Data Analytics in Cyber Security
CT115-3-M (Version E)

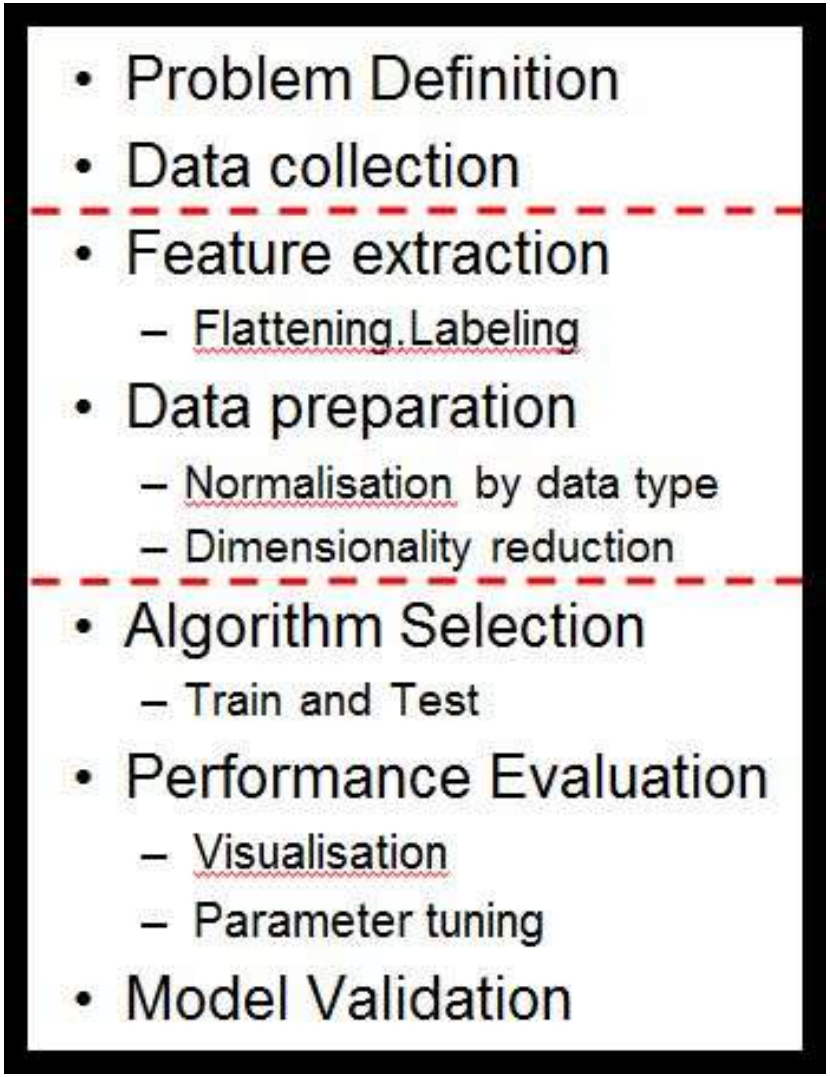
Model Optimisation Strategies

TOPIC LEARNING OUTCOMES

At the end of this topic, you should be able to:

1. Understand the concepts of Hyperparameter Tuning
2. Understand the concepts of Feature Selection
3. Understand the concepts of Re-Sampling

Machine Learning Pipeline



Iteration:

Model Validation

- The model validation phase should lead to a new round of performance evaluation, and the set of candidate algorithms will gradually be reduced until one algorithm (or one ensemble of algorithms) is selected.

Contents & Structure

- Hyperparameter tuning
- Feature selection
- Resampling

Feature selection

- The dataset may have a large number of features that may not all be relevant and significant.
  - For certain types of data, like genetics or text, the number of features can be very large compared to the number of data points.
  - **Curse of dimensionality**: error increases with the increase in the number of features.
- **Feature selection** is a process of selecting the most relevant variables. The goal is to determine which columns are more predictive of the output.
  - Also called "**dimensionality reduction**" and "**feature engineering**"

Feature Engineering

- The feature engineering process involves selecting the minimum required features to produce a valid model because the more features a model contains, the more complex it is (and the more sparse the data), therefore the more sensitive the model is to errors due to variance.
- A common approach to eliminating features is to find their relative importance, then eliminate weak features or combinations of features and re-evalute to see if the model fares better during cross-validation

Feature Covariance

- In the worst case, one feature can explain (or already determine) all the other features and makes them obsolete.
- This results in a high redundancy among the features, increasing computational overhead
- The covariance matrix can be used to find redundant features (those that measure the same thing), and make decisions about which can be removed

$$cov_{x,y} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{N - 1}$$

$cov_{x,y}$ = covariance between variable x and y

x_i = data value of x

y_i = data value of y

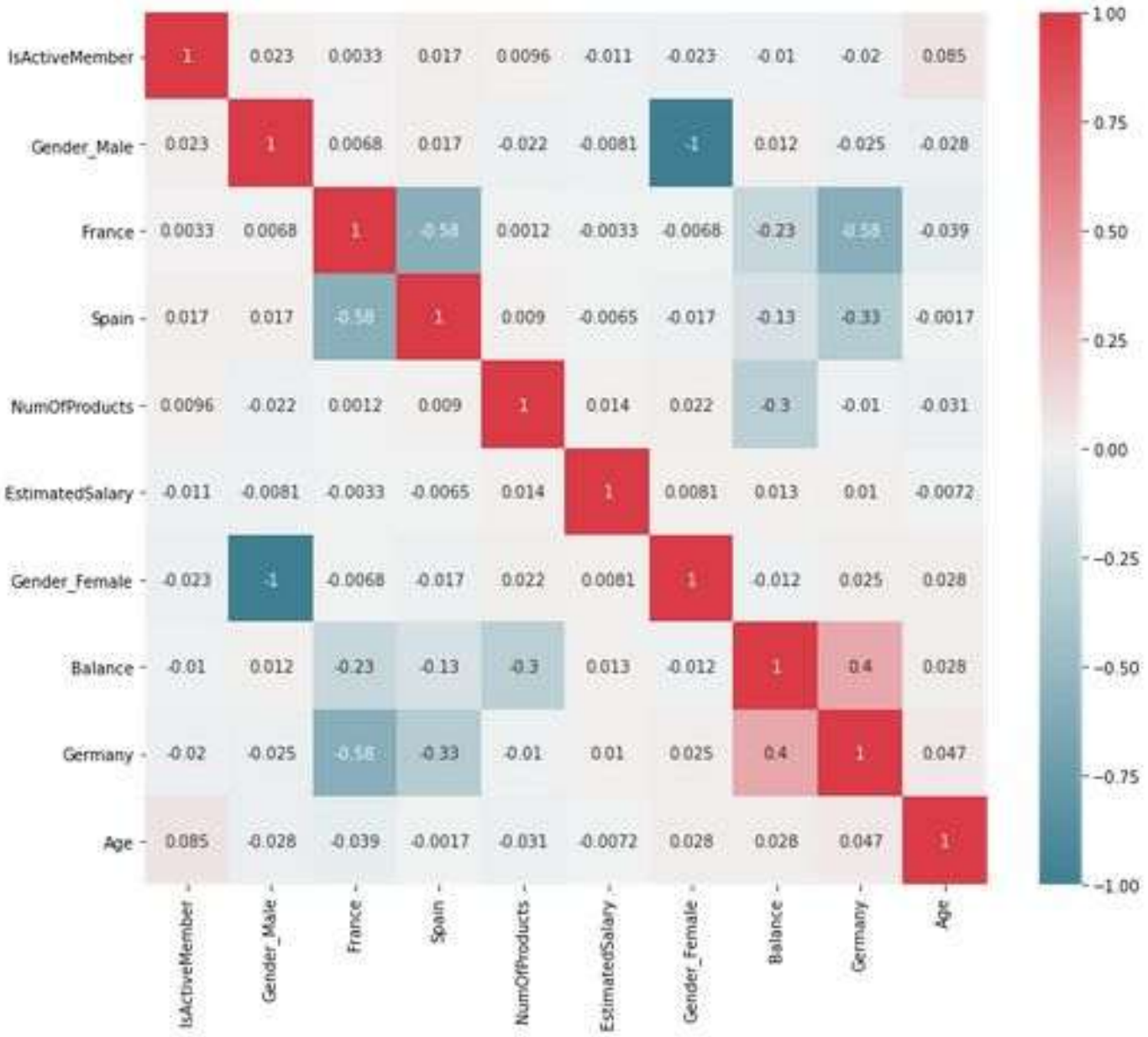
$\bar{x}$ = mean of x

$\bar{y}$ = mean of y

N = number of data values

Pearson Correlation

- The Pearson *r* is a standardized covariance, and ranges from -1, indicating a perfect negative linear relationship, and +1,indicating a perfect positive relationship.
- The covariance of two variables divided by the product of their standard deviations gives Pearson's correlation coefficient.
  $\rho (X,Y) = cov (X,Y) / \sigma X.\sigma Y$.
- A value of zero suggests no linear association, but does not mean two variables are independent, an extremely important point to remember.
- **Pearson r is not viable for understanding a great many dependencies**
- **The alternative is Mutual Information Correlation**




```
[24]: Status             1.000000
      IsActiveMember     0.156128
      Gender_Male        0.106512
      France             0.104955
      Spain              0.052667
      NumOfProducts      0.047820
      EstimatedSalary   -0.012097
      Gender_Female     -0.106512
      Balance           -0.118533
      Germany           -0.173488
      Age               -0.285323
      Name: Status, dtype: float64
```

High Correlations:

Check for greater than 0.7 and less than -0.7

Correlation Matrix "heatmap"

- *Correlations with classification target*

Mutual Information Correlation

- Mutual Information Correlation is based on a measure of **Entropy**
  - The Pearson correlation coefficient assumes normality and linearity of two random variables; Mutual Information removes these assumptions
- In essence, mutual information tells us *how useful the feature X is at predicting the random variable Y on a scale of zero to one*, with higher numbers indicating better predictors.
  - Mutual Information Correlation captures many different types of relationships (not just linear) and is considered the best metric
- However, it doesn't tell us if the feature is a predictor of success or failure.
- **Mutual Information and Pearson measures are complementary – they do not always move the same way**

Feature Filter

- There is a feature filter function in the sample code local library
- It selects all of the features with a Pearson or Mutual Information correlation with the target variable that is less than a given threshold (or “floor”)
- Low correlation with the target variable means these features are not very valuable as predictors *by themselves (we can’t say if they are more useful when combined with other variables)*
- *Nonetheless, this is a commonly used technique*

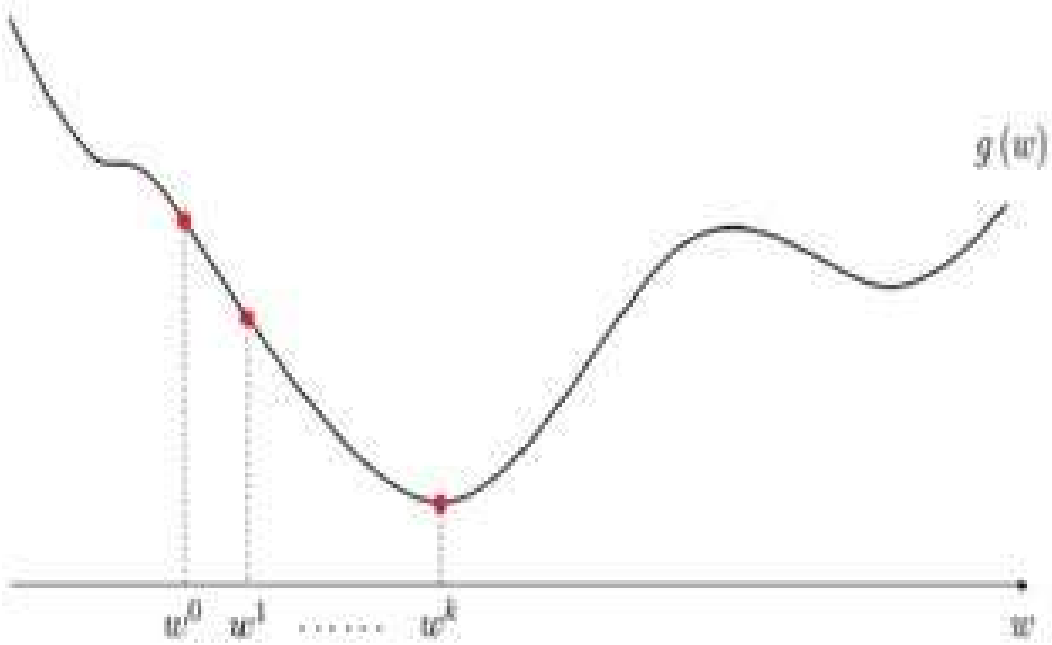
Hyperparameters

- Creating a machine learning model requires design choices as to how to define the model architecture
- Where the ***model parameters*** specify how to transform the input data into the desired output, the ***hyperparameters*** define how our model is actually structured.
  - hyperparameters define the model architecture
  - In *scikit-learn* they are passed as arguments to the constructor of the estimator classes.
- The process of searching for the ideal model architecture is referred to as *Hyperparameter Tuning*.

Many sets of Model parameters

Goal: to find the model/solution with minimum loss/error

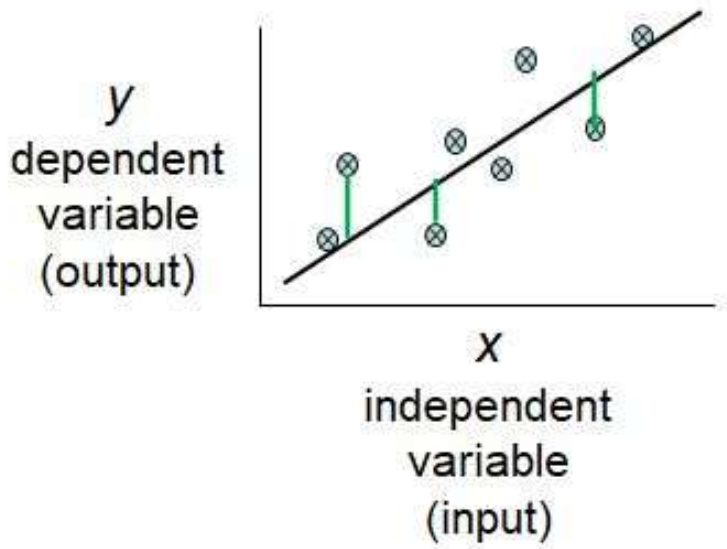
Mathematically, a "loss function" returns a measure of how good a prediction model does in terms of being able to predict the expected outcome.



- The curved line represents the solution space
- The dots represent the loss for a given set of model parameters
- Vertical lines represent the error between actual and predicted.

Many sets of Model parameters

The optimum model (or optimum solution) is the combination of model parameters that gives minimum error between the actual output and the modeled output



- The line depicts the predicted relationship
- The dots represent the actual values
- Vertical lines represent the error between actual and predicted.

The set of all possible models with unique sets of parameters is referred to as the "solution space".

The tuning of these parameters require the ***minimization of a cost function*** (or searching for the minimum cost function).

Bias / Variance Tradeoff

Reducing bias **generally** increases the variance but the relationship is NOT fixed and predictable

- In practice, optimisation of algorithm parameters is often a battle to find the desired balance for the bias/variance tradeoff.
- We quantitatively evaluate overfitting / underfitting using cross-validation –usually in conjunction with *hyperparameter tuning*
- Iterative – next steps, feeds back to previous steps

Hyperparameter Tuning

- Hyperparameter tuning methods allow us to automatically test possible combinations of values
- Tuning the hyper-parameters of an estimator is often referred to as "searching the hyperparameter space" for the optimum values.
- Two methods: Grid Search and Randomised Search
  - **GridSearchCV** evaluates all possible combinations of parameter values from a list
  - **RandomizedSearchCV** samples each setting from a distribution of possible parameter values.

Hyperparameter Tuning

Siddhardhan

Hyperparameter Tuning:

- GridSearchCV
- RandomizedSearchCV

https://youtu.be/DTcfH5W6o08

Hyperparameter Tuning Methods

- Both Grid Search and Randomised Search use the score function of the estimator to evaluate a parameter setting.
- The defaults are
  - sklearn.metrics.**accuracy_score for classification** and
  - Sklearn.metrics.**r2_score for regression**

A Grid Search strategy for hyperparameter tuning is commonly combined with cross validation

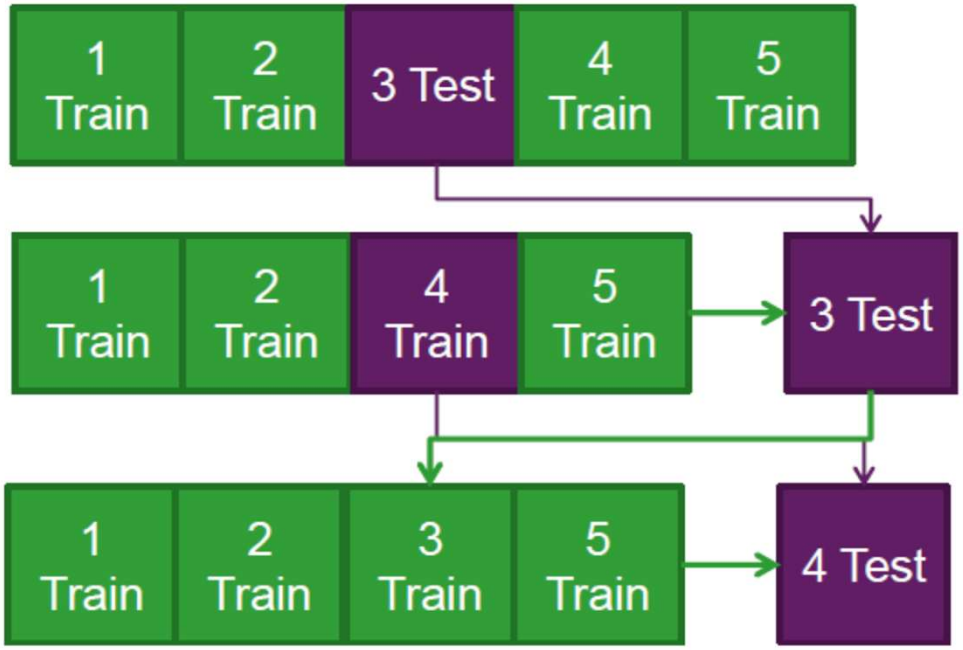
k-Fold Cross Validation

k-Fold divides all the samples into **k** groups of samples, called folds. The prediction function is learned using k-1 folds, and the remaining fold is used as the test set.

- **k** is typically 2, 5 or 10 for a balance between computational complexity and validation accuracy

1. A model is trained using k-1 folds as training data
2. The resulting model is validated on the remaining part of the data
   - It is used as a test set to compute a performance measure such as accuracy for classification or r^2 for regression
3. The performance measure reported by k-fold cross-validation is the average of the values computed in the loop.

K-fold Cross Validation Example



1. Split the data into 5 samples
2. Fit a model to the training samples and use the test sample to calculate a CV metric.
3. Repeat the process for the next sample, until all samples have been used to either train or test the model

The advantages are

- all observations are used for both training and validation, and each observation is used once for validation
- This can be done using the Train set from the original Test-Train split

Best Practice

(Other approaches generally follow the same principles)

The cross-validation information allows us to evaluate not only how much variance can be explained by the model, but also the predictive accuracy of the model.

Good models should have a high predictive AND explanatory power!

While this is a great way to make sure you've spanned the parameter space, the time required to train a model increases exponentially with the number of parameters.

The upside is that having many parameters typically indicates that an algorithm has greater flexibility. It can often achieve very good accuracy, provided you can find the right combination of parameter settings.

Permutation Feature Importance

- It is a model inspection technique that measures the contribution of each feature to a fitted model's statistical performance on a given tabular dataset.

- We measure the importance of a feature by calculating the increase in the model's prediction error after permuting the feature. A feature is "important" if shuffling its values increases the model error, because in this case the model relied on the feature for the prediction. A feature is "unimportant" if shuffling its values leaves the model error unchanged, because in this case the model ignored the feature for the prediction.

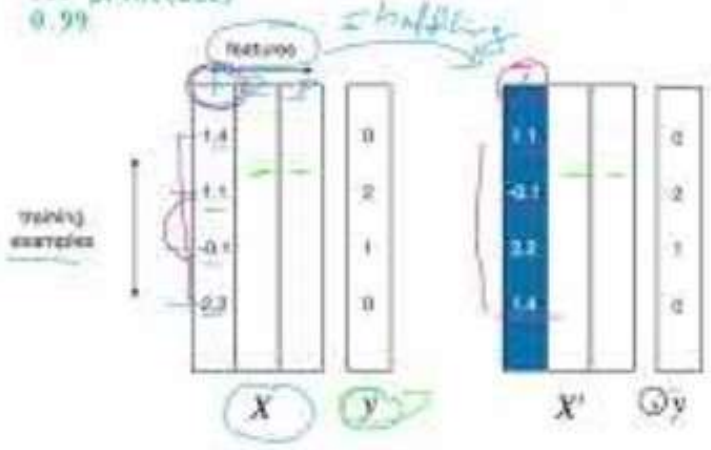
Permutation Feature Importance

Permutation Importance

intuitive & model-agnostic

1. Take a model that was fit to the training set
2. Estimate the predictive performance of the model on an independent dataset (e.g., validation dataset) and record it as the baseline performance
3. For each feature j
   a. randomly permute feature column j in the original dataset

```
>>> randomforest.fit(X_train, y_train)
>>> acc = randomforest.score(X_val, y_val)
>>> print(acc)
0.99
```



https://youtu.be/VUvShOEFdQo

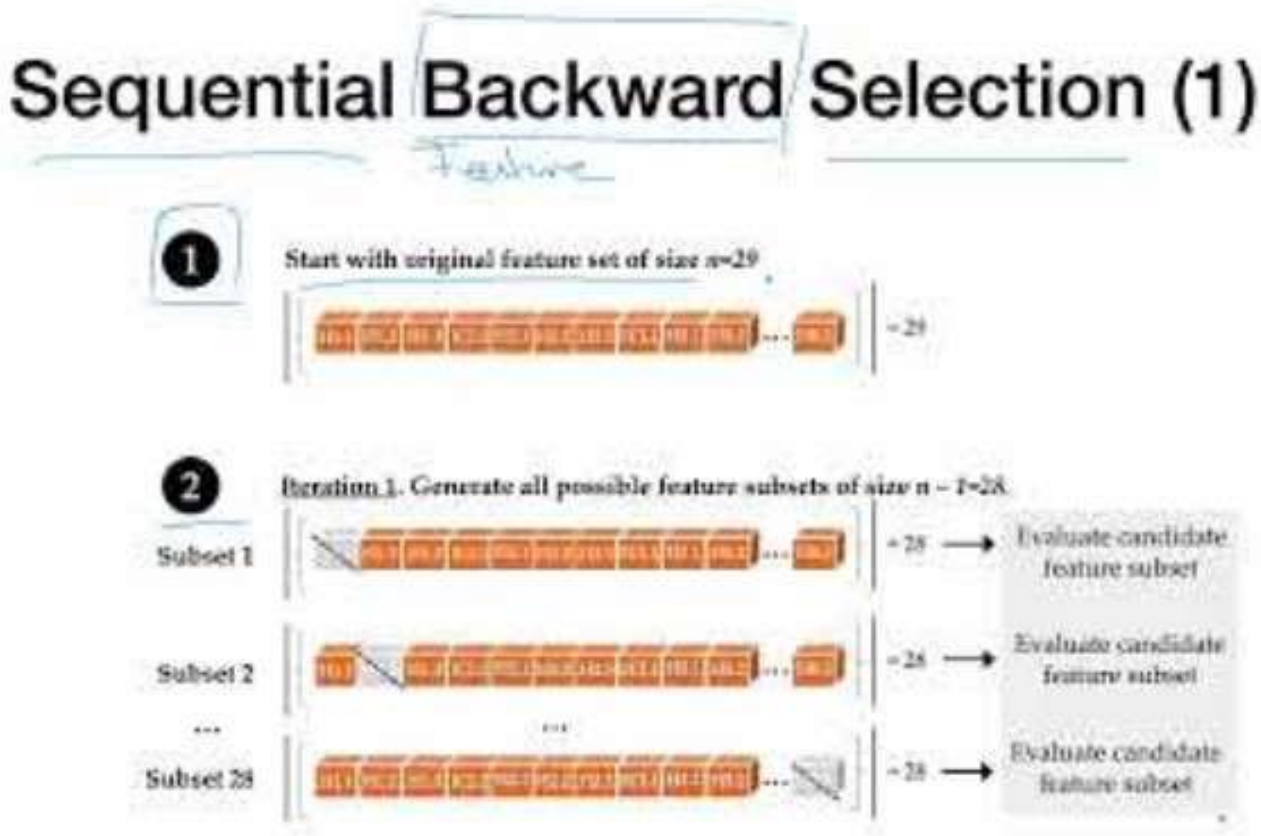
Permutation Feature Importance

- `mlxtend.evaluate.feature_importance_permutation`
- can be used with any classifier or regressor, and can be run on the test set as well
- The default metric is accuracy for classifiers and r2 for regressors. Optionally, metric= can designate a custom scoring function
- It returns two arrays:
  - the first array contains the actual importance values we are interested in.
  - When num_rounds > 1 the permutation is repeated multiple times with different random seeds, and the first array holds the average of the importance values, with all individual values from these runs in the second array.

Sequential Feature Selection

- `mlxtend.feature_selection.SequentialFeatureSelector`
- Sequential feature selection algorithms remove or add one feature at a time based on the classifier performance until a feature subset of the desired size is reached.
- Features are selected based on a performance metric hyperparameter *(like accuracy or AUC_ROC)* rather than feature weight coefficients *(coef_)*
- Each feature importance value has both a magnitude and a direction (positive or negative), which indicate how each feature affects a particular prediction.
  - A negative value means that feature makes the loss go up; in other words, the feature is worse than noise

Sequential Feature Selection



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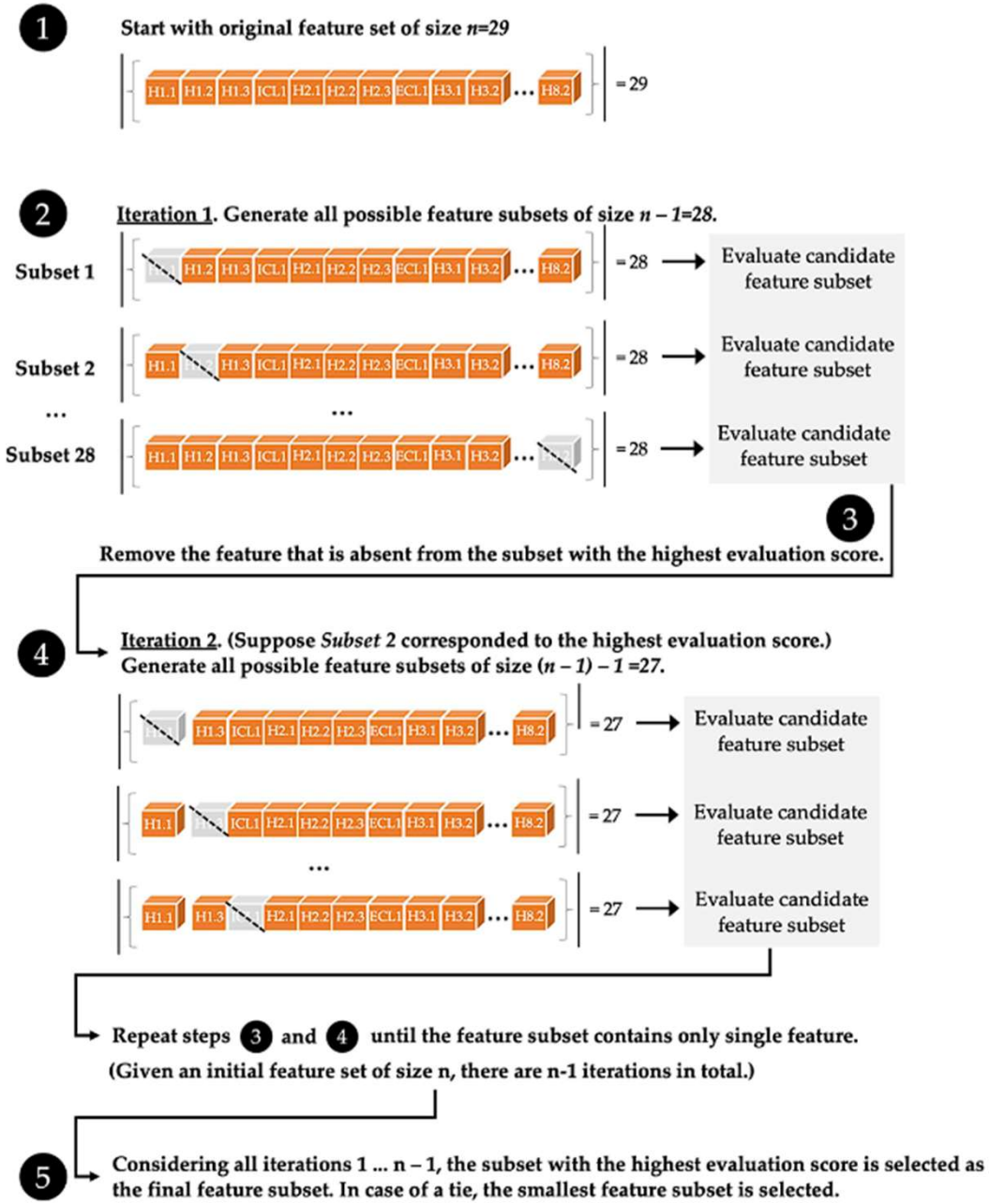
Sequential Feature Selection



http://rasbt.github.io/mlxtend/user_guide/feature_selection/SequentialFeatureSelector/

Resampling

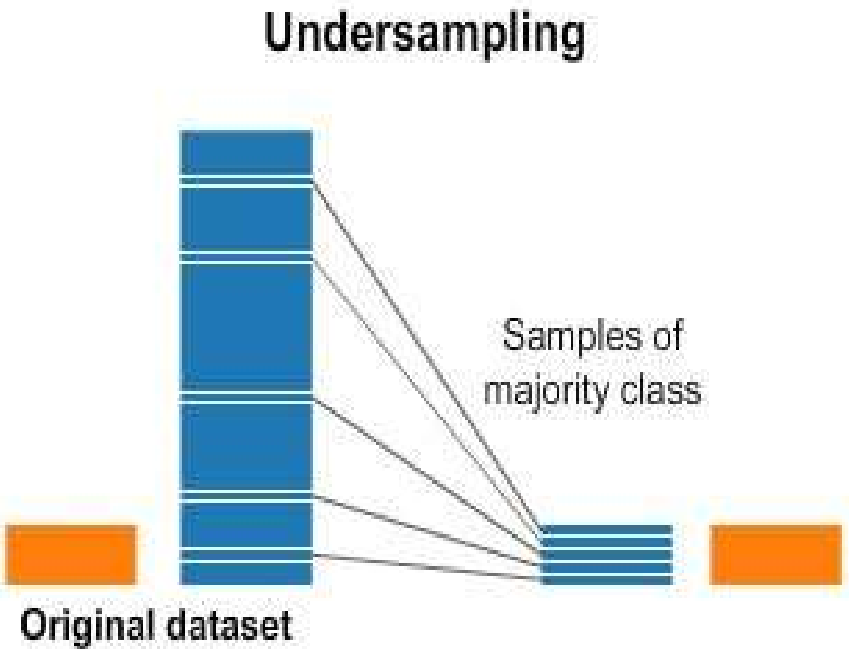
General Principle

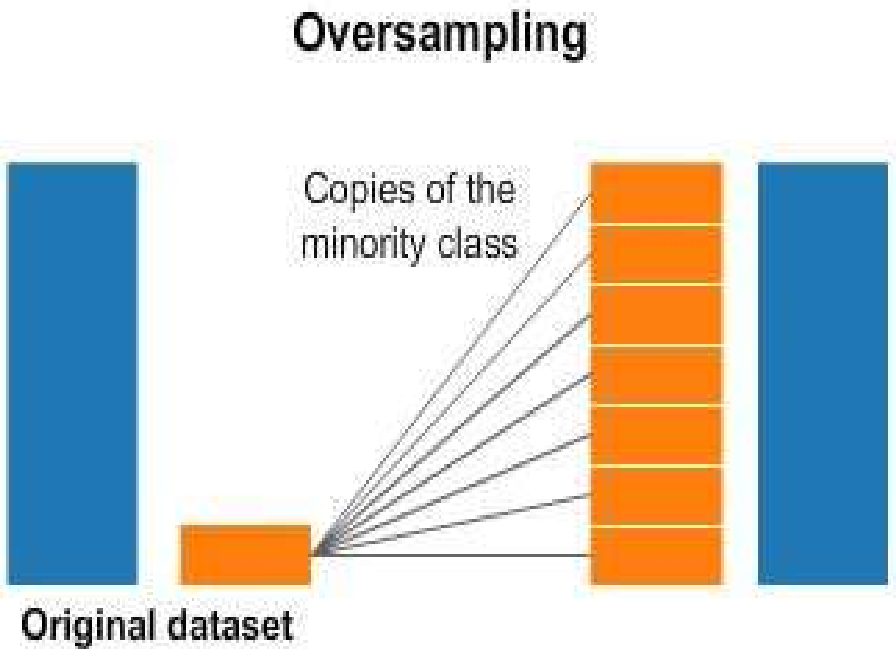
- Purpose of the **test** set is to represent the *population*
- Purpose of the **train** set is to represent the *characteristics of the classes*

So:

- An imbalanced **test** set is fine – *some classes naturally occur more frequently than others*
- An imbalanced **train** set is a problem – *there are not enough observations of some classes to distinguish their unique characteristics*

Resampling Strategies

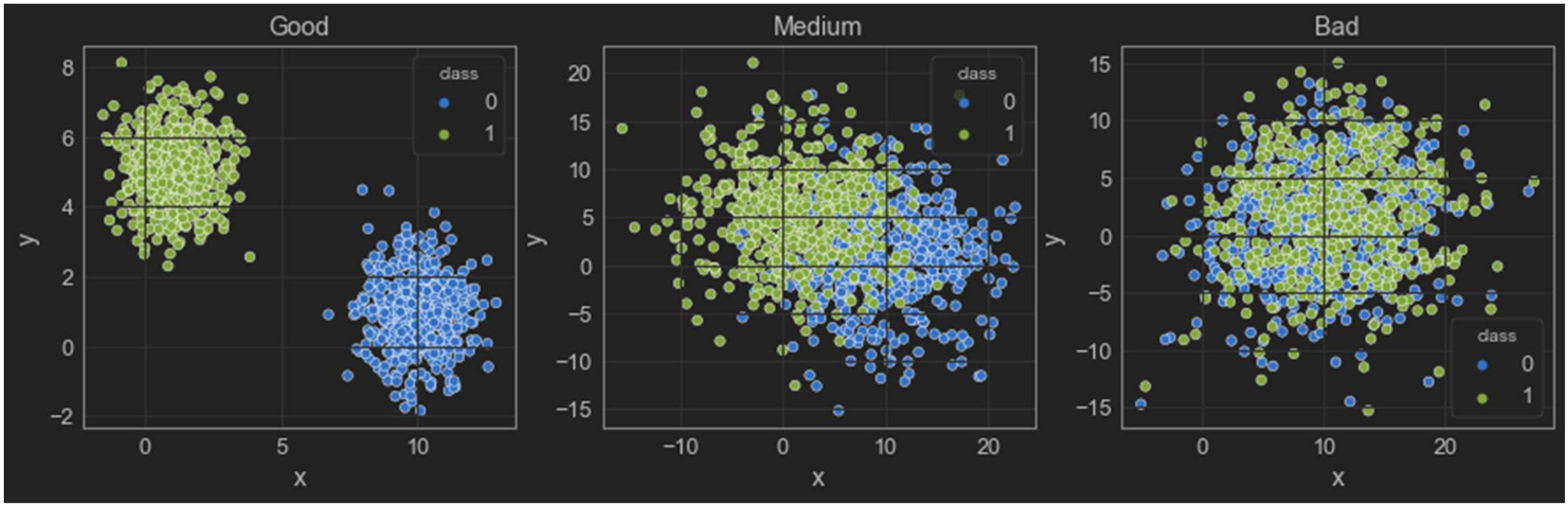




https://www.kaggle.com/code/rafjaa/resampling-strategies-for-imbalanced-datasets

Resampling: Class Separability

As an example, three artificial datasets with different levels of separation between classes



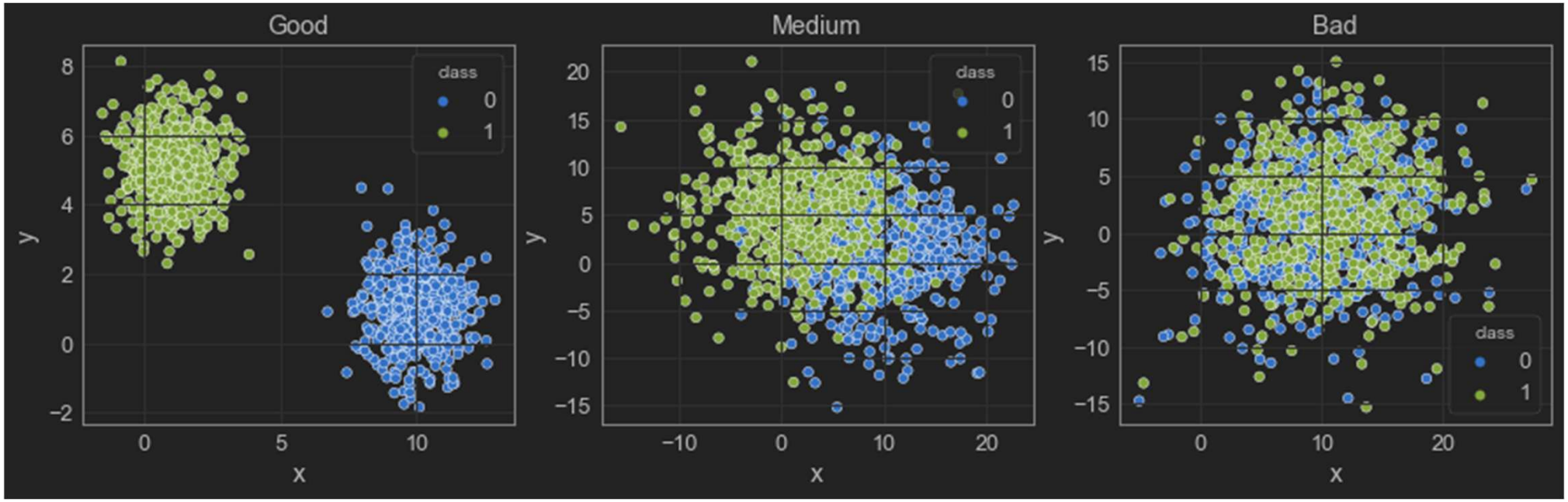
https://github.com/vinyluis/Articles/tree/main/Kolmogorov-Smirnov

https://towardsdatascience.com/evaluating-classification-models-with-kolmogorov-smirnov-ks-test-e211025f5573

Datasets (artificial)

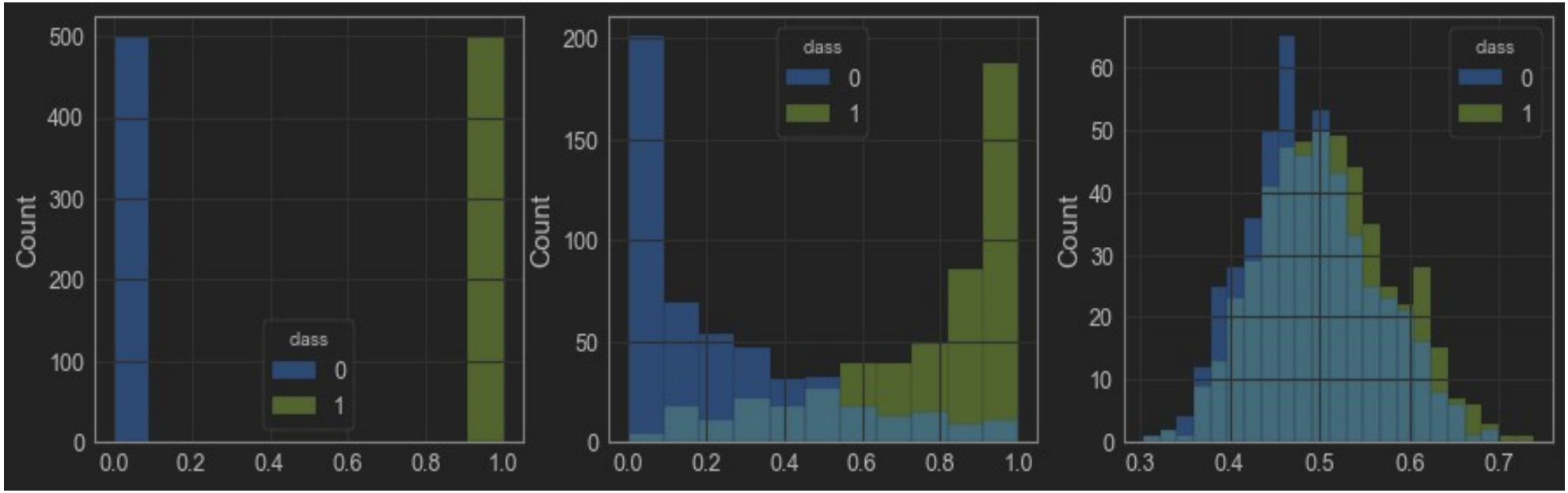
500 observations for each class: “True” [nonzero] and “False” [zero]

- In the “good” dataset, the classes don’t overlap, and they have a good noticeable gap between them.
- In the “medium” one there is enough overlap to confuse the classifier.
- In the “bad” dataset the overlap is so intense that the classes are almost inseparable.



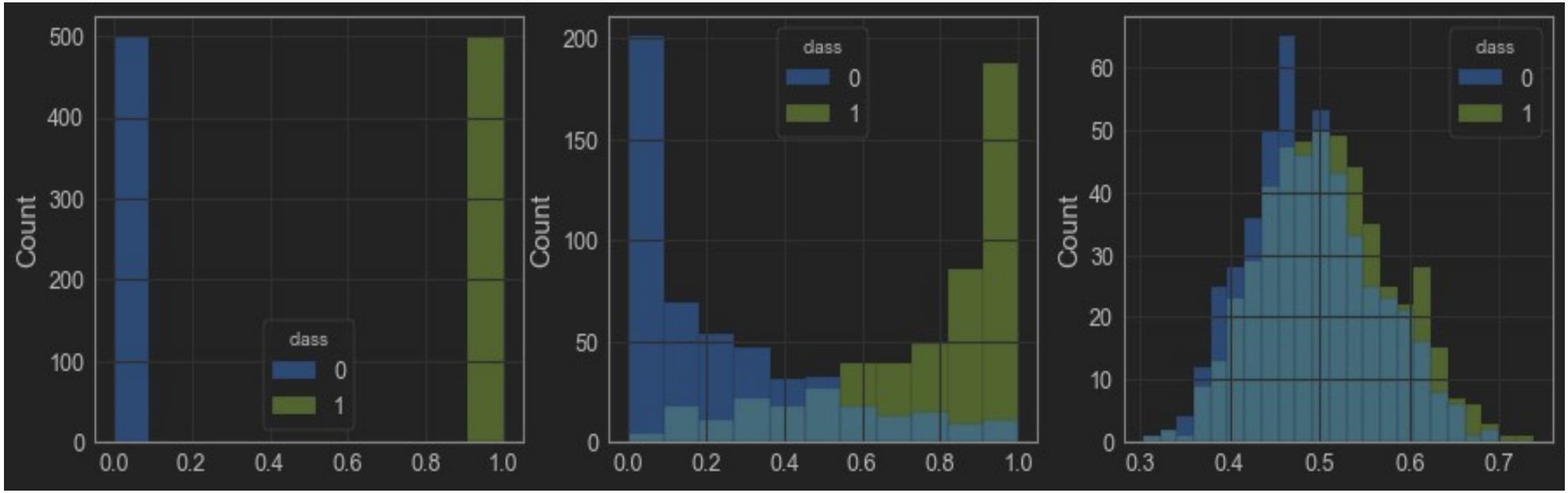
Probability of Predicted Class

- After training a default Naïve Bayes classifier for each dataset, we can see the distributions of the predictions for each class by plotting histograms.
- On the x-axis we have the probability of an observation being classified “True” [nonzero] and on the y-axis the count of observations in each bin of the graph:



Probability of Predicted Class

- The “good” example (left) has a perfect separation, as expected.
- The “medium” one (center) has a bit of an overlap, but most of the examples should be correctly classified *[Note the change in the scale of axis Y !]*.
- The classifier cannot separate the “bad” example (right) *[Note the change in the scale of axis X and Y !].*



UnderSampling Strategy

Three datasets based on the “medium” one:

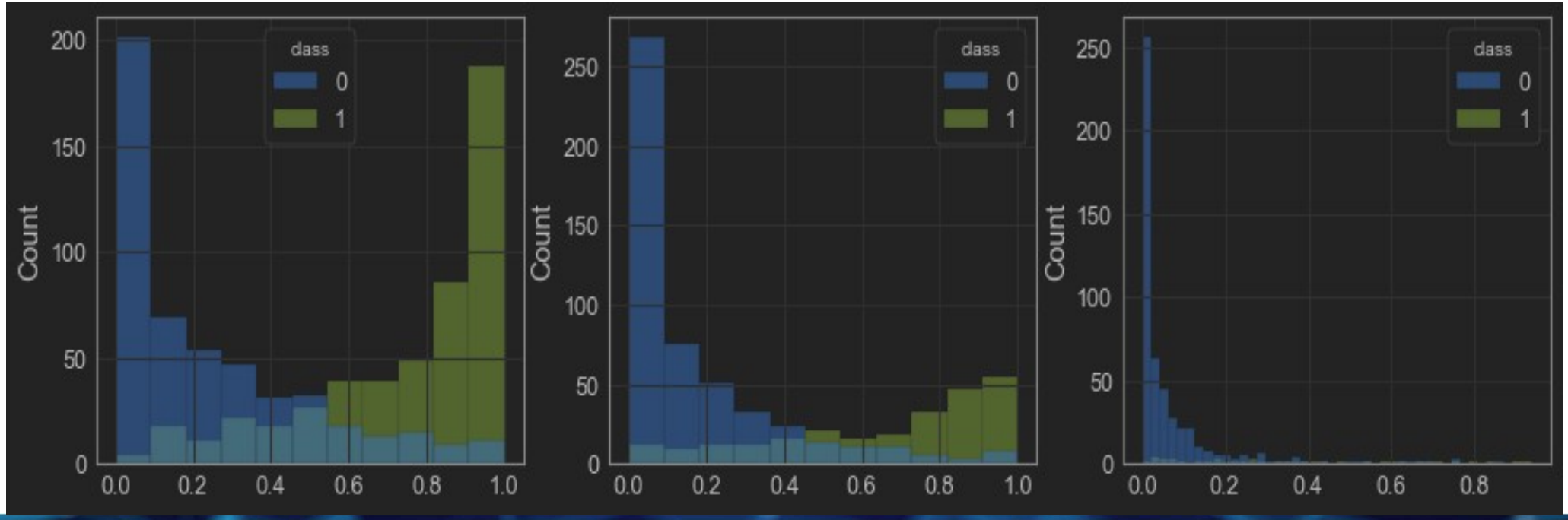
- The original, where the “True” class has 100% of the original examples (500)
- A new dataset where the “True” class has 50% of the original examples (250)
- A new dataset where the “True” class has only 10% of the original examples (50)

In all three cases, the “False” [zero] class will be unchanged with all 500 examples.

Resampling

Histograms after training the classifiers:

- The original “medium” dataset is on the left.
- The “50%” one (center) *[Note the change in the scale of axis Y !]*.
- The “10%” one (right) *[Note how the “True” class “disappears” !]*.



Resampling

- One approach to addressing imbalanced datasets is to oversample the minority class.
- The simplest approach involves duplicating examples in the minority class, although these examples don't add any new information to the model.
- Instead, new examples can be synthesized from the existing examples: the new examples are similar to the existing examples, but not exact copies.
- This type of data augmentation for the minority class is referred to as the Synthetic Minority Oversampling Technique, or SMOTE for short.

Review Questions

1. How to use hyperparameter tuning to improve the model performance?
2. How to use feature selection to improve model performance?
3. How to use re-sampling strategies to improve model performance?

Summary / Recap of Main Points

At the end of this topic, you should be able to:

1. Understand the concepts of Hyperparameter Tuning
2. Understand the concepts of Feature Selection
3. Understand the concepts of Re-Sampling