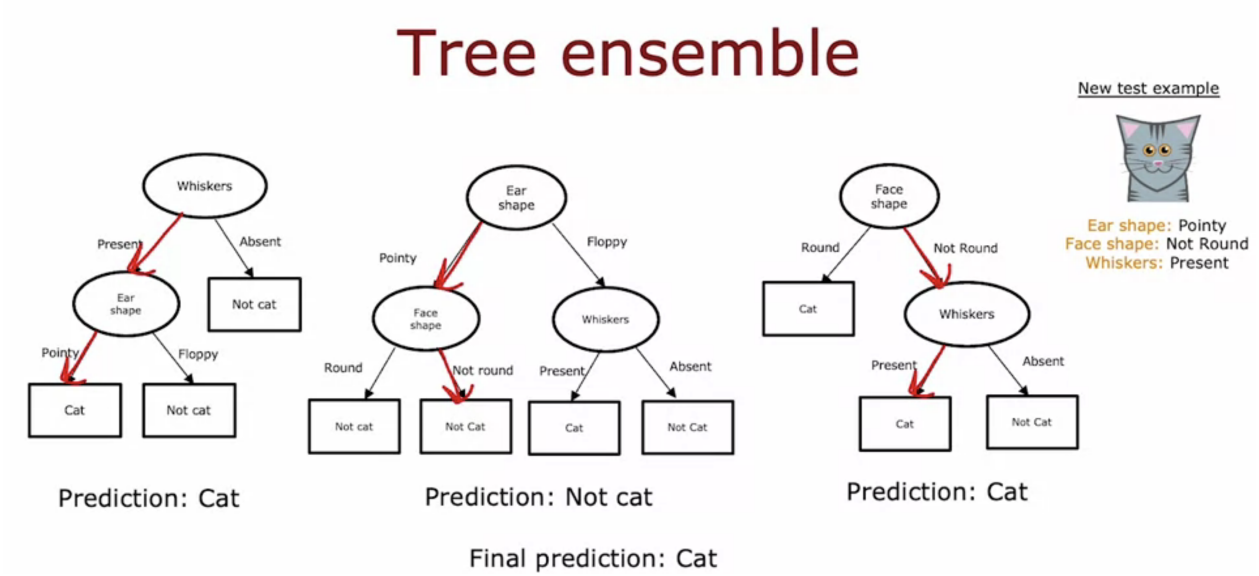
Ungraded Lab - Trees Ensemble

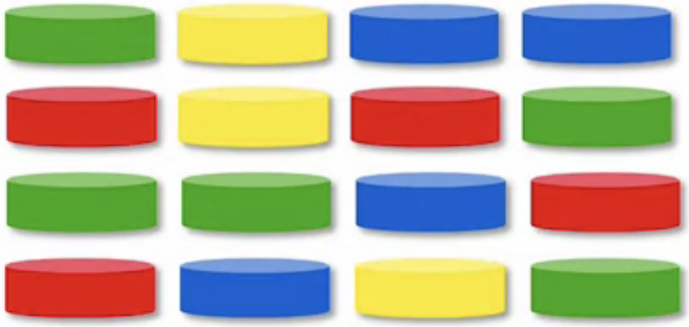
In this notebook, you will:

- Use Pandas to perform one-hot encoding of a dataset
- Use scikit-learn to implement a Decision Tree, Random Forest and XGBoost models



Sampling with replacement

Sampling with replacement:



Sampling with replacement

Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	1
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Pointy	Not round	Present	0
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Pointy	Round	Present	1
Floppy	Not round	Present	1
Floppy	Round	Absent	0
Pointy	Round	Absent	1

Generating a tree sample

Given training set of size m

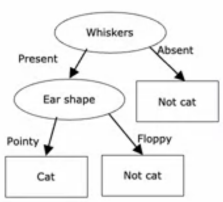
For $b = 1$ to B:

Use sampling with replacement to create a new training set of size m

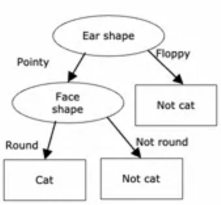
Train a decision tree on the new dataset

Use something with replacement to generate another training set of M or 10 training examples. This again looks a bit like the original training set but it's also a little bit different. You then train the decision tree on this new data set and you end up with a somewhat different decision tree. And so on. And you may do this a total of capital B times. Typical choice of capital B the number of such trees you built might be around a 100 people recommend any value from Say 64, 128. And having built an ensemble of say 100 different trees, you would then when you're trying to make a prediction, get these trees all votes on the correct final prediction. It turns out that setting capital B to be larger, never hurts performance, but beyond a certain point, you end up with diminishing returns and it doesn't actually get that much better when B is much larger than say 100 or so. And that's why I never use say 1000 trees that just slows down the computation significantly without meaningfully increasing the performance of the overall algorithm.

Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Round	Present	Yes
Pointy	Not Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Present	Yes
Pointy	Not Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Not Round	Present	Yes



Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Pointy	Round	Absent	Yes
Floppy	Not Round	Absent	No
Floppy	Not Round	Absent	No
Pointy	Round	Absent	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Round	Present	Yes



...

Bagged decision tree

Typesetting math: 0%

Randomizing the feature choice

At each node, when choosing a feature to use to split, if n features are available, pick a random subset of $k < n$ features and allow the algorithm to only choose from that subset of features.

we will instead pick a random subset of K less than N features. And allow the algorithm to choose only from that subset of K features. So in other words, you would pick K features as the allowed features and then out of those K features choose the one with the highest information gain as the choice of feature to use the split.

But for other training sets it's not uncommon that for many or even all capital B training sets, you end up with the same choice of feature at the root node and at a few of the nodes near the root node. So there's one modification to the algorithm to further try to randomize the feature choice at each node that can cause the set of trees and you learn to become more different from each other. So when you vote them, you end up with an even more accurate prediction.

$K = \sqrt{n}$

so this means that any little change further to the training set makes it less likely to have a huge impact on the overall output of the overall random forest algorithm. Because it's already explored and it's averaging over a lot of small changes to the training set.

Random forest algorithm

Boosted trees intuition

Given training set of size m

For $b = 1$ to B:

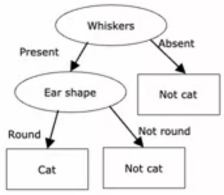
Use sampling with replacement to create a new training set of size m

But instead of picking from all examples with equal (1/m) probability, make it more likely to pick misclassified examples from previously trained trees

Train a decision tree on the new dataset

For example, if you're learning to play the piano and you're trying to master a piece on the piano rather than practicing the entire say five minute piece over and over, which is quite time consuming. If you instead play the piece and then focus your attention on just the parts of the piece that you aren't yet playing that well in practice those smaller parts over and over. Then that turns out to be a more efficient way for you to learn to play the piano well. And so this idea of boosting is similar. We're going to look at the decision trees, we've trained so far and look at what we're still not yet doing well on. And then when building the next decision tree, we're going to focus more attention on the examples that we're not yet doing well. So rather than looking at all the training examples, we focus more attention on the subset of examples is not yet doing well on and get the new decision tree, the next decision tree reporting ensemble to try to do well on them. And this is the idea behind boosting and it turns out to help the learning algorithm learn to do better more quickly. So in detail, we will look at this tree that we have just built and go back to the original training set. Notice that this is the original training set, not one generated through sampling with replacement. And we'll go through all ten examples and look at what this learned decision tree predicts on all ten examples. So this fourth most column are their predictions and put a checkmark across next to each example, depending on whether the trees classification was correct or incorrect.

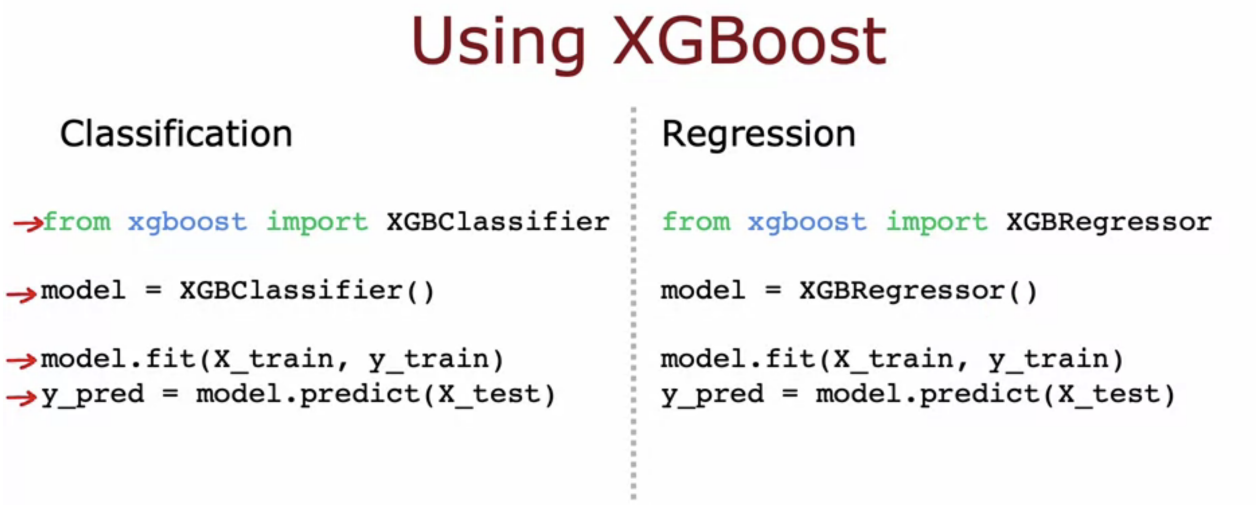
Ear shape	Face shape	Whiskers	Cat
Pointy	Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Absent	No
Pointy	Round	Present	Yes
Pointy	Not Round	Present	Yes
Floppy	Round	Absent	No
Floppy	Round	Present	Yes
Pointy	Not Round	Absent	No
Pointy	Not Round	Absent	No
Pointy	Not Round	Present	Yes



Ear shape	Face shape	Whiskers	Prediction
Pointy	Round	Present	Cat ✓
Floppy	Not Round	Present	Not cat ✗
Floppy	Round	Absent	Not cat ✓
Pointy	Not Round	Present	Not cat ✓
Pointy	Round	Present	Cat ✓
Pointy	Round	Absent	Not cat ✗
Floppy	Not Round	Absent	Not cat ✓
Pointy	Round	Absent	Not cat ✗
Floppy	Round	Absent	Not cat ✓
Floppy	Round	Absent	Not cat ✓

XGBoost (eXtreme Gradient Boosting)

- Open source implementation of boosted trees
- Fast efficient implementation
- Good choice of default splitting criteria and criteria for when to stop splitting
- Built in regularization to prevent overfitting
- Highly competitive algorithm for machine learning competitions (eg: Kaggle competitions)



Let's import the libraries we will use.

In [2]:
```
import numpy as np
import pandas as pd
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
from xgboost import XGBClassifier
import matplotlib.pyplot as plt
plt.style.use('./deeplearning.mplstyle')

RANDOM_STATE = 55 ## We will pass it to every sklearn call so we ensure reproducibility
```

1. Introduction

Datatset

- This dataset is obtained from Kaggle: Heart Failure Prediction Dataset (https://www.kaggle.com/datasets/fedesoriano/heart-failure-prediction)

Context

- Cardiovascular disease (CVDs) is the number one cause of death globally, taking an estimated 17.9 million lives each year, which accounts for 31% of all deaths worldwide. Four out of five CVD deaths are due to heart attacks and strokes, and one-third of these deaths occur prematurely in people under 70 years of age. Heart failure is a common event caused by CVDs.
- People with cardiovascular disease or who are at high cardiovascular risk (due to the presence of one or more risk factors such as hypertension, diabetes, hyperlipidaemia or already established disease) need early detection and management.
- This dataset contains 11 features that can be used to predict possible heart disease.
- Let's train a machine learning model to assist with diagnosing this disease.

Attribute Information

- Age: age of the patient [years]
- Sex: sex of the patient [M: Male, F: Female]
- ChestPainType: chest pain type [TA: Typical Angina, ATA: Atypical Angina, NAP: Non-Anginal Pain, ASY: Asymptomatic]
- RestingBP: resting blood pressure [mm Hg]
- Cholesterol: serum cholesterol [mm/dl]
- FastingBS: fasting blood sugar [1: if FastingBS > 120 mg/dl, 0: otherwise]
- RestingECG: resting electrocardiogram results [Normal: Normal, ST: having ST-T wave abnormality (T wave inversions and/or ST elevation or depression of > 0.05 mV), LVH: showing probable or definite left ventricular hypertrophy by Estes' criteria]
- MaxHR: maximum heart rate achieved [Numeric value between 60 and 202]
- ExerciseAngina: exercise-induced angina [Y: Yes, N: No]
- Oldpeak: oldpeak = ST [Numeric value measured in depression]
- ST_Slope: the slope of the peak exercise ST segment [Up: upsloping, Flat: flat, Down: downsloping]
- HeartDisease: output class [1: heart disease, 0: Normal]

Let's now load the dataset. As we can see above, the variables:

- Sex
- ChestPainType
- RestingECG
- ExerciseAngina
- ST_Slope

Are *categorical*, so we must one-hot encode them.

In [3]:
```
# Load the dataset using pandas
df = pd.read_csv("heart.csv")
```

In [4]:
```
df.head()
```

Out[4]:

	Age	Sex	ChestPainType	RestingBP	Cholesterol	FastingBS	RestingECG	MaxHR	ExerciseAngina	Oldpeak	ST_Slope	HeartDisease
0	40	M	ATA	140	289	0	Normal	172	N	0.0	Up	0
1	49	F	NAP	160	180	0	Normal	156	N	1.0	Flat	1
2	37	M	ATA	130	283	0	ST	98	N	0.0	Up	0
3	48	F	ASY	138	214	0	Normal	108	Y	1.5	Flat	1
4	54	M	NAP	150	195	0	Normal	122	N	0.0	Up	0

We must perform some data engineering before working with the models. There are 5 categorical features, so we will use Pandas to one-hot encode them.

2. One-hot encoding using Pandas

First we will remove the binary variables, because one-hot encoding them would do nothing to them. To achieve this we will just count how many different values there are in each categorical variable and consider only the variables with 3 or more values.

In [5]:
```
cat_variables = ['Sex',
'ChestPainType',
'RestingECG',
'ExerciseAngina',
'ST_Slope'
]
```

As a reminder, one-hot encoding aims to transform a categorical variable with `n` outputs into `n` binary variables.

Pandas has a built-in method to one-hot encode variables, it is the function `pd.get_dummies`. There are several arguments to this function, but here we will use only a few. They are:

- data: DataFrame to be used
- prefix: A list with prefixes, so we know which value we are dealing with
- columns: the list of columns that will be one-hot encoded. 'prefix' and 'columns' must have the same length.

For more information, you can always type `help(pd.get_dummies)` to read the function's full documentation.

In [6]:
```
# This will replace the columns with the one-hot encoded ones and keep the columns outside 'columns' argument as
df = pd.get_dummies(data = df,
                    prefix = cat_variables,
                    columns = cat_variables)
```

In [7]:
```
df.head()
```

Out[7]:

	Age	RestingBP	Cholesterol	FastingBS	MaxHR	Oldpeak	HeartDisease	Sex_F	Sex_M	ChestPainType_ASY	...	ChestPainType_NAP	ChestPainType_
0	40	140	289	0	172	0.0	0	0	1	0	...	0	
1	49	160	180	0	156	1.0	1	1	0	0	...	1	
2	37	130	283	0	98	0.0	0	0	1	0	...	0	
3	48	138	214	0	108	1.5	1	1	0	1	...	0	
4	54	150	195	0	122	0.0	0	0	1	0	...	1	

5 rows × 21 columns

Let's choose the variables that will be the input features of the model.

- The target is `HeartDisease`.
- All other variables are features that can potentially be used to predict the target, `HeartDisease`.

In [8]:
```
features = [x for x in df.columns if x not in 'HeartDisease'] ## Removing our target variable
```

We started with 11 features. Let's see how many feature variables we have after one-hot encoding.

In [9]:
```
print(len(features))
```

```
20
```

3. Splitting the Dataset

In [10]:
```
help(train_test_split)
```

```
Help on function train_test_split in module sklearn.model_selection._split:

train_test_split(*arrays, test_size=None, train_size=None, random_state=None, shuffle=True, stratify=None)
    Split arrays or matrices into random train and test subsets.

    Quick utility that wraps input validation and
    ``next(ShuffleSplit().split(X, y))`` and application to input data
    into a single call for splitting (and optionally subsampling) data in a
    oneliner.

    Read more in the :ref:`User Guide <cross_validation>`.

    Parameters
    ----------
    *arrays : sequence of indexables with same length / shape[0]
        Allowed inputs are lists, numpy arrays, scipy-sparse
        matrices or pandas dataframes.

    test_size : float or int, default=None
        If float, should be between 0.0 and 1.0 and represent the proportion
        of the dataset to include in the test split. If int, represents the
        absolute number of test samples. If None, the value is set to the
        complement of the train size. If ``train_size`` is also None, it will
        be set to 0.25.

    train_size : float or int, default=None
        If float, should be between 0.0 and 1.0 and represent the
        proportion of the dataset to include in the train split. If
        int, represents the absolute number of train samples. If None,
        the value is automatically set to the complement of the test size.

    random_state : int, RandomState instance or None, default=None
        Controls the shuffling applied to the data before applying the split.
        Pass an int for reproducible output across multiple function calls.
        See :term:`Glossary <random_state>`.

    shuffle : bool, default=True
        Whether or not to shuffle the data before splitting. If shuffle=False
        then stratify must be None.

    stratify : array-like, default=None
        If not None, data is split in a stratified fashion, using this as
        the class labels.
        Read more in the :ref:`User Guide <stratification>`.

    Returns
    -------
    splitting : list, length=2 * len(arrays)
        List containing train-test split of inputs.

        .. versionadded:: 0.16
            If the input is sparse, the output will be a
            ``scipy.sparse.csr_matrix``. Else, output type is the same as the
            input type.

    Examples
    --------
    >>> import numpy as np
    >>> from sklearn.model_selection import train_test_split
    >>> X, y = np.arange(10).reshape((5, 2)), range(5)
    >>> X
    array([[0, 1],
           [2, 3],
           [4, 5],
           [6, 7],
           [8, 9]])
    >>> list(y)
    [0, 1, 2, 3, 4]

    >>> X_train, X_test, y_train, y_test = train_test_split(
    ...     X, y, test_size=0.33, random_state=42)
    ...
    >>> X_train
    array([[4, 5],
           [0, 1],
           [6, 7]])
    >>> y_train
    [2, 0, 3]
    >>> X_test
    array([[2, 3],
           [8, 9]])
    >>> y_test
    [1, 4]

    >>> train_test_split(y, shuffle=False)
    [[0, 1, 2], [3, 4]]
```

In [11]:
```
X_train, X_val, y_train, y_val = train_test_split(df[features], df['HeartDisease'], train_size = 0.8, random_sta

# We will keep the shuffle = True since our dataset has not any time dependency.
```

In [12]:
```
print(f'train samples: {len(X_train)}')
print(f'validation samples: {len(X_val)}')
print(f'target proportion: {sum(y_train)/len(y_train):.4f}')
```

```
train samples: 734
validation samples: 184
target proportion: 0.5518
```

4. Building the Models

4.1 Decision Tree

In this section, let's work with the Decision Tree we previously learned, but now using the Scikit-learn implementation (https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html).

There are several hyperparameters in the Decision Tree object from Scikit-learn. We will use only some of them and also we will not perform feature selection nor hyperparameter tuning in this lab (but you are encouraged to do so and compare the results 😀)

The hyperparameters we will use and investigate here are:

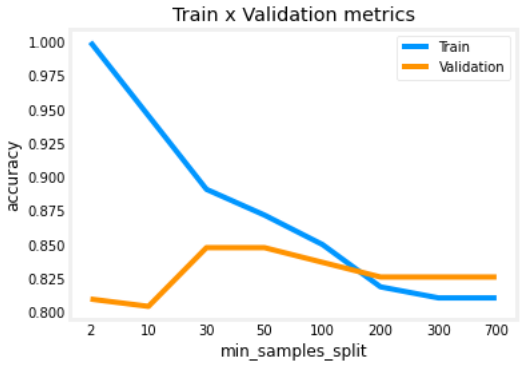
- min_samples_split: The minimum number of samples required to split an internal node.
  - Choosing a higher min_samples_split can reduce the number of splits and may help to reduce overfitting.
- max_depth: The maximum depth of the tree.
  - Choosing a lower max_depth can reduce the number of splits and may help to reduce overfitting.

In [13]:
```
min_samples_split_list = [2,10, 30, 50, 100, 200, 300, 700] ## If the number is an integer, then it is the actua
max_depth_list = [1,2, 3, 4, 8, 16, 32, 64, None] # None means that there is no depth limit.
```

In [14]:
```
accuracy_list_train = []
accuracy_list_val = []
for min_samples_split in min_samples_split_list:
    # You can fit the model at the same time you define it, because the fit function returns the fitted estimato
    model = DecisionTreeClassifier(min_samples_split = min_samples_split,
                                   random_state = RANDOM_STATE).fit(X_train,y_train)
    predictions_train = model.predict(X_train) ## The predicted values for the train dataset
    predictions_val = model.predict(X_val) ## The predicted values for the test dataset
    accuracy_train = accuracy_score(predictions_train,y_train)
    accuracy_val = accuracy_score(predictions_val,y_val)
    accuracy_list_train.append(accuracy_train)
    accuracy_list_val.append(accuracy_val)

plt.title('Train x Validation metrics')
plt.xlabel('min_samples_split')
plt.ylabel('accuracy')
plt.xticks(ticks = range(len(min_samples_split_list )),labels=min_samples_split_list)
plt.plot(accuracy_list_train)
plt.plot(accuracy_list_val)
plt.legend(['Train','Validation'])
```

Out[14]:
```
<matplotlib.legend.Legend at 0x7fa8c4d09dd0>
```



Note how increasing the the number of `min_samples_split` reduces overfitting.

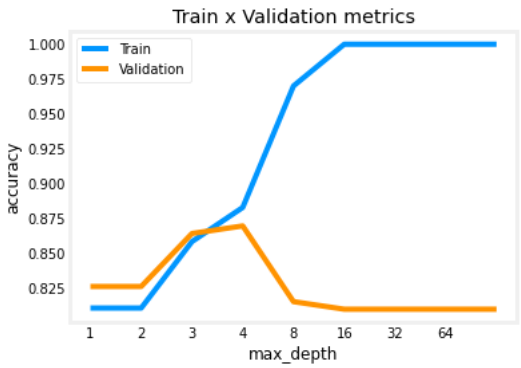
- Increasing `min_samples_split` from 10 to 30, and from 30 to 50, even though it does not improve the validation accuracy, it brings the training accuracy closer to it, showing a reduction in overfitting.

Let's do the same experiment with `max_depth` .

In [15]:
```
accuracy_list_train = []
accuracy_list_val = []
for max_depth in max_depth_list:
    # You can fit the model at the same time you define it, because the fit function returns the fitted estimato
    model = DecisionTreeClassifier(max_depth = max_depth,
                                   random_state = RANDOM_STATE).fit(X_train,y_train)
    predictions_train = model.predict(X_train) ## The predicted values for the train dataset
    predictions_val = model.predict(X_val) ## The predicted values for the test dataset
    accuracy_train = accuracy_score(predictions_train,y_train)
    accuracy_val = accuracy_score(predictions_val,y_val)
    accuracy_list_train.append(accuracy_train)
    accuracy_list_val.append(accuracy_val)

plt.title('Train x Validation metrics')
plt.xlabel('max_depth')
plt.ylabel('accuracy')
plt.xticks(ticks = range(len(max_depth_list )),labels=max_depth_list)
plt.plot(accuracy_list_train)
plt.plot(accuracy_list_val)
plt.legend(['Train','Validation'])
```

Out[15]:
```
<matplotlib.legend.Legend at 0x7fa8c446bf90>
```



We can see that in general, reducing `max_depth` can help to reduce overfitting.

- Reducing `max_depth` from 8 to 4 increases validation accuracy closer to training accuracy, while significantly reducing training accuracy.
- The validation accuracy reaches the highest at tree_depth=4.
- When the `max_depth` is smaller than 3, both training and validation accuracy decreases. The tree cannot make enough splits to distinguish positives from negatives (the model is underfitting the training set).
- When the `max_depth` is too high (>= 5), validation accuracy decreases while training accuracy increases, indicating that the model is overfitting to the training set.

So we can choose the best values for these two hyper-parameters for our model to be:

- `max_depth = 4`
- `min_samples_split = 50`

In [16]:
```
decision_tree_model = DecisionTreeClassifier(min_samples_split = 50,
                                             max_depth = 3,
                                             random_state = RANDOM_STATE).fit(X_train,y_train)
```

In [17]:
```
print(f"Metrics train:\n\tAccuracy score: {accuracy_score(decision_tree_model.predict(X_train),y_train):.4f}")
print(f"Metrics validation:\n\tAccuracy score: {accuracy_score(decision_tree_model.predict(X_val),y_val):.4f}")
```

```
Metrics train:
        Accuracy score: 0.8583
Metrics validation:
        Accuracy score: 0.8641
```

No sign of overfitting, even though the metrics are not that good.

4.2 Random Forest

Now let's try the Random Forest algorithm also, using the Scikit-learn implementation.

- All of the hyperparameters found in the decision tree model will also exist in this algorithm, since a random forest is an ensemble of many Decision Trees.
- One additional hyperparameter for Random Forest is called `n_estimators` which is the number of Decision Trees that make up the Random Forest.

Remember that for a Random Forest, we randomly choose a subset of the features AND randomly choose a subset of the training examples to train each individual tree.

- Following the lectures, if n is the number of features, we will randomly select $\sqrt{n}$ of these features to train each individual tree.
- Note that you can modify this by setting the `max_features` parameter.

You can also speed up your training jobs with another parameter, `n_jobs` .

- Since the fitting of each tree is independent of each other, it is possible fit more than one tree in parallel.
- So setting `n_jobs` higher will increase how many CPU cores it will use. Note that the numbers very close to the maximum cores of your CPU may impact on the overall performance of your PC and even lead to freezes.
- Changing this parameter does not impact on the final result but can reduce the training time.

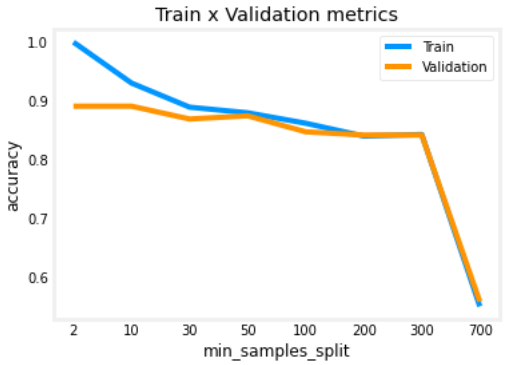
We will run the same script again, but with another parameter, `n_estimators`, where we will choose between 10, 50, and 100. The default is 100.

In [18]:
```
min_samples_split_list = [2,10, 30, 50, 100, 200, 300, 700]  ## If the number is an integer, then it is the actu
                                                              ## If it is a float, then it is the percentage of the dataset
max_depth_list = [2, 4, 8, 16, 32, 64, None]
n_estimators_list = [10,50,100,500]
```

In [19]:
```
accuracy_list_train = []
accuracy_list_val = []
for min_samples_split in min_samples_split_list:
    # You can fit the model at the same time you define it, because the fit function returns the fitted estimato
    model = RandomForestClassifier(min_samples_split = min_samples_split,
                                   random_state = RANDOM_STATE).fit(X_train,y_train)
    predictions_train = model.predict(X_train) ## The predicted values for the train dataset
    predictions_val = model.predict(X_val) ## The predicted values for the test dataset
    accuracy_train = accuracy_score(predictions_train,y_train)
    accuracy_val = accuracy_score(predictions_val,y_val)
    accuracy_list_train.append(accuracy_train)
    accuracy_list_val.append(accuracy_val)

plt.title('Train x Validation metrics')
plt.xlabel('min_samples_split')
plt.ylabel('accuracy')
plt.xticks(ticks = range(len(min_samples_split_list )),labels=min_samples_split_list)
plt.plot(accuracy_list_train)
plt.plot(accuracy_list_val)
plt.legend(['Train','Validation'])
```

Out[19]:
```
<matplotlib.legend.Legend at 0x7fa8c434c310>
```

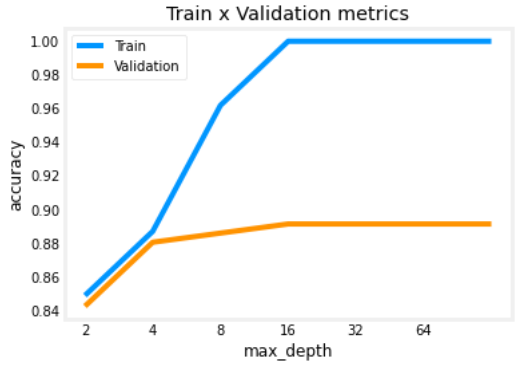


Notice that, even though the validation accuraty reaches is the same both at `min_samples_split = 2` and `min_samples_split = 10`, in the latter the difference in training and validation set reduces, showing less overfitting.

In [20]:
```
accuracy_list_train = []
accuracy_list_val = []
for max_depth in max_depth_list:
    # You can fit the model at the same time you define it, because the fit function returns the fitted estimato
    model = RandomForestClassifier(max_depth = max_depth,
                                   random_state = RANDOM_STATE).fit(X_train,y_train)
    predictions_train = model.predict(X_train) ## The predicted values for the train dataset
    predictions_val = model.predict(X_val) ## The predicted values for the test dataset
    accuracy_train = accuracy_score(predictions_train,y_train)
    accuracy_val = accuracy_score(predictions_val,y_val)
    accuracy_list_train.append(accuracy_train)
    accuracy_list_val.append(accuracy_val)

plt.title('Train x Validation metrics')
plt.xlabel('max_depth')
plt.ylabel('accuracy')
plt.xticks(ticks = range(len(max_depth_list )),labels=max_depth_list)
plt.plot(accuracy_list_train)
plt.plot(accuracy_list_val)
plt.legend(['Train','Validation'])
```

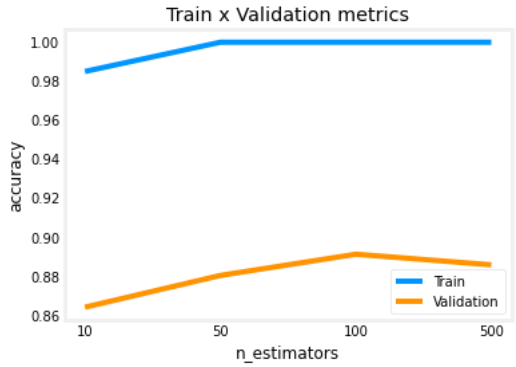
Out[20]:
```
<matplotlib.legend.Legend at 0x7fa8c42d7510>
```



In [21]:
```
accuracy_list_train = []
accuracy_list_val = []
for n_estimators in n_estimators_list:
    # You can fit the model at the same time you define it, because the fit function returns the fitted estimato
    model = RandomForestClassifier(n_estimators = n_estimators,
                                   random_state = RANDOM_STATE).fit(X_train,y_train)
    predictions_train = model.predict(X_train) ## The predicted values for the train dataset
    predictions_val = model.predict(X_val) ## The predicted values for the test dataset
    accuracy_train = accuracy_score(predictions_train,y_train)
    accuracy_val = accuracy_score(predictions_val,y_val)
    accuracy_list_train.append(accuracy_train)
    accuracy_list_val.append(accuracy_val)

plt.title('Train x Validation metrics')
plt.xlabel('n_estimators')
plt.ylabel('accuracy')
plt.xticks(ticks = range(len(n_estimators_list )),labels=n_estimators_list)
plt.plot(accuracy_list_train)
plt.plot(accuracy_list_val)
plt.legend(['Train','Validation'])
```

Out[21]:
```
<matplotlib.legend.Legend at 0x7fa8c4215790>
```



Let's then fit a random forest with the following parameters:

- max_depth: 16
- min_samples_split: 10
- n_estimators: 100

In [22]:
```
random_forest_model = RandomForestClassifier(n_estimators = 100,
                                             max_depth = 16,
                                             min_samples_split = 10).fit(X_train,y_train)
```

In [23]:
```
print(f"Metrics train:\n\tAccuracy score: {accuracy_score(random_forest_model.predict(X_train),y_train):.4f}\nMe
```

```
Metrics train:
        Accuracy score: 0.9346
Metrics test:
        Accuracy score: 0.8859
```

Note that we are searching for the best value one hyperparameter while leaving the other hyperparameters at their default values.

- Ideally, we would want to check every combination of values for every hyperparameter that we are tuning.
- If we have 3 hyperparameters, and each hyperparameter has 4 values to try out, we should have a total of 4 x 4 x 4 = 64 combinations to try.
- When we only modify one hyperparameter while leaving the rest as their default value, we are trying 4 + 4 + 4 = 12 results.
- To try out all combinations, we can use a sklearn implementation called GridSearchCV. GridSearchCV has a refit parameter that will automatically refit a model on the best combination so we will not need to program it explicitly. For more on GridSearchCV, please refer to its documentation (https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.GridSearchCV.html).

4.3 XGBoost

Next is the Gradient Boosting model, called XGBoost. The boosting methods train several trees, but instead of them being uncorrelated to each other, now the trees are fit one after the other in order to minimize the error.

The model has the same parameters as a decision tree, plus the learning rate.

- The learning rate is the size of the step on the Gradient Descent method that the XGBoost uses internally to minimize the error on each train step.

One interesting thing about the XGBoost is that during fitting, it can take in an evaluation dataset of the form `(X_val,y_val)`.

- On each iteration, it measures the cost (or evaluation metric) on the evaluation datasets.
- Once the cost (or metric) stops decreasing for a number of rounds (called early_stopping_rounds), the training will stop.
- More iterations lead to more estimators, and more estimators can result in overfitting.
- By stopping once the validation metric no longer improves, we can limit the number of estimators created, and reduce overfitting.

First, let's define a subset of our training set (we should not use the test set here).

In [24]:
```
n = int(len(X_train)*0.8) ## Let's use 80% to train and 20% to eval
```

In [25]:
```
X_train_fit, X_train_eval, y_train_fit, y_train_eval = X_train[:n], X_train[n:], y_train[:n], y_train[n:]
```

We can then set a large number of estimators, because we can stop if the cost function stops decreasing.

Note some of the `.fit()` parameters:

- `eval_set = [(X_train_eval,y_train_eval)]` :Here we must pass a list to the eval_set, because you can have several different tuples ov eval sets.
- `early_stopping_rounds` : This parameter helps to stop the model training if its evaluation metric is no longer improving on the validation set. It's set to 10.
  - The model keeps track of the round with the best performance (lowest evaluation metric). For example, let's say round 16 has the lowest evaluation metric so far.
  - Each successive round's evaluation metric is compared to the best metric. If the model goes 10 rounds where none have a better metric than the best one, then the model stops training.
  - The model is returned at its last state when training terminated, not its state during the best round. For example, if the model stops at round 26, but the best round was 16, the model's training state at round 26 is returned, not round 16.
  - Note that this is different from returning the model's "best" state (from when the evaluation metric was the lowest).

In [26]:
```
xgb_model = XGBClassifier(n_estimators = 500, learning_rate = 0.1,verbosity = 1, random_state = RANDOM_STATE)
xgb_model.fit(X_train_fit,y_train_fit, eval_set = [(X_train_eval,y_train_eval)], early_stopping_rounds = 10)
```

```
[0]     validation_0-logloss:0.64479
[1]     validation_0-logloss:0.60569
[2]     validation_0-logloss:0.57481
[3]     validation_0-logloss:0.54947
[4]     validation_0-logloss:0.52973
[5]     validation_0-logloss:0.51331
[6]     validation_0-logloss:0.49823
[7]     validation_0-logloss:0.48855
[8]     validation_0-logloss:0.47888
[9]     validation_0-logloss:0.47068
[10]    validation_0-logloss:0.46507
[11]    validation_0-logloss:0.45832
[12]    validation_0-logloss:0.45557
[13]    validation_0-logloss:0.45030
[14]    validation_0-logloss:0.44653
[15]    validation_0-logloss:0.44213
[16]    validation_0-logloss:0.43948
[17]    validation_0-logloss:0.44088
[18]    validation_0-logloss:0.44358
[19]    validation_0-logloss:0.44493
[20]    validation_0-logloss:0.44294
[21]    validation_0-logloss:0.44486
[22]    validation_0-logloss:0.44586
[23]    validation_0-logloss:0.44680
[24]    validation_0-logloss:0.44925
[25]    validation_0-logloss:0.45383
```

Out[26]:
```
XGBClassifier(base_score=0.5, booster='gbtree', callbacks=None,
              colsample_bylevel=1, colsample_bynode=1, colsample_bytree=1,
              early_stopping_rounds=None, enable_categorical=False,
              eval_metric=None, gamma=0, gpu_id=-1, grow_policy='depthwise',
              importance_type=None, interaction_constraints='',
              learning_rate=0.1, max_bin=256, max_cat_to_onehot=4,
              max_delta_step=0, max_depth=6, max_leaves=0, min_child_weight=1,
              missing=nan, monotone_constraints='()', n_estimators=500,
              n_jobs=0, num_parallel_tree=1, predictor='auto', random_state=55,
              reg_alpha=0, reg_lambda=1, ...)
```

Even though we initialized the model to allow up to 500 estimators, the algorithm only fit 26 estimators (over 26 rounds of training).

To see why, let's look for the round of training that had the best performance (lowest evaluation metric). You can either view the validation log loss metrics that were output above, or view the model's `.best_iteration` attribute:

In [27]:
```
xgb_model.best_iteration
```

Out[27]:
```
16
```

The best round of training was round 16, with a log loss of 4.3948.

- For 10 rounds of training after that (from round 17 to 26), the log loss was higher than this.
- Since we set `early_stopping_rounds` to 10, then by the 10th round where the log loss doesn't improve upon the best one, training stops.
- You can try out different values of `early_stopping_rounds` to verify this. If you set it to 20, for instance, the model stops training at round 36 (16 + 20).

In [28]:
```
dict(X_train),y_train):.4f}\nMetrics test:\n\tAccuracy score: {accuracy_score(xgb_model.predict(X_val),y_val):.4f
```

```
Metrics train:
        Accuracy score: 0.9251
Metrics test:
        Accuracy score: 0.8641
```

In this example, both Random Forest and XGBoost had similar performance (test accuracy).

Congratulations, you have learned how to use Decision Tree, Random Forest from the scikit-learn library and XGBoost!