Model Accuracy and Evaluation

Spring 2023

May 17 2023

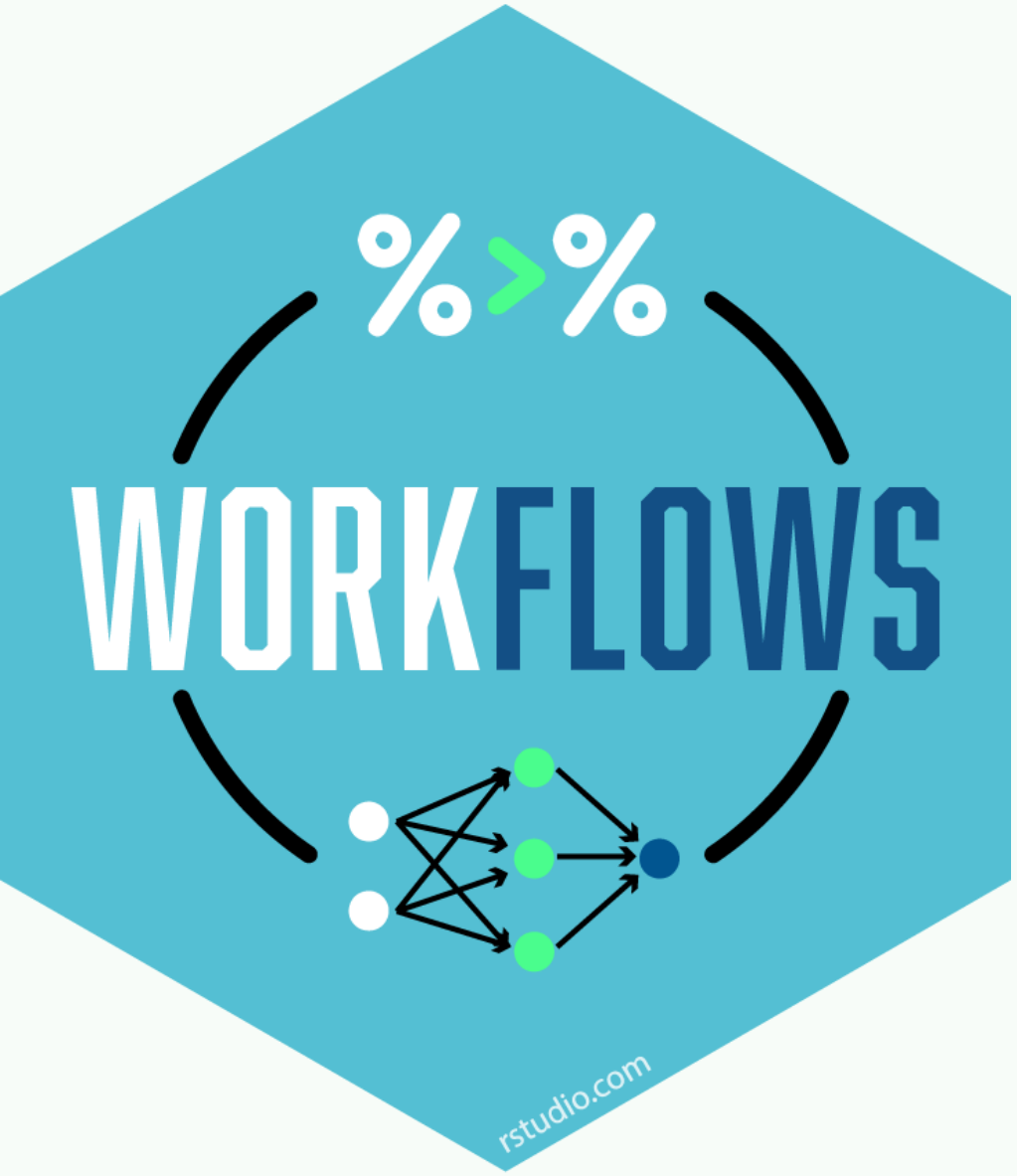
Recap: KNN (K- Nearest Neighbor)

- *Supervised machine learning algorithm i.e., it requires labeled data for training*
- *Need to tell the algorithm the exact number of neighbors (K) we want to consider*

Training and Testing

Training: *Fitting a model with certain hyper-parameters on a particular subset of the dataset*

Testing: *Test the model on a different subset of the dataset to get an estimate of a final, unbiased assessment of the model's performance*



Workflows

A machine learning workflow (the "black box") containing model specification and preprocessing recipe/formula

Forest Fire : Data Description (Recall!)

Variable	Description
Date	(DD-MM-YYYY) Day, month, year
Temp	Noon temperature in Celsius degrees: 22 to 42
RH	Relative Humidity in percentage: 21 to 90
Ws	Wind speed in km/h: 6 to 29
Rain	Daily total rain in mm: 0 to 16.8
Fine Fuel Moisture Code (FFMC) index	28.6 to 92.5
Duff Moisture Code (DMC) index	1.1 to 65.9
Drought Code (DC) index	7 to 220.4
Initial Spread Index (ISI) index	0 to 18.5
Buildup Index (BUI) index	1.1 to 68
Fire Weather Index (FWI) index	0 to 31.1
Classes	Two classes, namely **fire** and **not fire**

1. Create a workflow: Split the raw data

```
set.seed(123) # set seed for reproducibility

# Prepare the raw dataset
fire_raw <- fire %>% select(temperature, isi, classes)

fire_split <- initial_split(fire_raw, prop = 0.75)
```

```
# Create training data
(fire_train <- fire_split %>% training())
# A tibble: 182 × 3
   temperature   isi classes
         <dbl> <dbl> <chr>
 1          38   4.1 fire
 2          34  14.3 fire
 3          33   6.7 fire
 4          30   1   not fire
 5          35   7.5 fire
 6          34   7.3 fire
 7          33   2.8 fire
 8          31   2.5 not fire
 9          34   3   not fire
10          33  14.2 fire
# … with 172 more rows
```

```
# Create testing data
(fire_test <- fire_split %>% testing())
# A tibble: 61 × 3
   temperature   isi classes
         <dbl> <dbl> <chr>
 1          29   1   not fire
 2          26   0.3 not fire
 3          26   4.8 fire
 4          28   0.4 not fire
 5          31   0.7 not fire
 6          31   2.5 not fire
 7          34   9.2 fire
 8          32   7.6 fire
 9          32   2.2 not fire
10          29   1.1 not fire
# … with 51 more rows
```

2. Make a recipe

```
fire_recipe <- recipe(classes ~ ., data = fire_raw) %>%
  step_scale(all_predictors()) %>% # scale the predictors
  step_center(all_predictors()) %>% # center the predictors
  prep    # pre-process
```

3. Specify the model

```
fire_knn_spec <- nearest_neighbor(mode = "classification",
                                  engine = "kknn",
                                  weight_func = "rectangular",
                                  neighbors = 5)
```

4. Define the workflow object

```
fire_workflow <- workflow() %>% # initialize a workflow
  add_recipe(fire_recipe) %>% # add recipe
  add_model(fire_knn_spec) # add model specification
```

5. Fit the model

```
fire_fit <- fit(fire_workflow, data = fire_train)
```

Fitted workflow

```
fire_fit
══ Workflow [trained] ══════════════════════════════════════════════════════════
Preprocessor: Recipe
Model: nearest_neighbor()

── Preprocessor ────────────────────────────────────────────────────────────────
2 Recipe Steps

• step_scale()
• step_center()

── Model ───────────────────────────────────────────────────────────────────────

Call:
kknn::train.kknn(formula = ..y ~ ., data = data, ks = min_rows(5,     data, 5), kernel = ~"rectangular")

Type of response variable: nominal
Minimal misclassification: 0.03296703
Best kernel: rectangular
Best k: 5
```

6. Evaluate the model on test dataset

```
test_features <- fire_test %>% select(temperature, isi)
fire_pred <- predict(fire_fit, test_features)
fire_results <- fire_test %>%
  select(classes) %>%
  bind_cols(predicted = fire_pred)
```

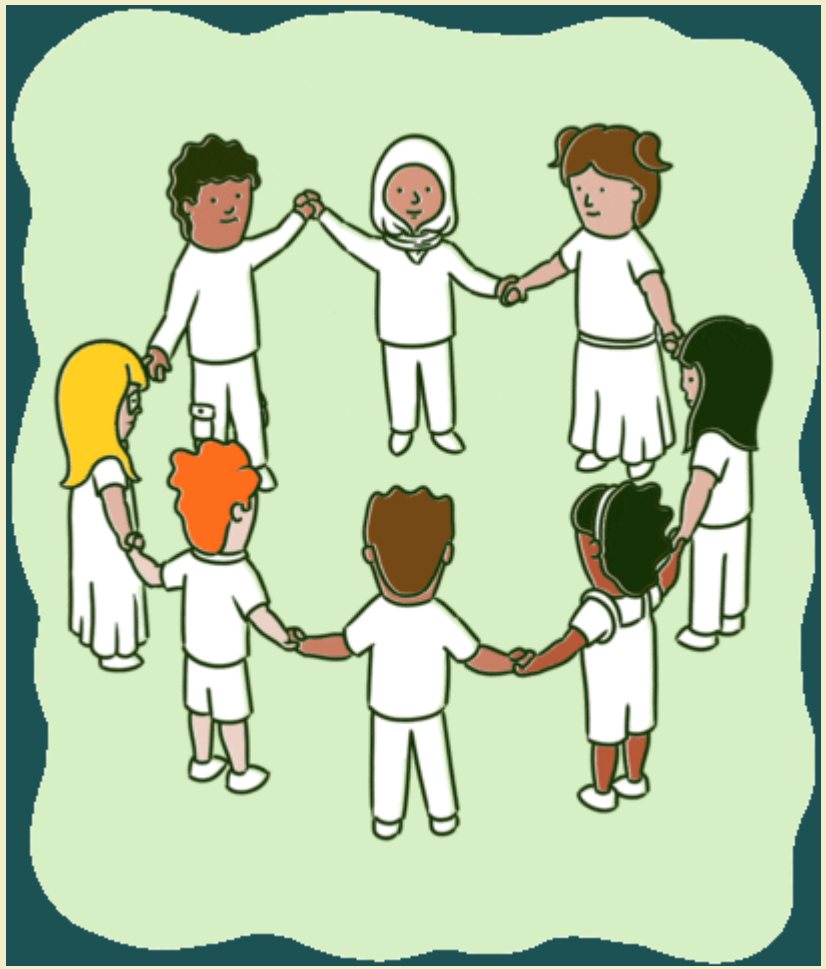
7. Compare the known labels and predicted labels

```
knitr::kable(fire_results)
```

classes	.pred_class
not fire	not fire
not fire	not fire
fire	fire
not fire	not fire
not fire	not fire
not fire	not fire
fi	fi

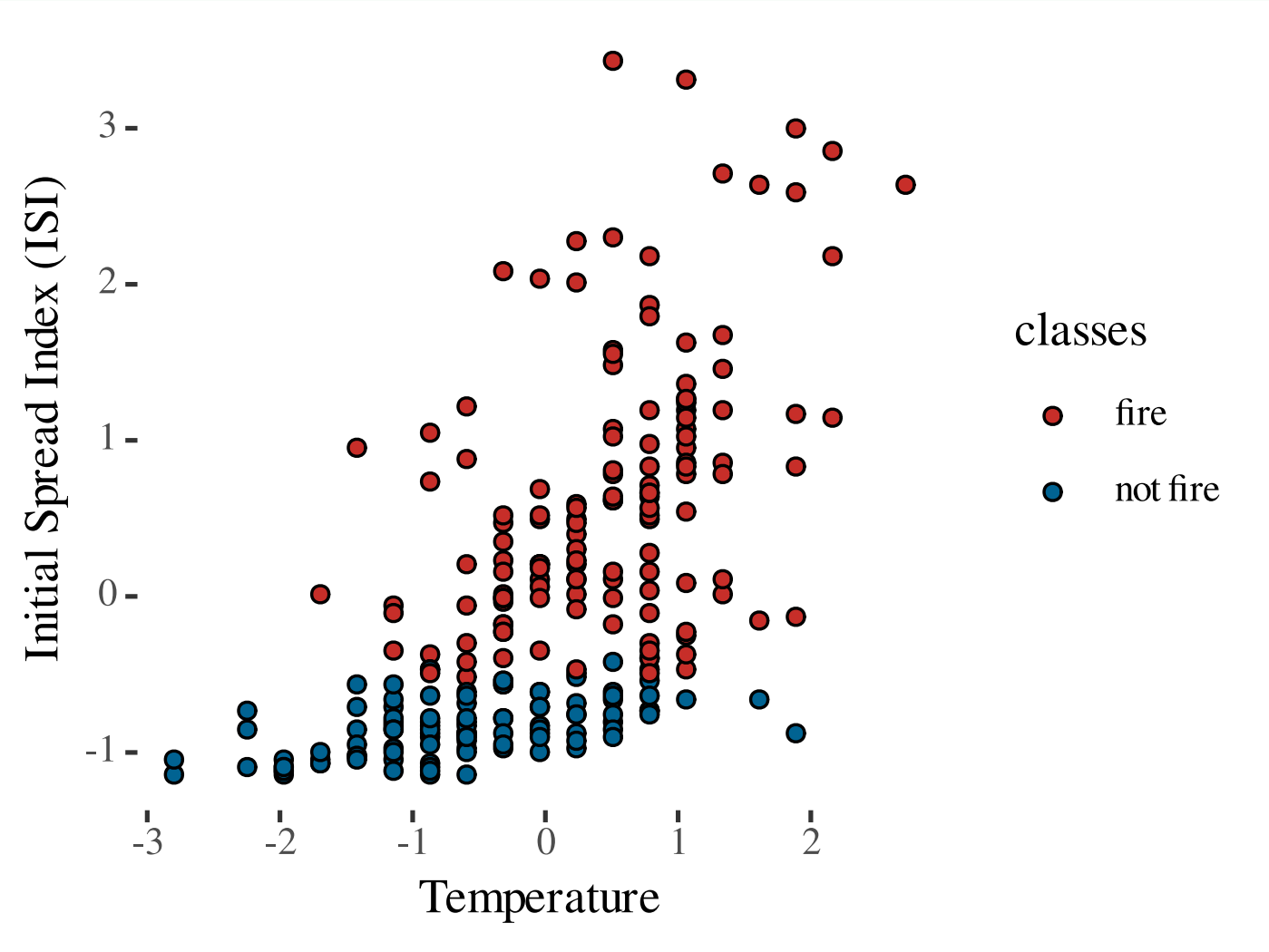
GROUP ACTIVITY 1

05:00



- Get the class activity 22.Rmd file from moodle
- Let's work on group activity 1 together

How do we choose the number of neighbors in a principled way?

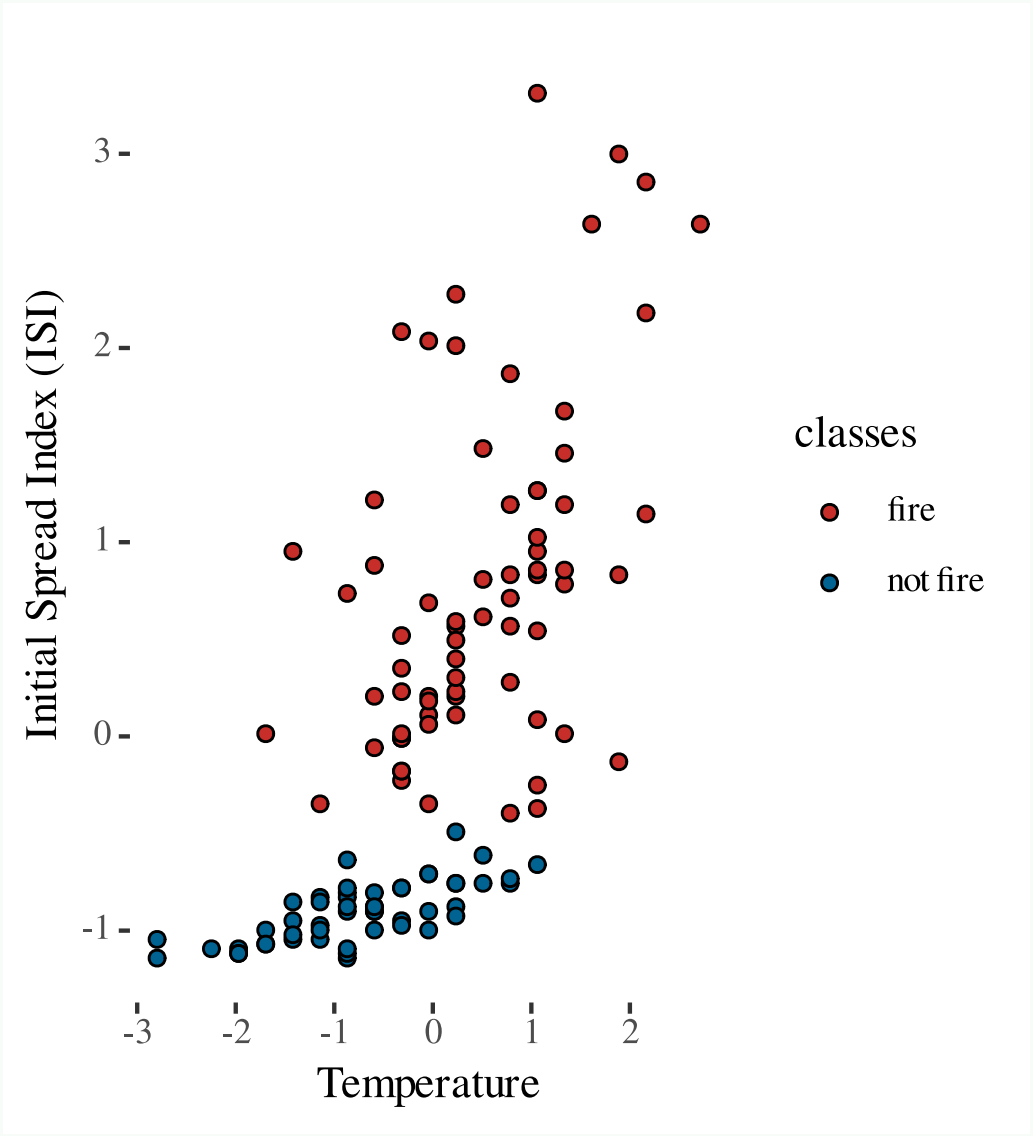

Initial Spread Index (ISI)
3
2
1
0
-1
-3
-2
-1
0
1
2
Temperature
classes
fire
not fire

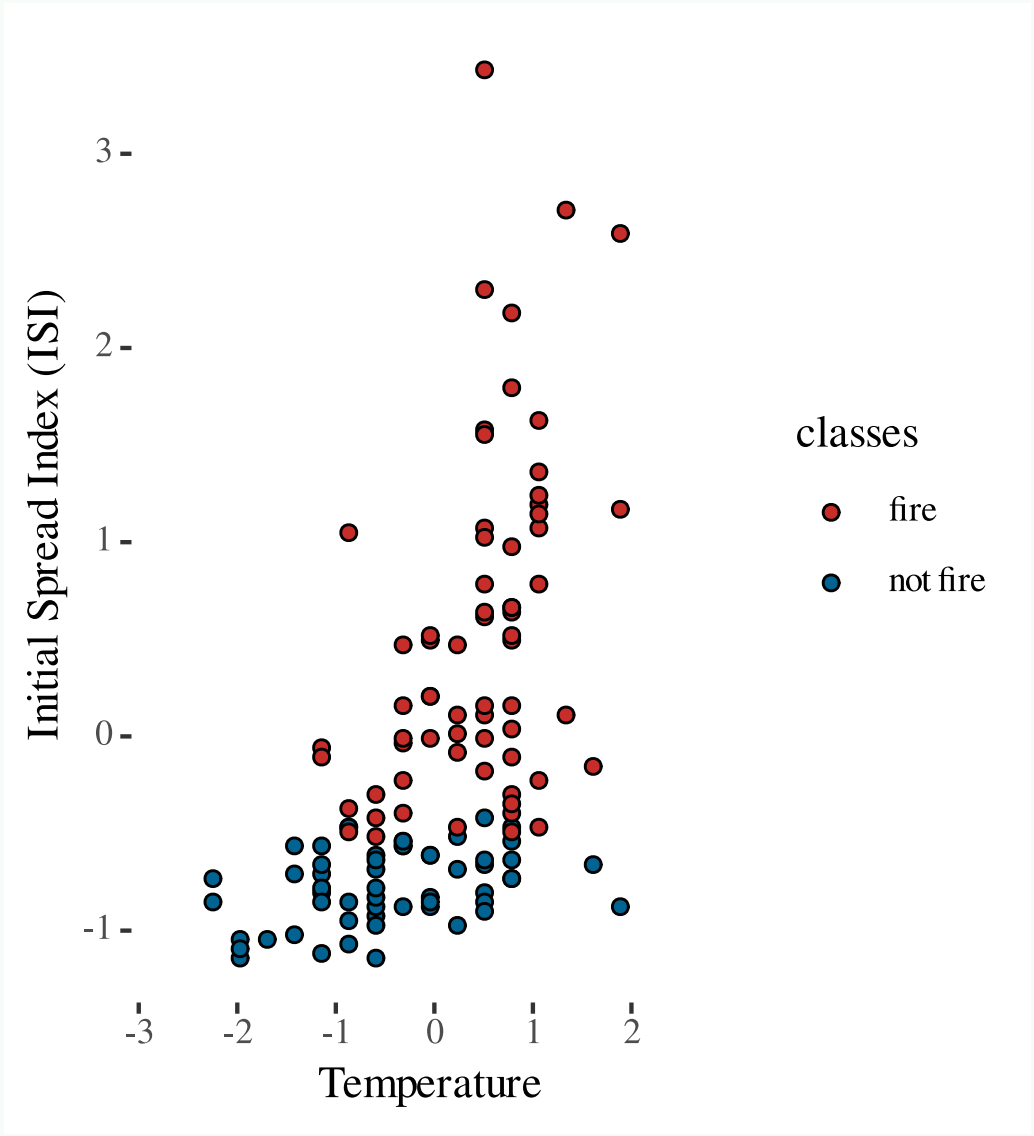
Evaluating accuracy

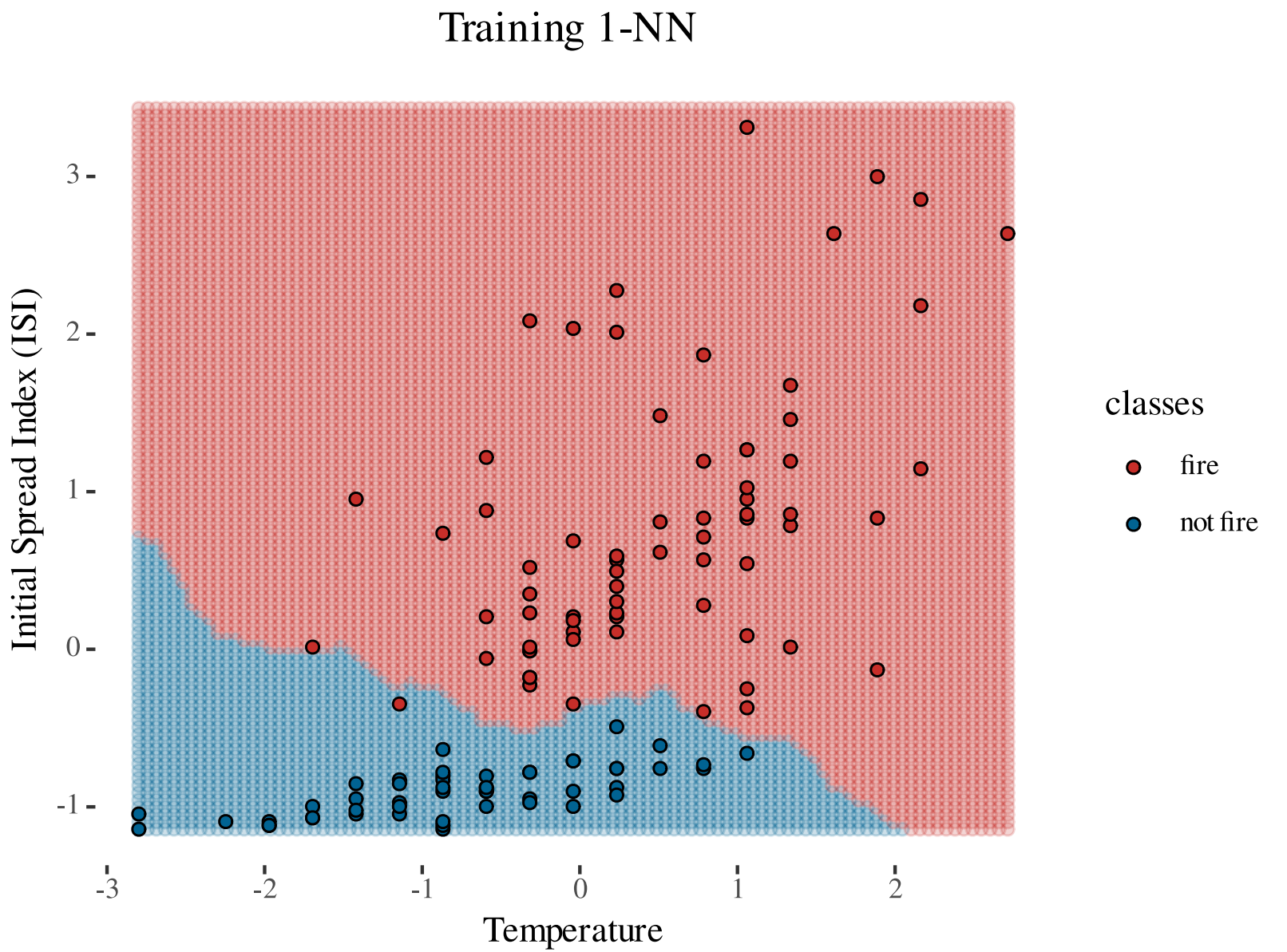
We want to evaluate classifiers based on some accuracy metrics.

- **Randomly split data set into two pieces: training set and test set**
- **Train (i.e. fit) KNN on the training set**
- **Make predictions on the test set**
- **See how good those predictions are**

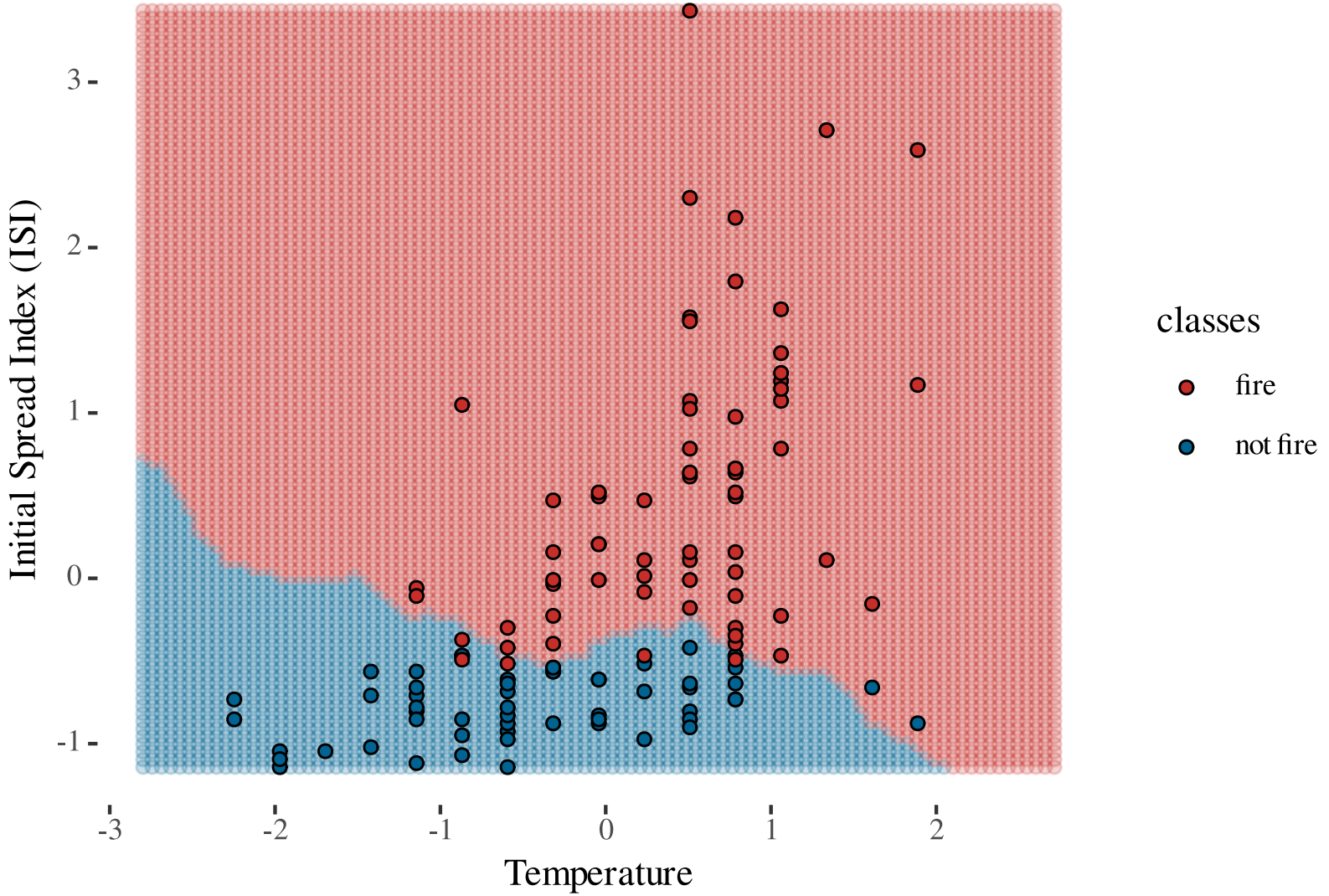
Train (left) and test (right) dataset (50-50)

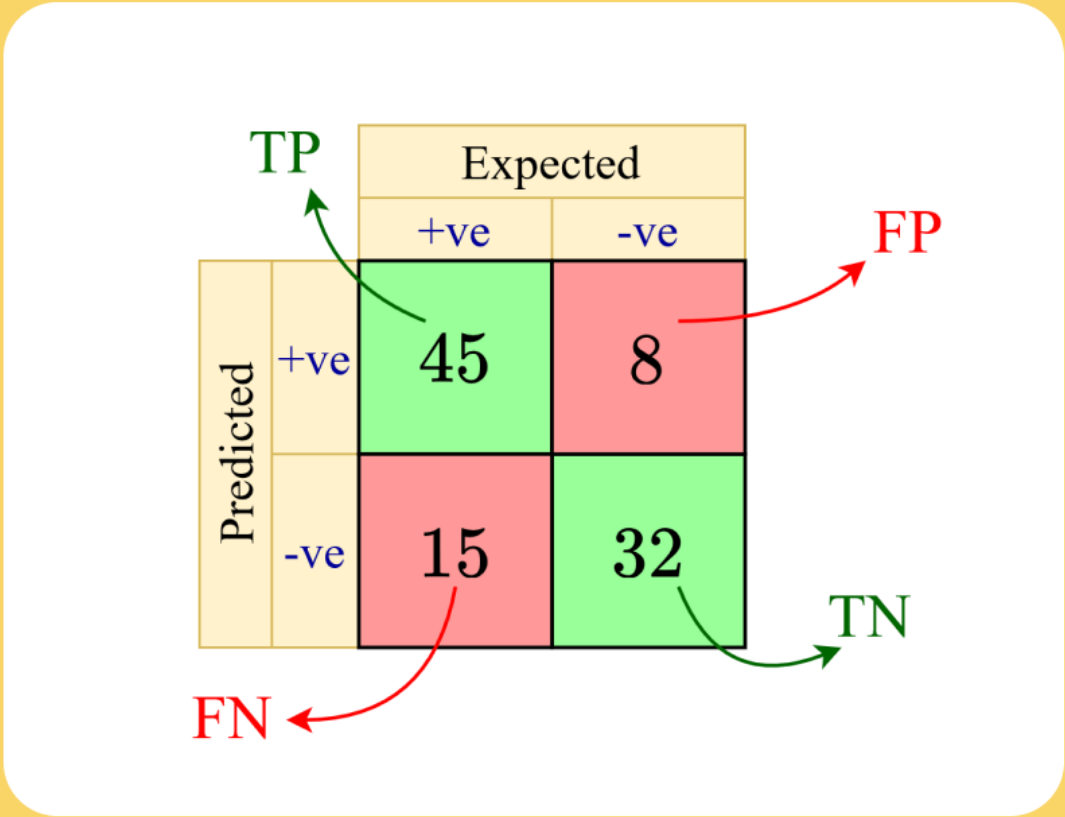


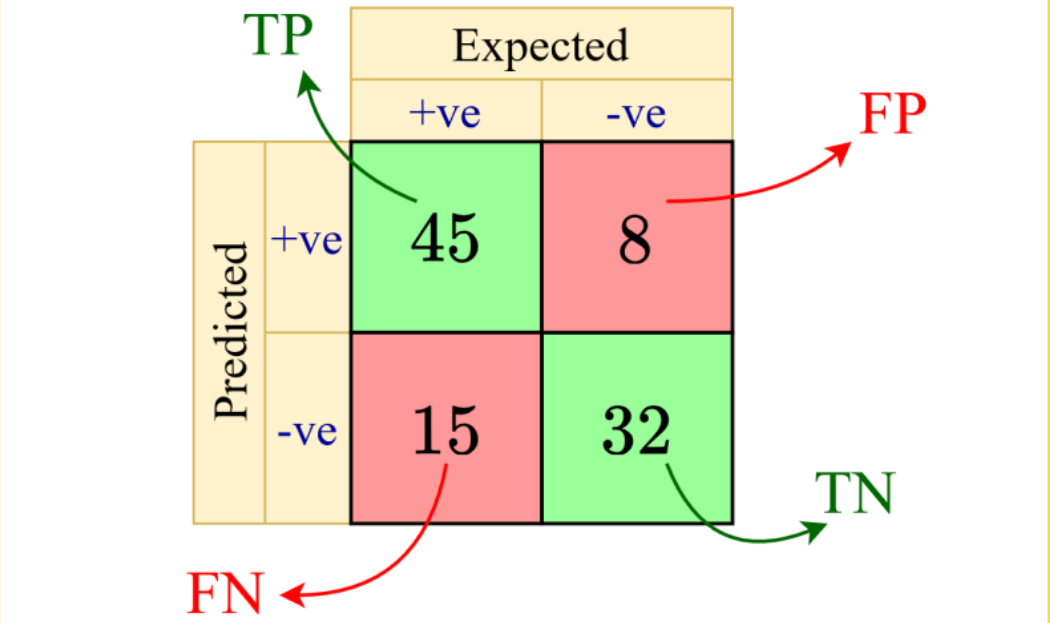



Training 1-NN
Initial Spread Index (ISI)
3
2
1
0
-1
-3
-2
-1
0
1
2
Temperature
classes
fire
not fire

Evaluating performance




TP
Expected
+ve
-ve
FP
Predicted
+ve
45
8
-ve
15
32
TN
FN



Confusion matrix: tabulation of true (i.e. expected) and predicted class labels

Common metrics include:

- accuracy
- sensitivity
- specificity
- positive predictive value (PPV)

```
conf_mat(fire_results, truth = classes, estimate = predicted)
          Truth
Prediction fire not fire
  fire       61        2
  not fire    6       53
```

Accuracy

Proportion of correctly classified cases

$$\text{Accuracy} = \frac{\text{true positives} + \text{true negatives}}{n}$$

```
          Truth
Prediction fire not fire
  fire       61        2
  not fire    6       53
```

```
accuracy(fire_results, truth = classes,
         estimate = predicted)
# A tibble: 1 × 3
  .metric  .estimator .estimate
  <chr>    <chr>          <dbl>
1 accuracy binary         0.934
```

Sensitivity

Proportion of positive cases that are predicted to be positive

$$\text{Sensitivity} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

Also called... true positive rate or recall

```
          Truth
Prediction fire not fire
  fire       61        2
  not fire    6       53
```

```
sens(fire_results, truth = classes,
          estimate = predicted)
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 sens    binary         0.910
```

Specificity

Proportion of negative cases that are predicted to be negative

$$\text{Specificity} = \frac{\text{true negatives}}{\text{false positives} + \text{true negatives}}$$

Also called... true negative rate

```
            Truth
Prediction fire not fire
  fire       61        2
  not fire    6       53
```

```
spec(fire_results, truth = classes,
         estimate = predicted)
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 spec    binary         0.964
```

Positive predictive value (PPV)

Proportion of cases that are predicted to be positives that are truly positives

$$\text{PPV} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

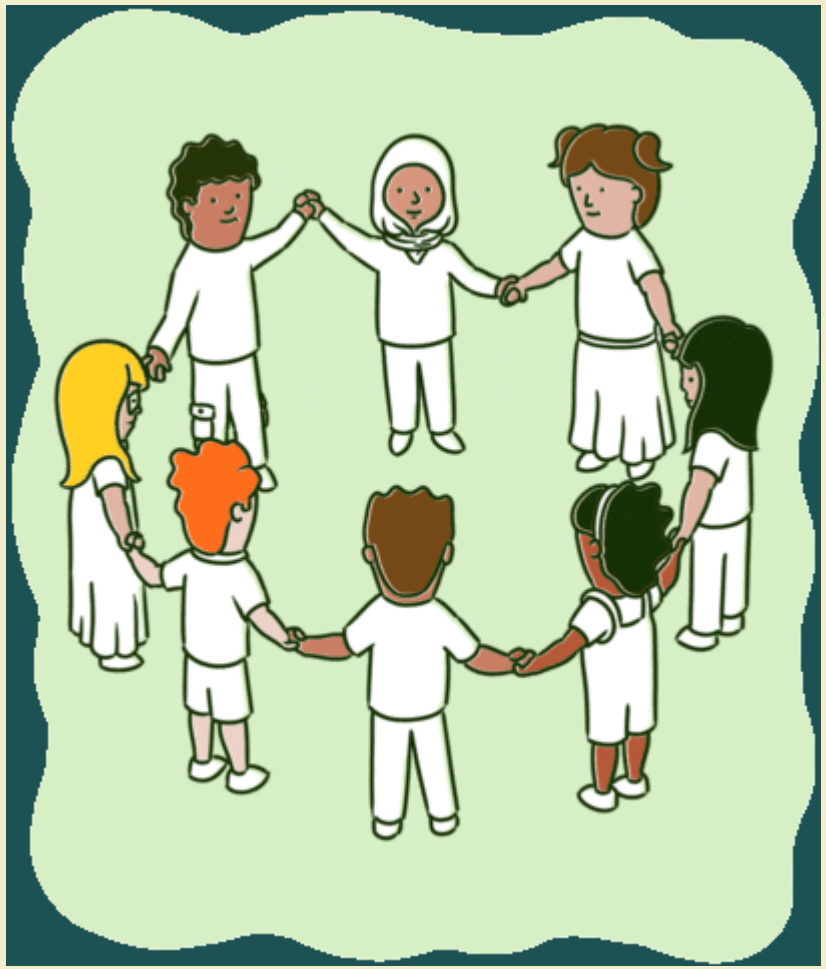
Also called... precision

```
          Truth
Prediction fire not fire
  fire       61        2
  not fire    6       53
```

```
ppv(fire_results, truth = classes,
          estimate = predicted)
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 ppv     binary         0.968
```

GROUP ACTIVITY 2

15:00



- Please continue working on group activity 2
- Consider calculating the accuracy metrics by hand
- Verify your calculations with R-code

Tabulate the metrics !!

```
custom_metrics <- metric_set(accuracy, sens, spec, ppv) # select custom metrics
metrics <- custom_metrics(fire_results, truth = classes, estimate = predicted)
metrics
# A tibble: 4 × 3
  .metric  .estimator .estimate
  <chr>    <chr>          <dbl>
1 accuracy binary         0.934
2 sens     binary         0.910
3 spec     binary         0.964
4 ppv      binary         0.968
```

Choose the optimal K based on majority of the metrics!