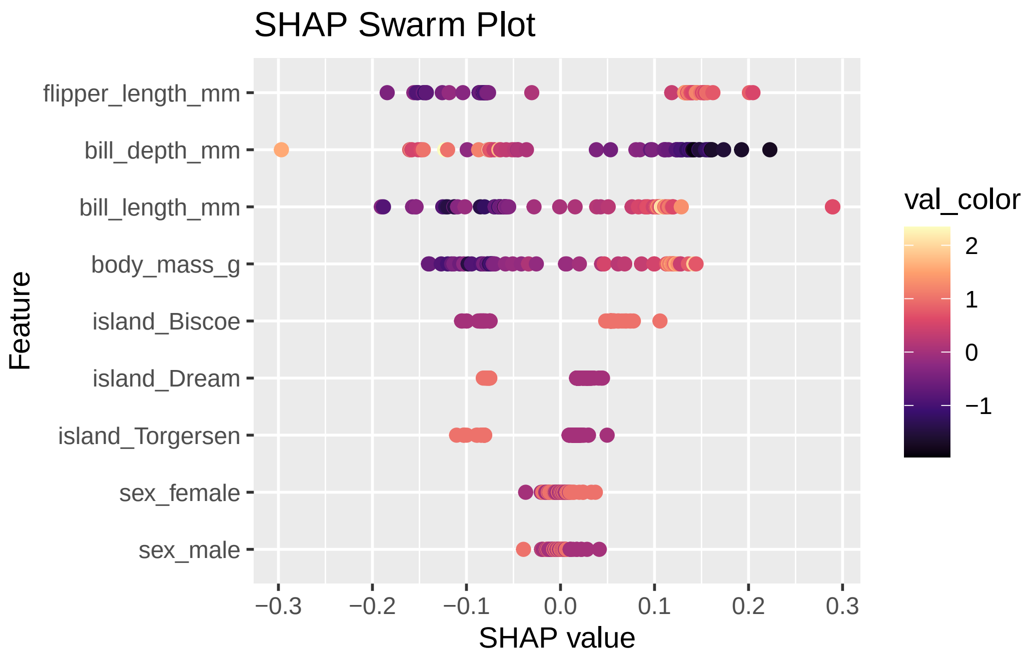
We can also perform sensitivity analysis for our fitted model using the ***sensitivity_analysis()*** function. There are currently different methods implemented, some of these methods only work for particular models:

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")
```


Mean |SHAP| value
Feature
flipper_length_mm
bill_depth_mm
bill_length_mm
body_mass_g
island_Biscoe
island_Dream
island_Torgersen
sex_female
sex_male
0.12 ± 0.03
0.12 ± 0.05
0.1 ± 0.05
0.09 ± 0.03
0.07 ± 0.02
0.03 ± 0.02
0.03 ± 0.03
0.01 ± 0.01
0.01 ± 0.01
0.00
0.05
0.10
0.15
value


SHAP Value Distribution
SHAP value
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
flipper_length_mm
bill_depth_mm
bill_length_mm
body_mass_g
island_Biscoe
island_Dream
island_Torgersen
sex_female
sex_male
Feature



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)
```

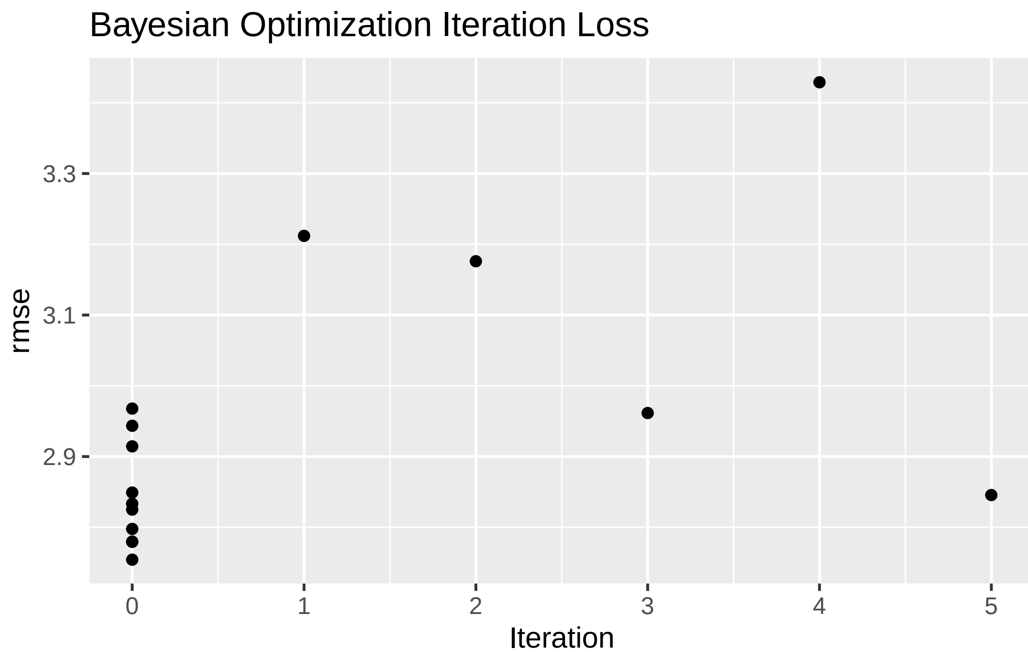
The Pipe (%>%) Operator

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:

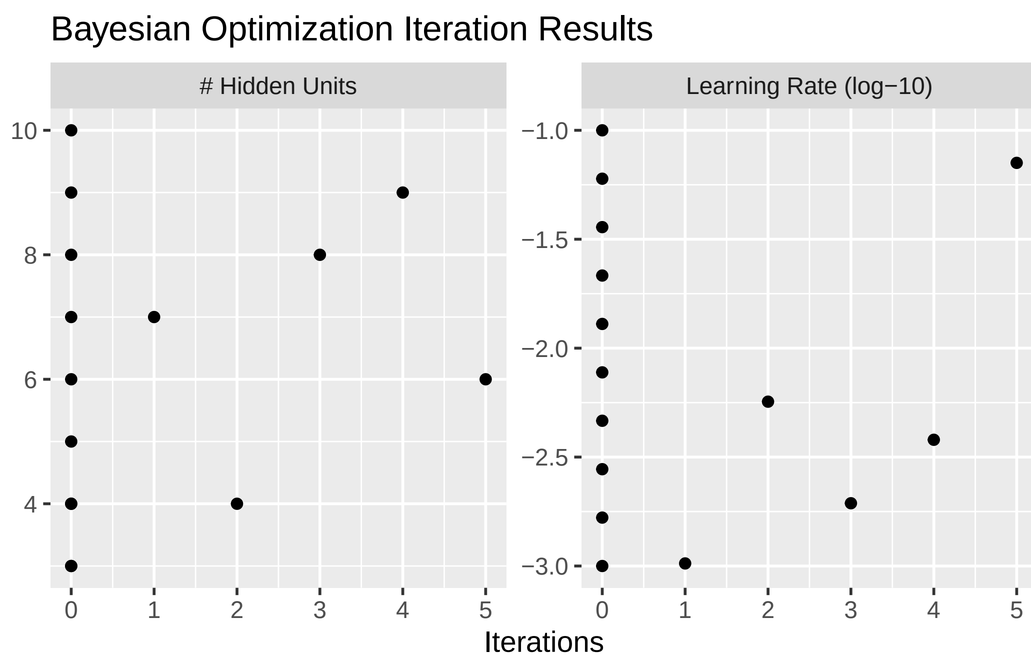
```
formula = "bill_length_mm ~ ."

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"
              )
```

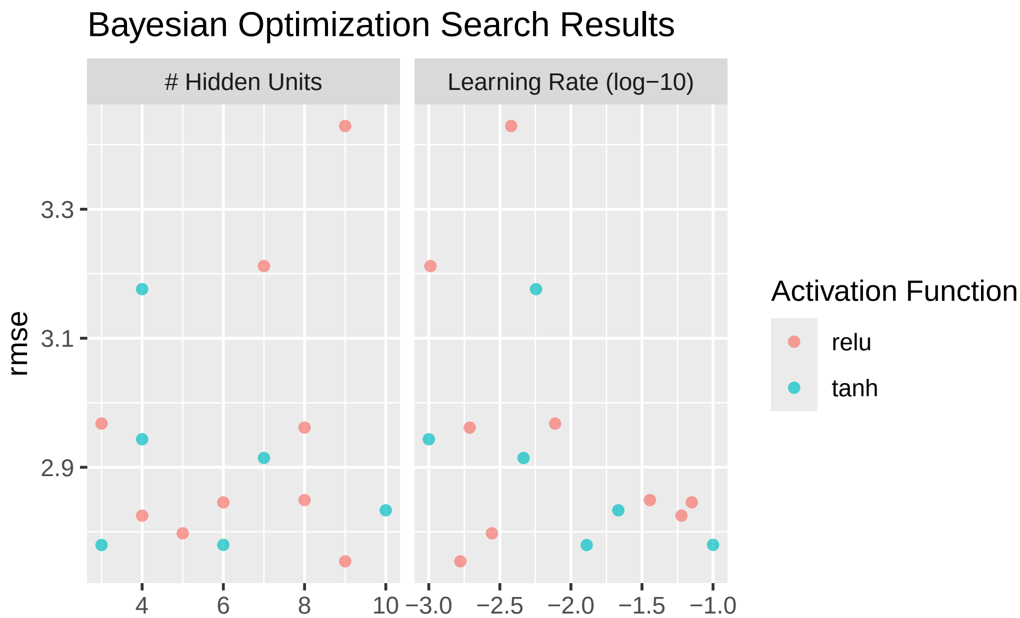
```
[1] "Commencing Tuning..."

! No improvement for 5 iterations; returning current results.

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



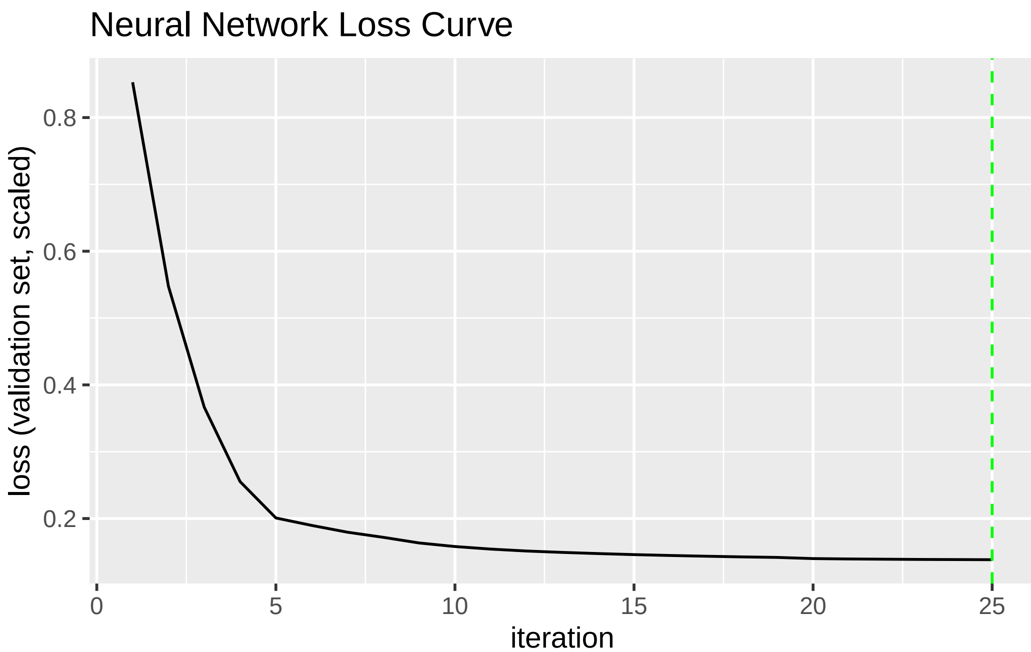
Bayesian Optimization Iteration Loss
rmse
3.3
3.1
2.9
0
1
2
3
4
5
Iteration



Bayesian Optimization Iteration Results
Hidden Units
Learning Rate (log−10)
10
8
6
4
−1.0
−1.5
−2.0
−2.5
−3.0
0
1
2
3
4
5
Iterations

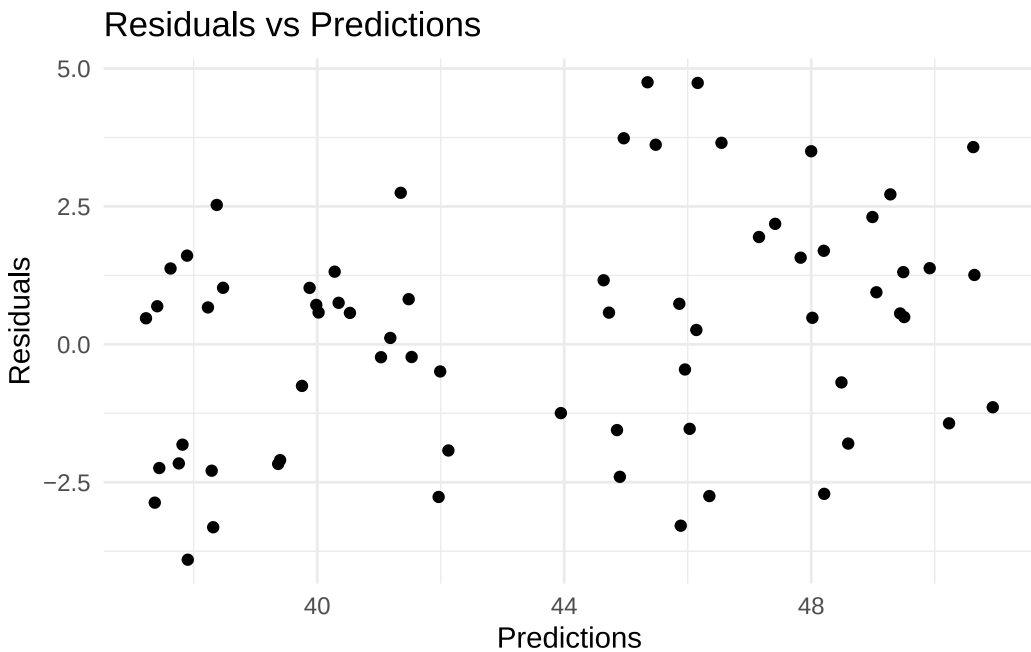


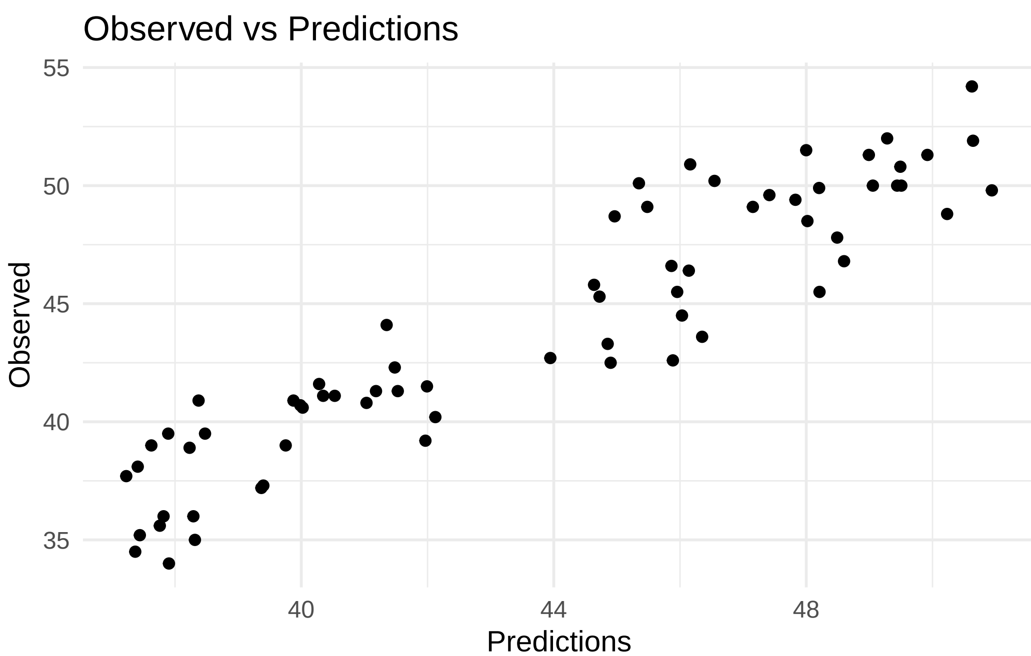

```
[1] "############# Best Hyperparameters Found:"
# A tibble: 1 x 10
  hidden_units activation learn_rate .metric .estimator  mean     n std_err
         <int> <chr>           <dbl> <chr>   <chr>      <dbl> <int>   <dbl>
1            9 relu          0.00167 rmse    standard    2.75     1      NA
# i 2 more variables: .config <chr>, .iter <int>
[1] "############# Loss Curve"
```

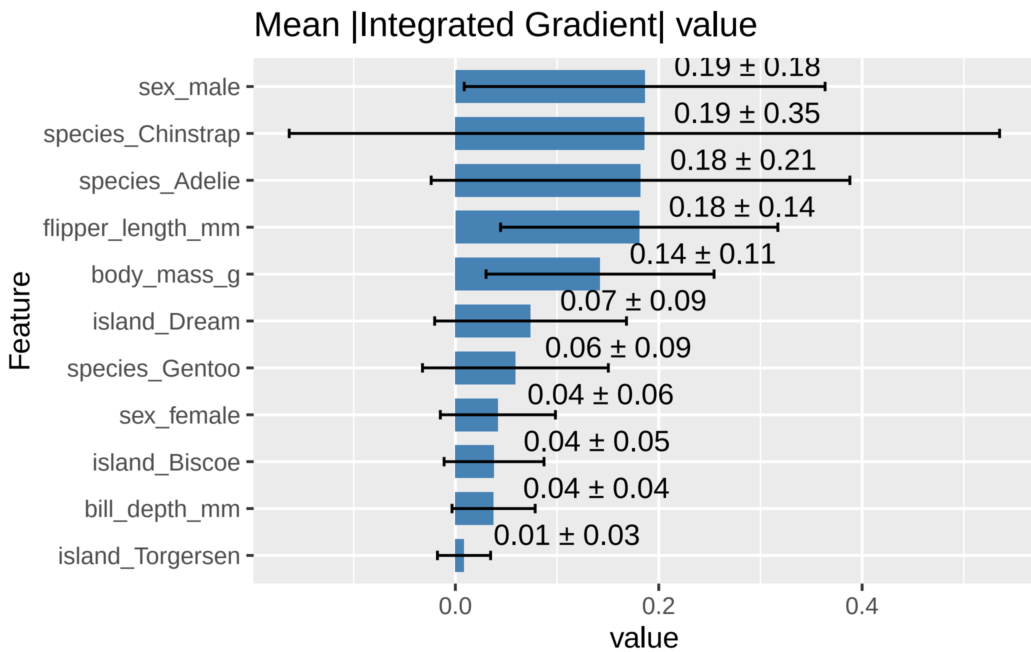


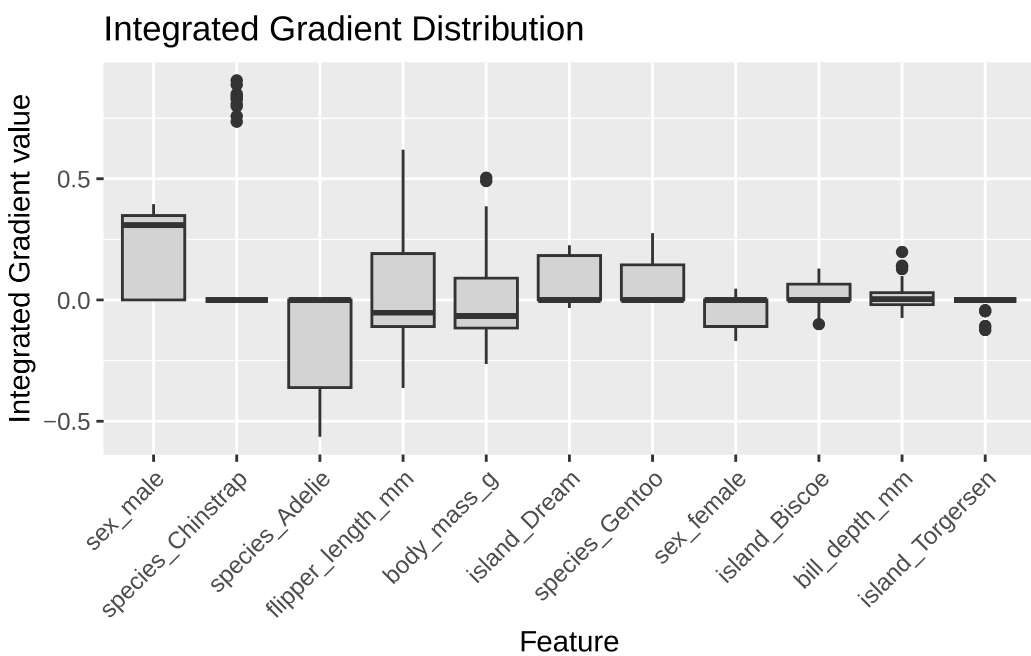

```
[1] "############# Showing Results"
```

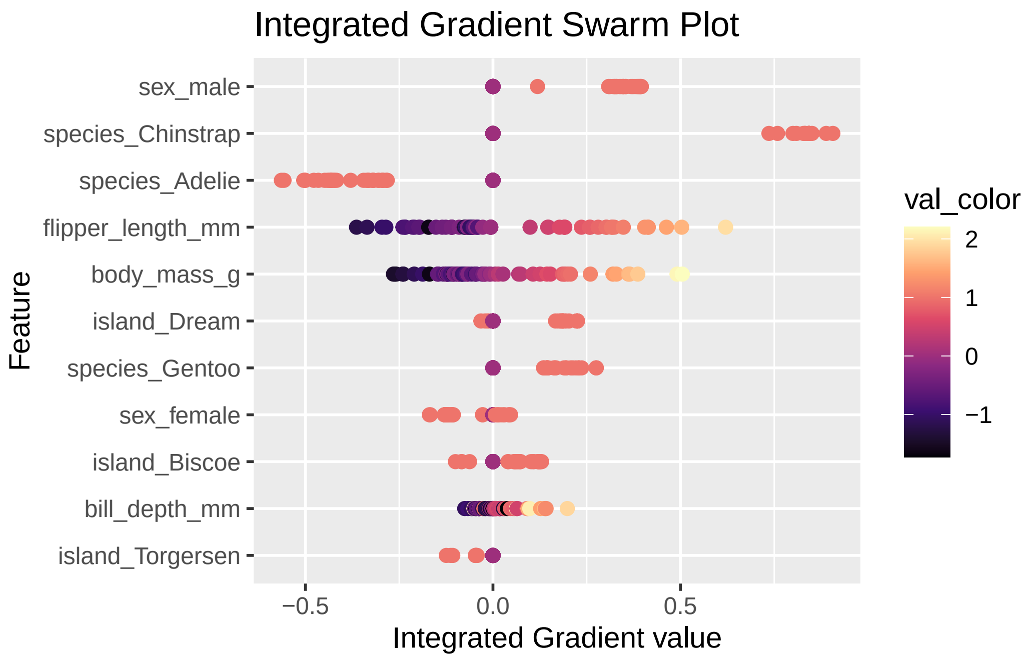
Metric	Value
RMSE	2.080
MAE	1.740
MAPE	3.990
MPE	0.175
CCC	0.910
SMAPE	3.990
RPIQ	4.510
RSQ	0.864

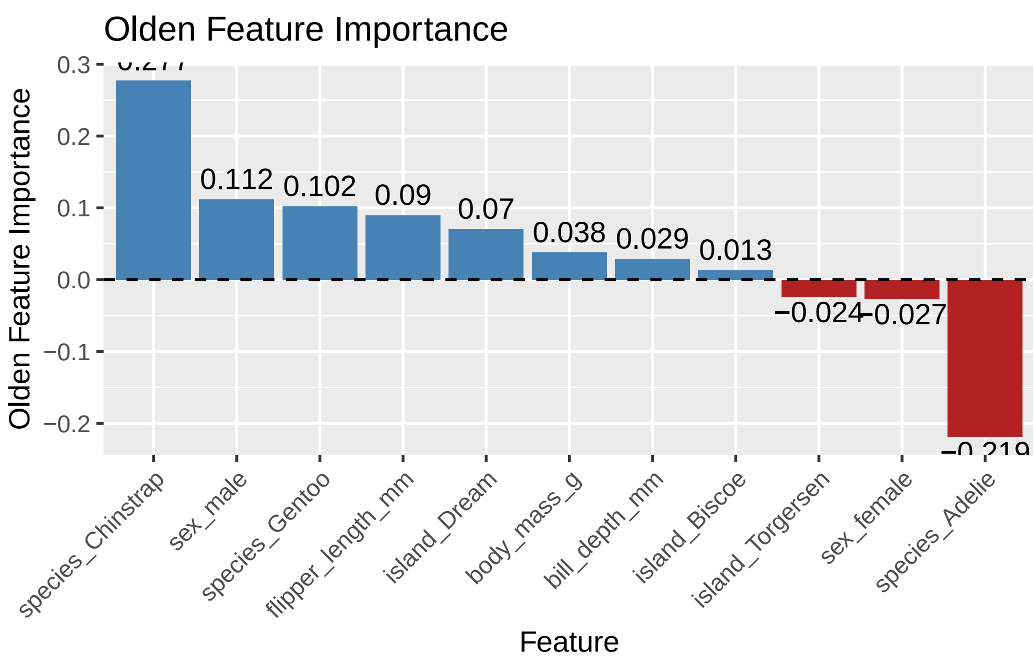

Residuals vs Predictions
5.0
2.5
0.0
−2.5
Residuals
40
44
48
Predictions


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


Mean |Integrated Gradient| value
Feature
sex_male
species_Chinstrap
species_Adelie
flipper_length_mm
body_mass_g
island_Dream
species_Gentoo
sex_female
island_Biscoe
bill_depth_mm
island_Torgersen
0.19 ± 0.18
0.19 ± 0.35
0.18 ± 0.21
0.18 ± 0.14
0.14 ± 0.11
0.07 ± 0.09
0.06 ± 0.09
0.04 ± 0.06
0.04 ± 0.05
0.04 ± 0.04
0.01 ± 0.03
0.0
0.2
0.4
value


Integrated Gradient Distribution
Integrated Gradient value
0.5
0.0
−0.5
sex_male
species_Chinstrap
species_Adelie
flipper_length_mm
body_mass_g
island_Dream
species_Gentoo
sex_female
island_Biscoe
bill_depth_mm
island_Torgersen
Feature


Integrated Gradient Swarm Plot
sex_male
species_Chinstrap
species_Adelie
flipper_length_mm
body_mass_g
island_Dream
species_Gentoo
sex_female
island_Biscoe
bill_depth_mm
island_Torgersen
Feature
−0.5
0.0
0.5
Integrated Gradient value
val_color
2
1
0
−1


Olden Feature Importance
0.3
0.2
0.1
0.0
−0.1
−0.2
Olden Feature Importance
0.277
0.112
0.102
0.09
0.07
0.038
0.029
0.013
−0.024
−0.027
−0.219
species_Chinstrap
sex_male
species_Gentoo
flipper_length_mm
island_Dream
body_mass_g
bill_depth_mm
island_Biscoe
island_Torgersen
sex_female
species_Adelie
Feature