Machine Learning Workflow

Lesson Goals

In this lesson you will learn:

- The procedure to apply Machine Learning.
- The inputs and outputs of every stage of the procedure.
- The role of experiments in Machine Learning.

Introduction

At this moment you may be wondering how to apply Machine Learning to a problem. This lesson provides the answers by breaking down the process into stages and explaining each stage, including the expected inputs and outputs. The Machine Learning workflow is composed of a series of subprocesses, or stages, so that the output of one subprocess is fed as input to the next subprocess. A helpful visual image is a pipeline connecting multiple processing machines.

Let's consider as a running example for this lesson an application to eHealth: a project for mining eHRs (electronic Health Records) to improve the quality and effectiveness of health care. More concretely, let's consider the problem of predicting the outcome of a medical treatment prescribed to a patient. Every patient is represented by an instance composed of a set of attributes describing the patient, for example: age, gender, height, weight, risk factors, medication, daily dosage, amount of intakes per day, dosage per intake, lowest blood pressure value, highest blood presure value, etc.

You can think of a patient as a vector of values, which are the independent variables. We use Machine Learning to learn a model to estimate the value of the dependent variable "efficacy of treatment" that we can model as a real variable in the range [0, 1] with 0 meaning that the treatment is totally ineffective, and 1 meaning totally effective. To evaluate the estimation produced by Machine Learning, we can compare the estimated value to the actual value, and consider the estimation as accurate enough if the difference is 3% at most.

In this lesson we will demonstrate the different stages of a machine learning workflow using the census dataset used in previous lessons.

ETL

ETL stands for **Extraction, Transformation and Loading** of data. And it is a preliminary process that has to be completed before proceeding to the application of Machine Learning.

In the **Extraction** phase, data is imported from data sources to a data storage with a single unified view, like a Data Warehouse. The data sources may be heterogeneous and distributed. For instance, in our eHealth example, the medical history of a patient may be distributed across different databases belonging to the same or different health systems.

In the **Transformation** phase, the extracted data is homogenized. This includes transforming the data in the following ways:

- **Conversion:** magnitudes expressed in different units are all converted to a single reference unit. For instance, all volume magnitudes are converted to milliliters (ml).

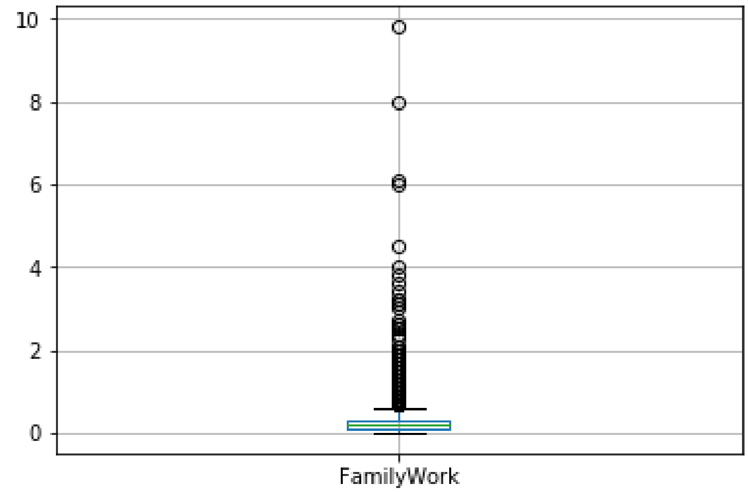
- **Remove outliers:** an outlier is a data point that clearly does not belong to the distribution of the rest of the dataset. In our eHealth example we can consider that an age of 150 years is certainly an outlier not belonging to the distribution of a representative sample of the general population. Whatever Machine Learning learns from the analysis of this instance is highly likely to not be applicable to the rest of the population. So the outlier is removed. There is another reason to remove the outlier from the data quality perspective. As we will see in the next bullet point, scaling the range of the age variable so that the highest age is mapped to 1, would make the rest of the mapped values to be inadequately compressed.

Recall our census dataset. Let's look at the dataset using the describe function.

```
census.describe()
```

	CensusId	TotalPop	Men	Women	Hispanic	White	...	Employed	PrivateWork	PublicWork	SelfEmployed
count	3220.000000	3.220000e+03	3.220000e+03	3.220000e+03	3220.000000	3220.000000	...	3.220000e+03	3220.000000	3220.000000	3220.000000
mean	31393.605280	9.940935e+04	4.889694e+04	5.051241e+04	11.011522	75.428789	...	4.559352e+04	74.219348	17.560870	7.931801
std	16292.078954	3.193055e+05	1.566813e+05	1.626620e+05	19.241380	22.932890	...	1.496995e+05	7.863188	6.510354	3.914974
min	1001.000000	8.500000e+01	4.200000e+01	4.300000e+01	0.000000	0.000000	...	6.200000e+01	25.000000	5.800000	0.000000
25%	19032.500000	1.121800e+04	5.637250e+03	5.572000e+03	1.900000	64.100000	...	4.550750e+03	70.500000	13.100000	5.400000
50%	30024.000000	2.603500e+04	1.293200e+04	1.305700e+04	3.900000	84.100000	...	1.050800e+04	75.700000	16.200000	6.900000
75%	46105.500000	6.643050e+04	3.299275e+04	3.348750e+04	9.825000	93.200000	...	2.863275e+04	79.700000	20.500000	9.400000
max	72153.000000	1.003839e+07	4.945351e+06	5.093037e+06	99.900000	99.800000	...	4.635465e+06	88.300000	66.200000	36.600000

Let's look for outliers in our census data. Even though the census data is thoroughly cleaned before it is released, for the sake of this exercise, let's pick the `FamilyWork` feature in our dataset. This column show the percent of people in each county that primarily perform unpaid family work. We can plot the boxplot of the feature to see how many points are extreme outliers.



As we can see, quite a bit of data is considered extreme outliers in this boxplot. To get rid of these outliers, we typically remove the entire row that contains the outlier. We compute the outer fence which is 3 times the IQR from the first and third quartiles. We then remove the outliers using the following code.

```
import numpy as np

q1 = np.percentile(census.FamilyWork, 25)
q3 = np.percentile(census.FamilyWork, 75)
iqr = q3 - q1
upper_fence = q3 + 3 * iqr
lower_fence = q1 - 3 * iqr
census_without_outliers = census[census.FamilyWork < upper_fence & census.FamilyWork > lower_fence]
census_without_outliers
```

	CensusId	State	County	TotalPop	Men	Women	Hispanic	White	Black	Native	Asian	Pacific	Citizen	Income	IncomeErr	IncomePerCap
0	1001	Alabama	Autauga	55221	26745	28476	2.6	75.8	18.5	0.4	1.0	0.0	40725	51281.0	2391.0	24974
1	1003	Alabama	Baldwin	195121	95314	99807	4.5	83.1	9.5	0.6	0.7	0.0	147695	50254.0	1263.0	27317
2	1005	Alabama	Barbour	26932	14497	12435	4.6	46.2	46.7	0.2	0.4	0.0	20714	32964.0	2973.0	16824
3	1007	Alabama	Bibb	22604	12073	10531	2.2	74.5	21.4	0.4	0.1	0.0	17495	38678.0	3995.0	18431
4	1009	Alabama	Blount	57710	28512	29198	8.6	87.9	1.5	0.3	0.1	0.0	42345	45813.0	3141.0	20532
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
3215	72145	Puerto Rico	Vega Baja	56858	27379	29479	96.4	3.4	0.1	0.0	0.0	0.0	43656	16948.0	1234.0	9102
3216	72147	Puerto Rico	Vieques	9130	4585	4545	96.7	2.9	0.0	0.0	0.0	0.0	7085	18104.0	3771.0	8821
3217	72149	Puerto Rico	Villalba	24685	12086	12599	99.7	0.0	0.0	0.0	0.0	0.0	18458	17818.0	1255.0	8420
3218	72151	Puerto Rico	Yabucoa	36279	17648	18631	99.8	0.2	0.0	0.0	0.1	0.0	27924	15627.0	1836.0	7960
3219	72153	Puerto Rico	Yauco	39474	19047	20427	99.5	0.5	0.0	0.0	0.0	0.0	30661	14708.0	1245.0	7743

3022 rows × 59 columns

Our initial dataset has 3220 rows and after removing outliers we have only 3022 rows. A total of 198 rows were removed.

> **Scaling:** all variables are scaled so that they take values from the same range, typically this range is [0, 1] (also known as *Normalization*). This is done to avoid bias effects in error metrics. For instance, consider variable A whose range is [0, 1] and variable B whose range is [0, 100]. A 10% error in the measurement of A would cause a "noise" of 0.01, but the same percentage of error in variable B would add a "noise" of 10. Thus the overall error might be dominated by errors in B due to scaling reasons, but not necessarily because of the right reason (possibly B has more influence in estimating the right value). Note that if we use an algorithm to scale the training data, then we will have to scale input data with the same algorithm before inputting it to the model learned by Machine Learning.

One thing we note in our dataset is that many columns in this dataset are expressed as a percent of the county population. These columns contain a number between 0 and 100. It might be easier for our calculations if we used a number between 0 and 1 and divided all these columns by 100.

We can do this one column at a time, for example, here we convert the `Hispanic` column:

```
census['HispanicRate'] = census['Hispanic'] / 100
```

However, this is not very efficient. It is more efficient to convery all columns at once. First we make a list of the columns to be converted and then convert them.

```
def to_percent(x):
   return(x/100)

conversion_list = ['Hispanic', 'White', 'Black', 'Native', 'Asian', 'Pacific', 'Poverty', 'ChildPoverty',
'Professional', 'Service', 'Office', 'Construction', 'Production', 'Drive', 'Carpool', 'Transit', 'Walk',
'OtherTransp', 'WorkAtHome', 'Employed', 'PrivateWork', 'PublicWork']



new_column_list = [x+'Rate' for x in conversion_list]
census[new_column_list] = census[conversion_list].apply(to_percent)



census.BlackRate
'SelfEmployed', 'FamilyWork'
```

```
0       0.185
1       0.095
2       0.467
3       0.214
4       0.015
        ...
3215    0.001
3216    0.000
3217    0.000
3218    0.000
3219    0.000
Name: BlackRate, Length: 3220, dtype: float64
```

> **Rounding:** all real values are rounded to the same amount of decimal figures. For instance 0.333333333333 becomes 0.3333.

Rounding can be done using the `round` function in Python.

We can round one of the rate columns that we generated. For example, we can round the `NativeRate` column to reduce the decimal places to 3.

```
census['NativeRateRounded'] = round(census['NativeRate'], 3)
census.NativeRateRounded
```

```
0       0.004
1       0.006
2       0.002
3       0.004
4       0.003
        ...
3215    0.000
3216    0.000
3217    0.000
3218    0.000
3219    0.000
Name: NativeRateRounded, Length: 3220, dtype: float64
```

> **Standardization:** transform the data so that it has zero mean (mean removal) and unit variance (variance rescaling). For instance, w = (x-mean) / sigma.

We can demonstrate this by standardizing the population size in each county. Scikit-learn (which is a library that we will introduce in greater detail in subsequent lessons) has a function that performs this task called `MinMaxScaler`.

```
from sklearn.preprocessing import MinMaxScaler
```

```
census['TotalPopScaled'] = MinMaxScaler().fit_transform(census.TotalPop.values.reshape(-1,1))
census.TotalPopScaled.describe()
```

Note: If you have not installed Scikit-learn yet, you can install it directly in your Jupyter notebook by typing:

```
count    3220.000000
mean        0.009895
std         0.031809
min         0.000000
25%         0.001109
50%         0.002585
75%         0.006609
max         1.000000
Name: TotalPopScaled, dtype: float64
```

Dummy Variables/One Hot Encoding: In order to use categorical variables in our models, we perform a transformation that is known in statistics as creating dummy variables and as one hot encoding in computer science. The main idea is to add a variable to the dataset for each value of the categorical variable but one. These variables then take a value of either zero or one to indicate whether the original feature was equal to the value in the new dummy variable column. For example, in the census dataset, we can create a dummy variable for the state feature. We will create a variable for every state and territory but one. The reason for this is that since only one of the dummy variables can be 1 for each row, this means that we can exactly predict the value of one column using the sum of all the rest. This will add a perfectly correlated column to our dataset. As we have shown in previous lessons, this scenario should be avoided.

Here is the code for creating a dummy variable for the `State` feature.

```
states = pd.get_dummies(census.State, drop_first=True)
census_dummy = pd.concat([census, states], axis=1)
census_dummy.columns.values
```

```
array(['CensusId', 'State', 'County', 'TotalPop', 'Men', 'Women',
       'Hispanic', 'White', 'Black', 'Native', 'Asian', 'Pacific',
       'Citizen', 'Income', 'IncomeErr', 'IncomePerCap',
       'IncomePerCapErr', 'Poverty', 'ChildPoverty', 'Professional',
       'Service', 'Office', 'Construction', 'Production', 'Drive',
       'Carpool', 'Transit', 'Walk', 'OtherTransp', 'WorkAtHome',
       'MeanCommute', 'Employed', 'PrivateWork', 'PublicWork',
       'SelfEmployed', 'FamilyWork', 'Unemployment', 'HispanicRate',
       'WhiteRate', 'BlackRate', 'NativeRate', 'AsianRate', 'PacificRate',
       'PovertyRate', 'ChildPovertyRate', 'ProfessionalRate',
       'ServiceRate', 'OfficeRate', 'ConstructionRate', 'ProductionRate',
       'DriveRate', 'CarpoolRate', 'TransitRate', 'WalkRate',
       'OtherTranspRate', 'WorkAtHomeRate', 'EmployedRate',
       'PrivateWorkRate', 'PublicWorkRate', 'NativeRateRounded',
       'TotalPopScaled', 'Alaska', 'Arizona', 'Arkansas', 'California',
       'Colorado', 'Connecticut', 'Delaware', 'District of Columbia',
       'Florida', 'Georgia', 'Hawaii', 'Idaho', 'Illinois', 'Indiana',
       'Iowa', 'Kansas', 'Kentucky', 'Louisiana', 'Maine', 'Maryland',
       'Massachusetts', 'Michigan', 'Minnesota', 'Mississippi',
       'Missouri', 'Montana', 'Nebraska', 'Nevada', 'New Hampshire',
       'New Jersey', 'New Mexico', 'New York', 'North Carolina',
       'North Dakota', 'Ohio', 'Oklahoma', 'Oregon', 'Pennsylvania',
       'Puerto Rico', 'Rhode Island', 'South Carolina', 'South Dakota',
       'Tennessee', 'Texas', 'Utah', 'Vermont', 'Virginia', 'Washington',
       'West Virginia', 'Wisconsin', 'Wyoming'], dtype=object)
```

> **Shuffling:** when working with datasets contained in files (for instance ARFF files or CSV files), it makes sense to shuffle the rows. Otherwise other operations that will happen later in this workflow might be biased. In our eHealth example, if we have the dataset ordered by gender, train the model on the first half, and test it with the second, we would be applying the knowledge learned from the female population to the male population, which might bias the estimations.

In Pandas, we can shuffle rows using the `sample` function. We can take a random sample where we select 100% of our original data (sample proportion = 1). This will result in a random ordering of the data.

```
shuffled_census = census.sample(frac=1)
```

After the dataset has been transformed, the **Loading** phase is executed to store the resulting dataset into a data store, for instance a database.

Sampling

After we have performed ETL on the raw data, we need to split the transformed dataset. At this point you have the option to apply Machine Learning in different ways (that will be explained in the following sections). The option that you choose to use is called your "Experimental Design". Depending on this experimental design you will need to split your transformed dataset in different ways. For the time being, it is enough to know about the simplest experimental design, known as train-test split. The train-test split means that the transformed dataset is divided into two disjoint subsets: one subset that will be used for training Machine Learning (known as the **Training Set**), and another to test the model learned by Machine Learning (known as the **Test Set**).

Note that the sampling used to select the train set and the test set must be random. If the transformed dataset is contained in a text file, it is very helpful to have this file shuffled during ETL (as mentioned in the preceding section).

Sampling is done using the `sample` function. Using this function, we can determine the number of rows we want in our sample or the proportion of the dataset.

```
census_prop_sample = census.sample(frac=0.5)

census_size_sample = census.sample(n=1000)
```

Holdout Set

A Holdout Set is a subset that we obtain from the transformed dataset and that is not available to Machine Learning during the training phase (this phase is explained in the next section). In the case of the train-test split, the subset used to test the Machine Learning model is a holdout set known as the **Test Set**. And it is very important that this test set not be available to Machine Learning during training.

Training

After the Training Set is available as a result of the completion of the sampling phase, we are ready to put Machine Learning to work. Our first step is to select the Machine Learning algorithm. After selecting the Machine Learning algorithm, we train it on the Training Set.

If we want to perform a train test split, there is a specific function to perform this task called `train_test_split` in Scikit-learn. Using this function, we pick what proportion of the data will be in the training set and the remainder will be in the test set. Typically we like to have the majority of the dataset in our training set. This is because the more data we use for training, the more accurate our model will be.

```
from sklearn.model_selection import train_test_split
```

```
census_train, census_test = train_test_split(census, test_size = 0.2)
census_train
```

	CensusId	State	County	TotalPop	Men	Women	Hispanic	White	Black	Native	Asian	Pacific	Citizen	Income	IncomeErr	IncomePerCap
416	13061	Georgia	Clay	3104	1510	1594	4.9	31.6	61.1	0.0	0.0	0.0	2304	20438.0	3369.0	12790
2713	48381	Texas	Randall	126782	62256	64526	18.8	75.0	2.6	0.4	1.4	0.0	92898	60972.0	1404.0	30480
870	19163	Iowa	Scott	169994	83437	86557	6.1	81.6	7.6	0.2	2.3	0.0	126135	55114.0	1052.0	29391
2641	48237	Texas	Jack	8946	5121	3825	15.8	78.6	4.9	0.3	0.0	0.0	6786	50324.0	7203.0	23573
1160	22095	Louisiana	St. John the Baptist	44161	21467	22694	5.3	38.0	54.2	0.1	0.5	0.3	32034	50921.0	1889.0	22660
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
3012	54041	West Virginia	Lewis	16434	8181	8253	1.1	96.7	0.5	0.0	0.3	0.1	12926	37849.0	1922.0	21067
1714	31121	Nebraska	Merrick	7776	3826	3950	4.0	93.2	0.5	0.2	0.1	0.0	5904	51012.0	1769.0	26136
1390	27153	Minnesota	Todd	24466	12500	11966	5.5	91.9	0.3	0.4	0.4	0.0	17968	46414.0	1967.0	23808
3185	72085	Puerto Rico	Las Piedras	38605	18671	19934	99.6	0.1	0.1	0.0	0.0	0.0	29394	18838.0	1703.0	9833
235	6099	California	Stanislaus	527367	261045	266322	43.6	44.7	2.4	0.5	5.2	0.7	323587	50125.0	718.0	21922

2576 rows × 61 columns

```
census_test
```

	CensusId	State	County	TotalPop	Men	Women	Hispanic	White	Black	Native	Asian	Pacific	Citizen	Income	IncomeErr	IncomePerCap
2676	48307	Texas	McCulloch	8273	4086	4187	30.8	65.7	1.6	0.0	0.0	0.0	6061	40561.0	3136.0	22194
2360	45089	South Carolina	Williamsburg	33238	16166	17072	2.2	31.4	65.5	0.1	0.2	0.0	25611	28297.0	2230.0	16344
2597	48149	Texas	Fayette	24849	12267	12582	19.6	72.6	7.2	0.0	0.1	0.0	18420	47808.0	4108.0	28458
1911	37043	North Carolina	Clay	10656	5081	5575	3.0	96.0	0.5	0.0	0.1	0.0	8516	37076.0	7525.0	22106
1718	31129	Nebraska	Nuckolls	4391	2175	2216	2.3	95.9	0.0	0.0	0.8	0.0	3460	40488.0	5223.0	24447
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
1522	29079	Missouri	Grundy	10256	4916	5340	0.9	95.2	0.6	1.2	0.3	0.1	7768	37656.0	2389.0	19365
549	15007	Hawaii	Kauai	69691	34971	34720	10.5	30.1	0.6	0.2	33.6	9.1	49430	65101.0	2955.0	27441
3211	72137	Puerto Rico	Toa Baja	85242	40215	45027	99.5	0.3	0.1	0.0	0.0	0.0	64551	23303.0	983.0	11673
194	6017	California	El Dorado	182093	90970	91123	12.5	79.0	0.9	0.6	3.9	0.1	135584	69584.0	1835.0	35588
2898	51165	Virginia	Rockingham	77785	38141	39644	5.9	90.3	1.8	0.1	0.7	0.0	57657	53744.0	1500.0	26472

644 rows × 61 columns

What Happens During Training?

During training, we apply the machine learning algorithm to our data. The algorithm typically comprised of two mathematical equations. The first equation is the mathematical model. The model describes the mathematical relationship between the features in the data. The second part of the algorithm is the loss function. The loss function quantifies how much information was lost using our model by comparing the actual data with the predicted data that is outputted by the model. Our goal is to optimize the loss. Some machine learning algorithms will continue iterating until achieving an optimal loss.

The output of the training phase is a trained model that incorporates the knowledge learned by Machine Learning, which can be queried to solve unseen problems (new problems different from those present in the training set).

Testing

Now, you might be wondering "how good is the model for solving new problems?" This is the question that the testing phase answers by computing the value of a **quality metric**. Usually you will have a threshold value for this quality metric, meaning that for the model to be usefull the value of its quality metric must be equal or greater to the threshold value.

It is important to note that the test set cannot be used for training. The fact that Machine Learning is trained with a training set of solved problems (supervised Machine Learning), and the fact that it solves those problems well, does not provide any useful information on how well it generalizes (how well it solves *new* problems).

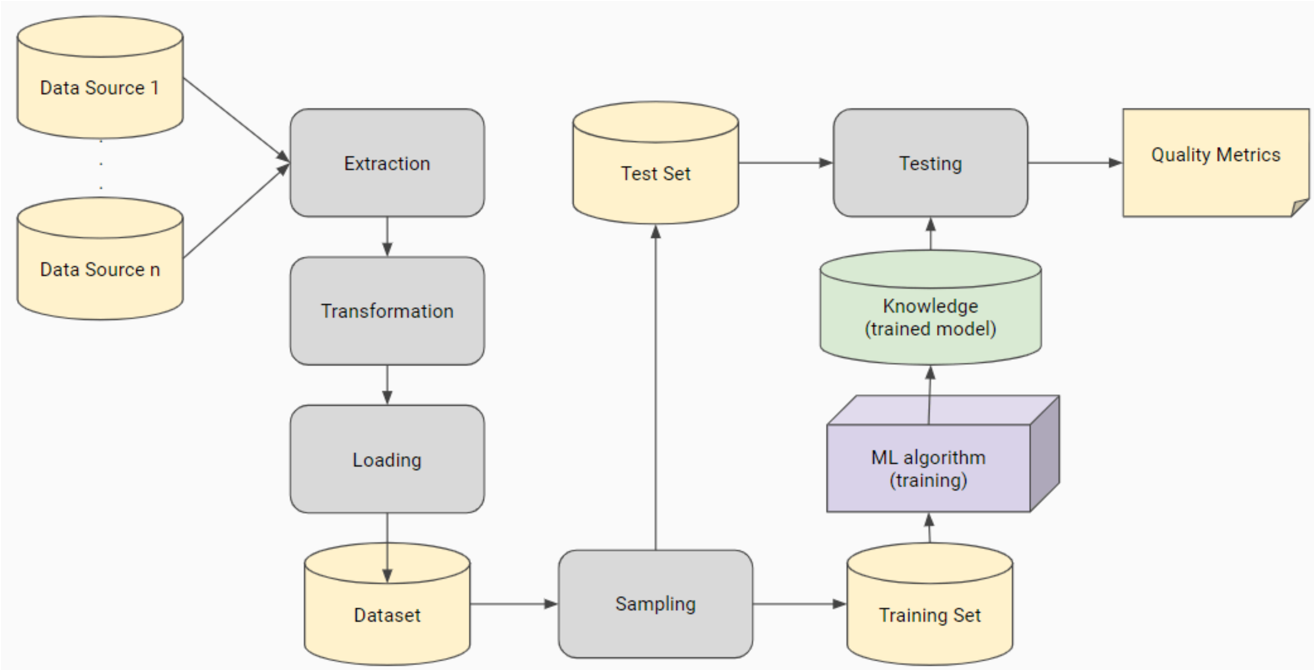
Experimental Design

Machine Learning is an experimental science. This means that when you approach a new problem, you don't know beforehand what Machine Learning algorithm will solve the problem satisfactorily. So you have to try different algorithms and analyze what happens. Every time you perform one of these trials you are actually making a Machine Learning experiment. That is why it is said that Machine Learning is an experimental science.

Before you perform any Machine Learning experiment, you have to think about how you will proceed. This is what is called the experimental design. Next, you will learn about the most common expèrimental designs that you can try out in solving Machine Learning problems.

Train-Test Split

We have already introduced this experimental design in the preceding sections. You proceed by randomly splitting the dataset into disjoint training and test sets. Then you train with the training set and evaluate how good the learned model is by feeding it the test set and comparing the model's estimations to those of the test set. This figure summarizes the workflow from the beginning:



Cross Validation

There is a probability that the train-test split tests the model on the only subset where it performs well, thus providing an unreliable quality metric. To reduce this probability, you can test on many different test sets and compute an average of the individual quality metrics obtained. This is what cross validation does. The procedure is:

1. Randomly partition the dataset in *n* bins.
2. For every bin (*b*):
   - Train with the remaining (*n-1*) bins.
   - Test with *b* and obtain quality metric.
3. Output the average of the *n* quality metrics obtained.

Train-Validation-Test Split

The training of some Machine Learning algorithms may be interpreted as learning a set of parameters that minimize the estimation error of the resulting model. How these parameters are learned is controlled by another set of parameters, that are called *hyper parameters* to avoid the confusion between both sets of parameters. Typical examples of this kind of Machine Learning paradigms are SVMs (Support Vector Machines) and Artificial Neural Networks.

The basic procedure is:

- Randomly partition the dataset in 3 disjoint subsets (training, validation, and test sets).
- Initialize the hyperparameters
- Train with the train set.

- Evaluate on validation set.
- Update best performing hyperparameters.
- Recompute/modify the hyperparameters while maximum number of iterations not reached.
- Using the best performing hyperparameters, compute the definitive quality metric on the test set.

Summary

In this chapter, you have learned the workflow of Machine Learning: ETL, sampling, training, and testing. Every time you execute this workflow you have performed one Machine Learning experiment, for which you have obtain a quality metric. At this point, you may wish to improve the quality metric, and consequently you may want to perform another experiment changing something, for instance the Machine Learning algorithm being used. As you see, this is an iterative process, and Machine Learning is an experimental science.