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Cross Validation and its Types

FUNDAMENTALS EXPLAINED
BY ROBOFIED

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01

What is Cross-Validation?

Cross-Validation is a data re-sampling technique in which we keep some percentage of the data for testing and the remaining data is used for training.

Steps:

1. Keep some part of data as testing set.
2. Train the model on rest of the data aka training set.
3. Test the model on the testing set.

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Need?

Used to check the predictive performance of the model by investigating how well it performs on the test or unseen data.

Allows us to compare different machine learning model and get a sense of how well they will perform in practice.

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Types of Cross-Validation

1. Hold-out Validation
2. Leave-One-Out Cross-Validation (LOOCV)
3. K-Fold Cross-Validation
4. Stratified K-Fold Cross-Validation
5. Cross-validation for Time series

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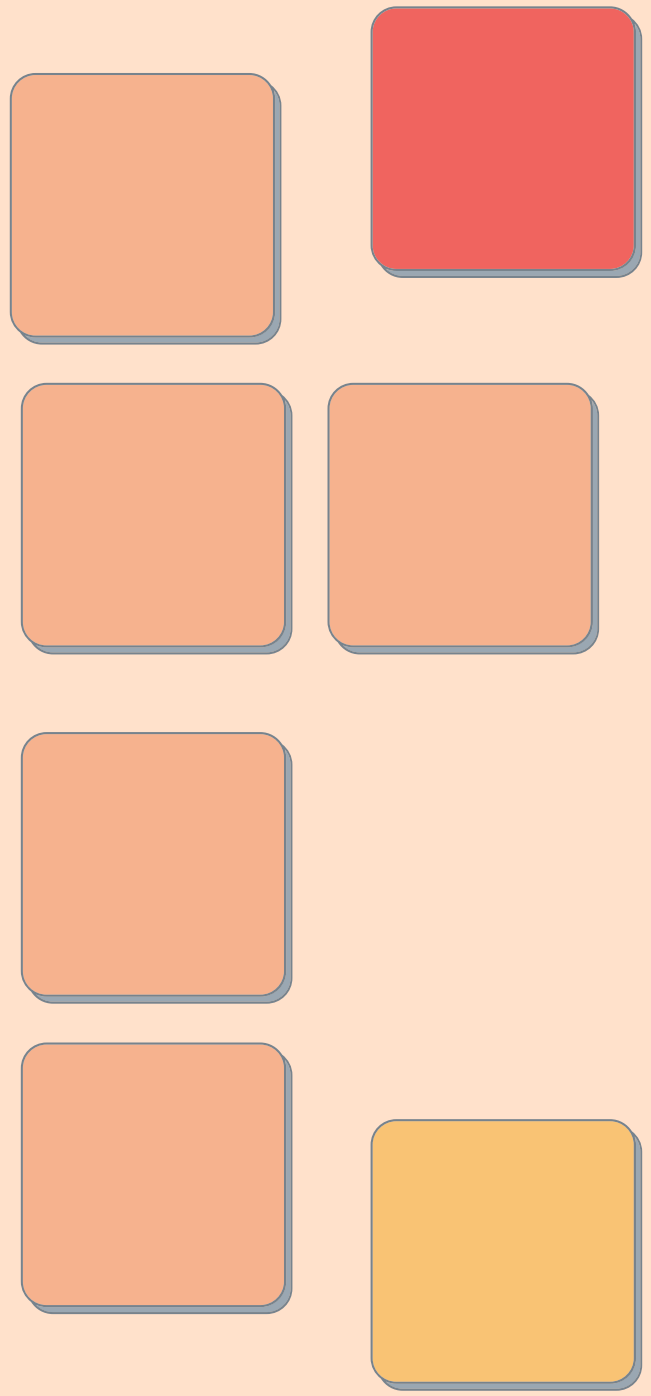
Hold-Out Cross Validation

Simplest kind of Cross-Validation.

Dataset is separated into training set and testing set. Then, training set is again separated into training set and validation set.



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Code

```
from sklearn.model_selection import train_test_split
x_train, x_test, y_train, y_test = train_test_split(x, y,
                                                    test_size = 0.20,
                                                    random_state = 42)
```

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06 Pros & Cons

Pros:

Needs only one iteration hence the computation costs are much lower.

Cons:

Provides a high variance estimate since changing which observations happen to be in the testing set can significantly change testing accuracy.

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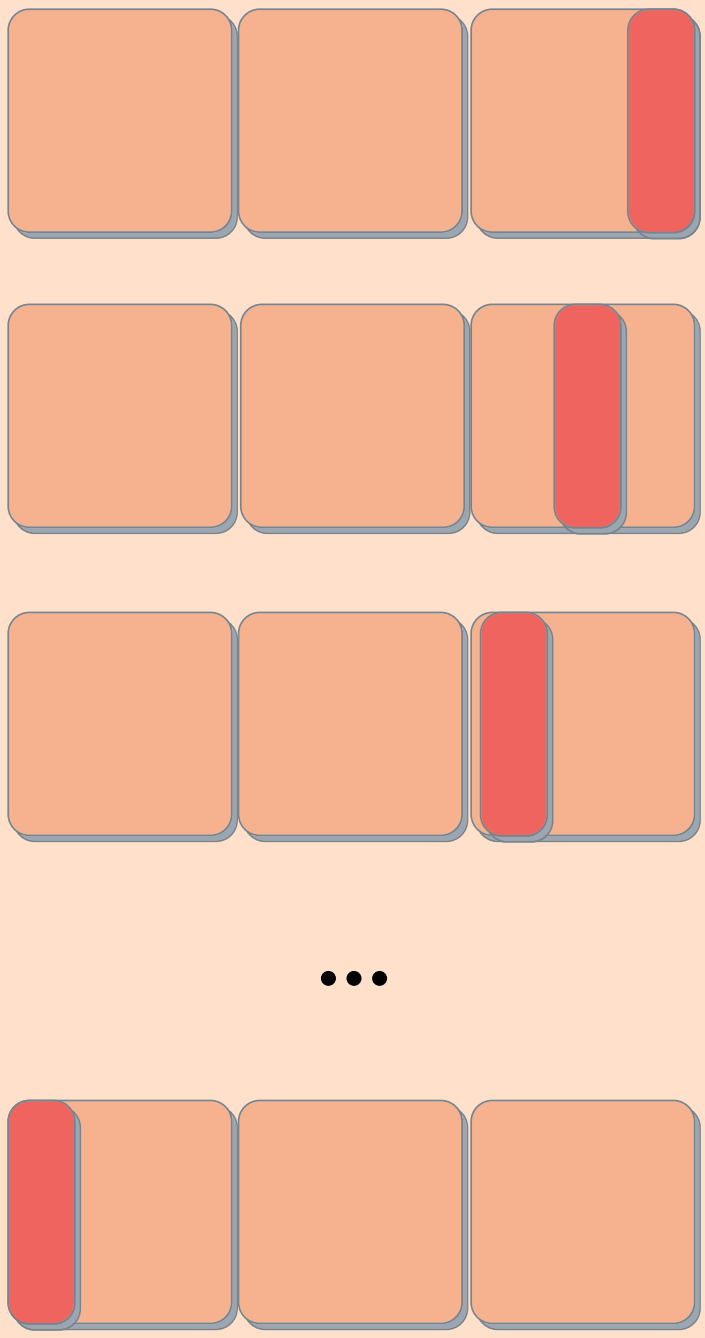
Leave-One-Out Cross Validation (LOOCV)

Only one data point is kept as testing set and model is trained on rest of the data.

This process is iterated for each data point.

For example: If we have 1000 data it will repeat 1000 times, at each iteration one data point for testing and the remaining for training.



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08 Pros & Cons

Pros:

Covers all the data points and learns everything, hence the bias will be very low.

Cons:

Since we repeat the process n time where n is the total number of data points, it results in high execution time.

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Code

```
from sklearn.model_selection import LeaveOneOut

loo = LeaveOneOut()
loo.get_n_splits(X)

for train_index, test_index in loo.split(X):
  X_train, X_test = X.iloc[train_index], X.iloc[test_index]
  y_train, y_test = y[train_index], y[test_index]
```

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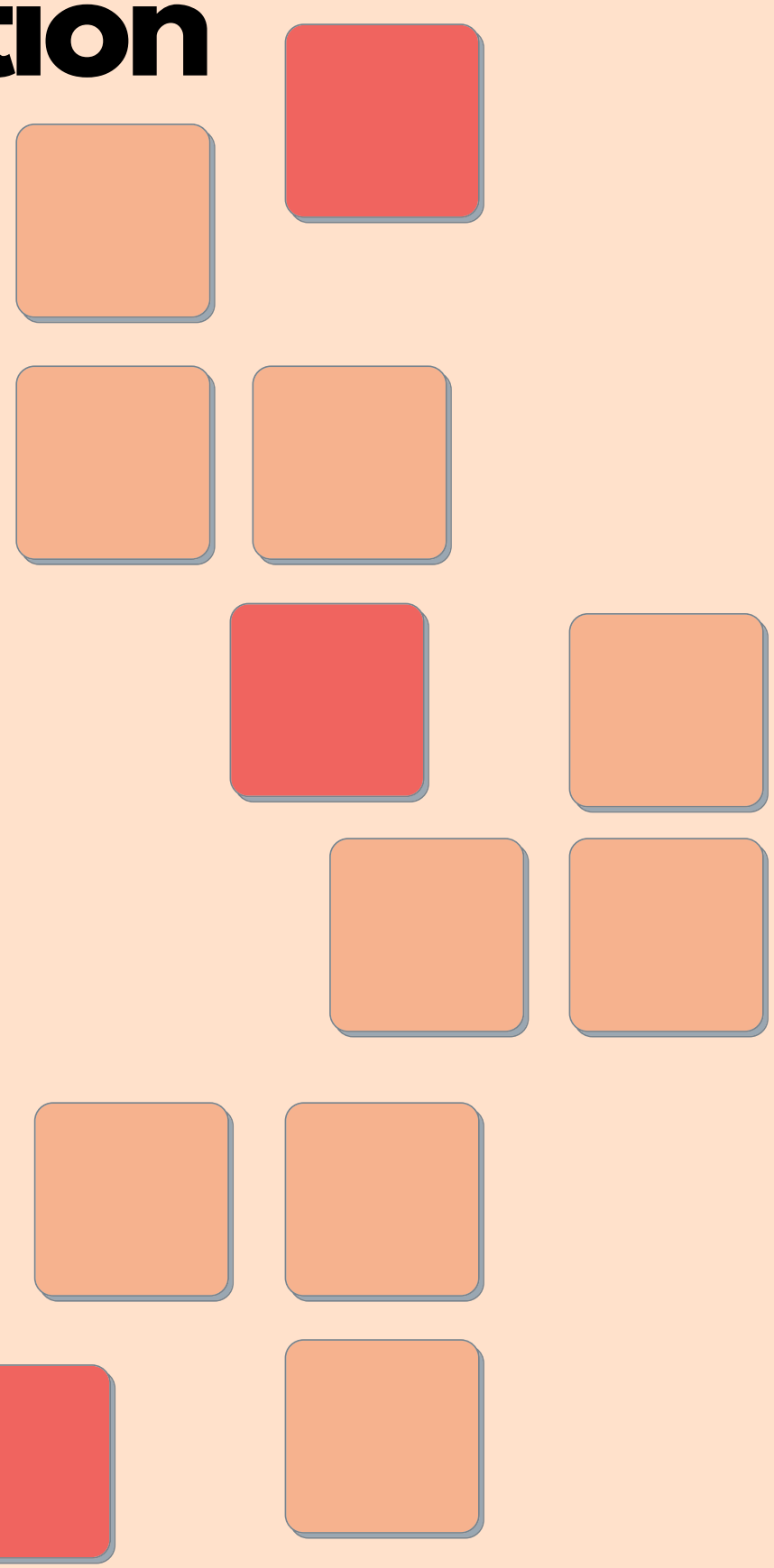
k-Folds Cross-Validation

Simply splitting data into train and test doesn't help due to variance it provided.

Creating a bunch of train/test splits, calculating the testing accuracy for each, and averaging the results together?

This is k-Folds Cross Validation.



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11 Steps

1. Split the dataset into **k** groups randomly. Take one group as testing set and rest as training set.
2. Fit the model on the training set and evaluate it on test set.
3. Set aside this evaluation score.
4. Take another group as test set and rest as training set.
5. Repeat the train test model fit setup until each group has become a test set.

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08 Pros & Cons

Pros:

Validates the performance of your model on multiple **folds** of your data.

Cons:

Doesn't work well with sequential data like time series.

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Code

```
from sklearn.model_selection import KFold
kf = KFold(n_splits = 5,
           random_state = None,
           shuffle = False)

for train_index, test_index in kf.split(X):
  print("Train:", train_index, "Test:", test_index)
  X_train, X_test = X[train_index], X[test_index]
  y_train, y_test = y[train_index], y[test_index]
```

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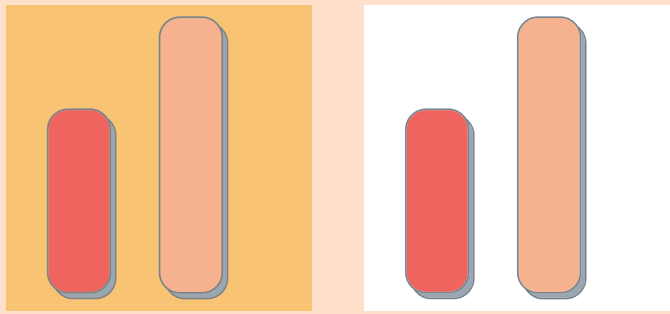
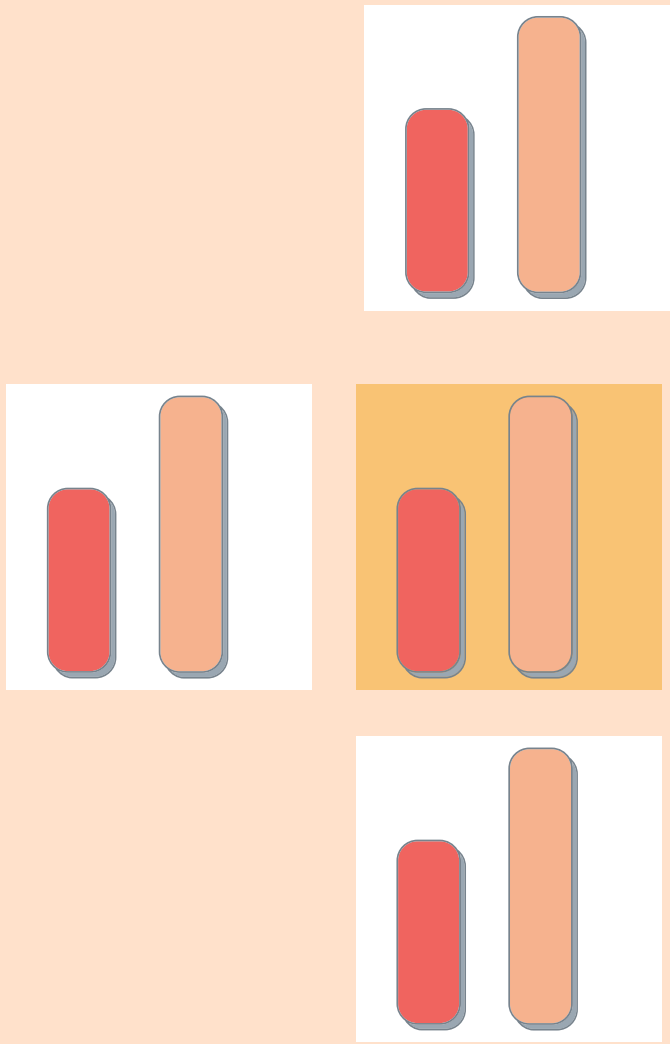
Stratified k-Folds Cross-Validation

Due to random sampling, there could be improper division of data between train and test sets.



For example, in case of binary classification problems, there could be more negative samples in one test set and in another test set, it could be very less.



To rectify this problem, stratification is required which means to rearrange in such a way that each fold is good representative of whole.

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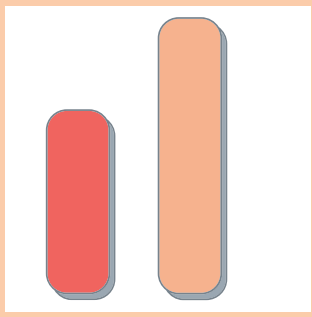
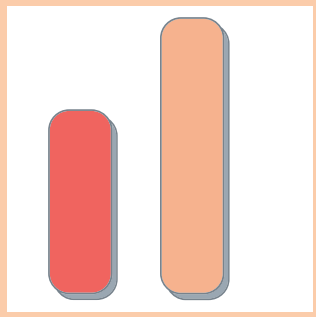
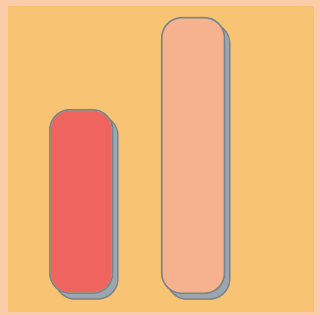
Cases

In case of categorical variables:



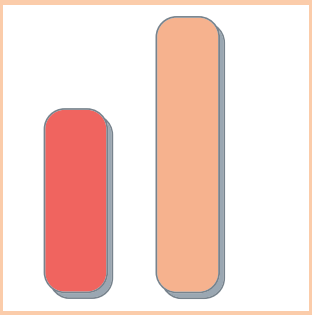


In each set, there are equal or close to results from each categories.



In case of continuous variables:

Means of all outcomes are comparable.



Class Distributions

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```python
from sklearn.model_selection import StratifiedKFolds

kf = StratifiedKFold(n_splits=5, random_state=None)

# X is the feature set and y is the target
for train_index, test_index in skf.split(X,y):
  print("Train:", train_index, "Test:", test_index)
  X_train, X_test = X.iloc[train_index], X.iloc[test_index]
  y_train, y_test = y[train_index], y[test_index]
```

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Cross-Validation for Time-Series

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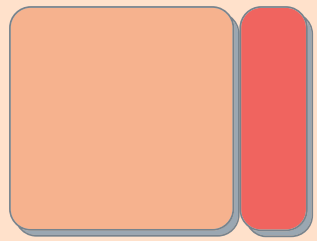
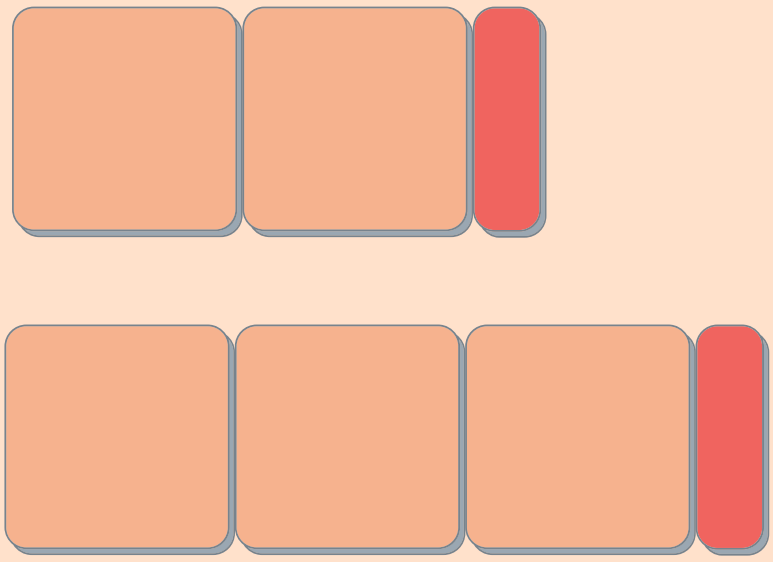
Splitting simply into train and test sets, doesn't help due to the time aspect of the data.



Folds for time-series data are created in forward chaining fashion. In each time step, train and test sets are changed. Later, we can average the forecast accuracy of test sets.



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Code

```python
from sklearn.model_selection import TimeSeriesSplit

tscv = TimeSeriesSplit(n_splits=3)

for train_index, test_index in tscv.split(X):
  print("Train:", train_index, "Test:", val_index)
  X_train, X_test = X.iloc[train_index], X.iloc[val_index]
  y_train, y_test = y[train_index], y[val_index]
```

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