

Overview

In this notebook we will learn about

- Categorical variables
 - non-numeric
- Classification task
 - Supervised Learning, with categorical target

We begin with the Binary Classification task, in which the targets are one of two possible values

- Positive/Negative

Recipe Step A: Get the data

Frame the problem

Borrowed from [Wikipedia \(https://en.wikipedia.org/wiki/RMS_Titanic\)](https://en.wikipedia.org/wiki/RMS_Titanic).

RMS Titanic was a British passenger liner that sank in the North Atlantic Ocean in 1912 after the ship struck an iceberg during her maiden voyage from Southampton to New York City. Of the estimated 2,224 passengers and crew aboard, more than 1,500 died, making it one of modern history's deadliest peacetime commercial marine disasters

The goal is to predict whether a passenger survives, based on passenger characteristics.

- target: { "Survive", "Not Survive" }
- features: vector of passenger characteristics

That is: a Binary Classification Task

- Positive: "Survive"
- Negative: "Not survive"

Aside: What does the Titanic have to do with Finance or Risk ?

- Credit risk: will borrower default ?
- Mortgage prepayment risk: Will mortgage Prepay ?

Recipe A.1: Get the data

The data comes in two CSV format files

- train
- test

We will read them into a Pandas DataFrame.

- Observe our use of *relative paths* for file names
- Using relative rather than absolute paths will allow us to grade your assignment on our machine
 - Files in different absolute locations, but same relative location

```
In [5]: # Note the use of *relative path*; you should all use relative rather than absolute paths  
TITANIC_PATH = th.TITANIC_PATH  
print("Data directory: ", TITANIC_PATH)  
  
train_data = pd.read_csv( os.path.join(TITANIC_PATH, "train.csv") )  
test_data  = pd.read_csv( os.path.join(TITANIC_PATH, "test.csv") )
```

Data directory: ./data/titanic

```
In [6]: train_data.shape  
        test_data.shape
```

```
Out[6]: (891, 12)
```

```
Out[6]: (418, 11)
```

Recipe A.2: Have a look at the data

Let's examine the first few records to get a feel for the shape of the data.

This will help us understand the features and the target.


```
In [7]: train_data.columns  
train_data.head()
```

```
Out[7]: Index(['PassengerId', 'Survived', 'Pclass', 'Name', 'Sex', 'Age', 'SibSp',  
              'Parch', 'Ticket', 'Fare', 'Cabin', 'Embarked'],  
              dtype='object')
```

```
Out[7]:
```

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C85	C
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S

The attributes have the following meaning:

- **Survived:** that's the target
 - 0 means passenger did not survive (Negative)
 - 1 means passenger survived (Positive)
- **Pclass:** passenger class.
- **Name, Sex, Age:** self-explanatory
- **SibSp:** how many siblings & spouses of the passenger aboard the Titanic.
- **Parch:** how many children & parents of the passenger aboard the Titanic.
- **Ticket:** ticket id
- **Fare:** price paid (in pounds)
- **Cabin:** passenger's cabin number
- **Embarked:** where the passenger embarked the Titanic

How many observations are there ?

```
In [8]: (num_obs, num_features) = train_data.shape  
        print("There are {nr} observations and {nf} attributes (including the target)".format(nr=num_obs, nf=num_features) )
```

There are 891 observations and 12 attributes (including the target)

Observation

- The data covers many fewer examples than the number of described in the problem statement
- Is the data not truly representative ?

We'll ignore this for now.

Let's try to understand the types of the attributes

In [9]: train_data.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 891 entries, 0 to 890
Data columns (total 12 columns):
PassengerId    891 non-null int64
Survived        891 non-null int64
Pclass         891 non-null int64
Name           891 non-null object
Sex            891 non-null object
Age           714 non-null float64
SibSp          891 non-null int64
Parch          891 non-null int64
Ticket         891 non-null object
Fare           891 non-null float64
Cabin          204 non-null object
Embarked       889 non-null object
dtypes: float64(2), int64(5), object(5)
memory usage: 83.7+ KB
```

Non-numeric attributes

We can see the non-numeric attributes (type is "object") are:

- Name
- Sex
- Cabin
- Embarked

Data issues: missing attributes

We can also see that we have some missing data issues to deal with.

Any attribute with less than num_obs values has observations with a missing value in the attribute

- Age
- Cabin
- Embarked

Other issues

- Shouldn't `Survived` be non-numeric (Positive/Negative or Survived/Not) ?
 - looks like this has been encoded as the integer 1/0
- What about `Pclass` ? Shouldn't it be non-numeric ?
 - This could have just as easily been encoded as non-numeric "First", "Second", "Third"
 - Is the fact that it has been encoded as small integers significant ?
 - This is much deeper than it sounds.
 - We will revisit when discussing Categorical variables.

For our first pass at the problem: we will ignore issues concerning `Survived` and `Pclass`.

Let's get a summary of the distribution of each attribute

(n.b., `describe` operates *only* on the numeric attributes)

In [10]: `train_data.describe()`

Out[10]:

	PassengerId	Survived	Pclass	Age	SibSp	Parch	Fare
count	891.000000	891.000000	891.000000	714.000000	891.000000	891.000000	891.000000
mean	446.000000	0.383838	2.308642	29.699118	0.523008	0.381594	32.204208
std	257.353842	0.486592	0.836071	14.526497	1.102743	0.806057	49.693429
min	1.000000	0.000000	1.000000	0.420000	0.000000	0.000000	0.000000
25%	223.500000	0.000000	2.000000	20.125000	0.000000	0.000000	7.910400
50%	446.000000	0.000000	3.000000	28.000000	0.000000	0.000000	14.454200
75%	668.500000	1.000000	3.000000	38.000000	1.000000	0.000000	31.000000
max	891.000000	1.000000	3.000000	80.000000	8.000000	6.000000	512.329200

- You can also observe the attributes with missing values by looking at the "count"
- You can clearly see that `Survived` is a binary, *integer* variable
- Only 38 % of the passengers survived ("mean")

```
In [11]: train_data["Survived"].value_counts()
```

```
Out[11]: 0    549  
         1    342  
         Name: Survived, dtype: int64
```



Recipe A.3: Select a performance measure

Our performance measure for the Classification task will be **accuracy**, the fraction of correct predictions.

$$\text{Accuracy} = \frac{\text{number of correct predictions}}{\text{number of predictions}}$$

There are several drawbacks with this definition, which we will address later.

But let's start with it for now.

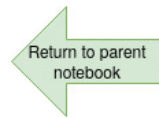
Recipe A.4: Create a test set and put it aside !

The train/test split was done for us: it came as two separate files

We might later choose to combine the two and do our own split (or better yet: multiple splits) but for now, we'll take what we are given.

Note that the test set provided *does not have targets* associated with each example

- The dataset was from a Kaggle competition. The "answers" (targets) to the test set were known only to the judges.
- This means you can't use the provided test set to evaluate the Performance Measure. Either
 - Create your own test set
 - Use Cross Validation



Recipe Step B: Exploratory Data Analysis (EDA)

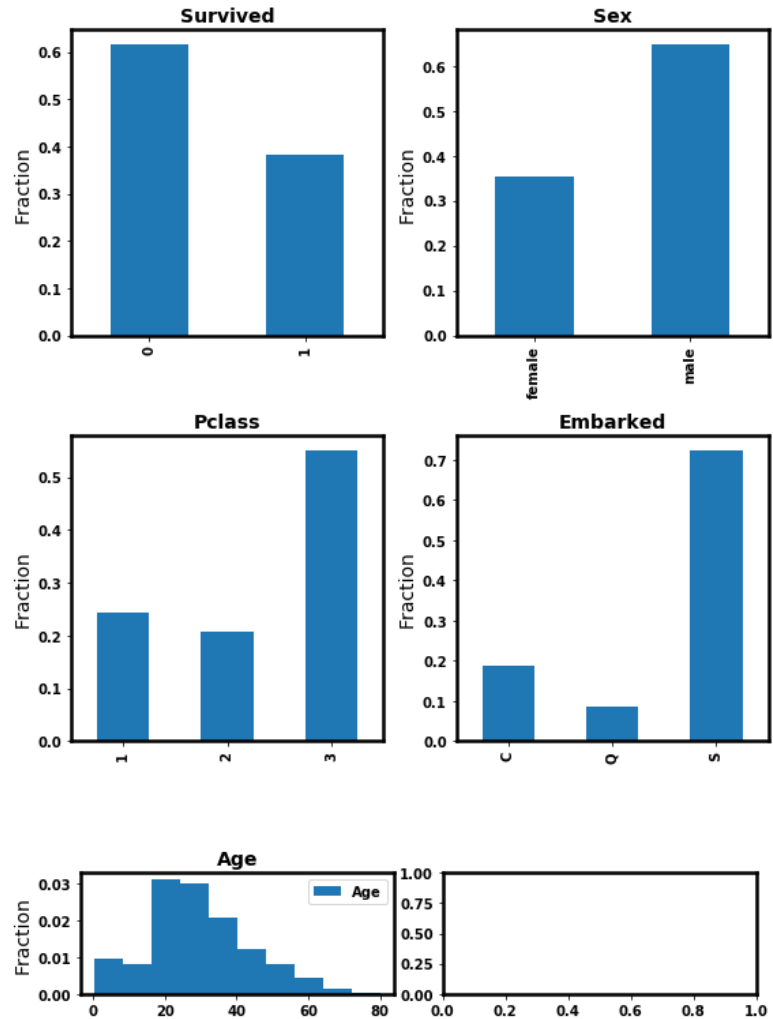
Visualize Data to gain insights

Distribution of each attribute

Let's start by looking at the (unconditional) distribution of the target and some attributes

First let's look at them normalized (i.e, as fractions or probabilities)

```
In [12]: clh.plot_attrs(train_data, [ "Survived", "Sex", "Pclass", "Embarked" ], attr_type
e="Cat", plot=True, normalize=True)
clh.plot_attrs(train_data, [ "Age" ], attr_type="Num", normalize=True)
```



One important observation is apparent:

The dataset is very *imbalanced*

- the number of Positive (Survive) examples is much less than the number of Negative (Not Survive) examples
- this is a problem: just look at the Loss that is being minimized

$$\begin{aligned}\mathcal{L}_{\Theta} &= \frac{1}{m} \sum_{i=1}^m \mathcal{L}_{\Theta}^{(i)} \\ &= \frac{1}{m} \left(\sum_{i \in \text{Positive}} \mathcal{L}_{\Theta}^{(i)} + \sum_{i \in \text{Negative}} \mathcal{L}_{\Theta}^{(i)} \right)\end{aligned}$$

The cumulative weight of the Positive examples is much less than the Negative

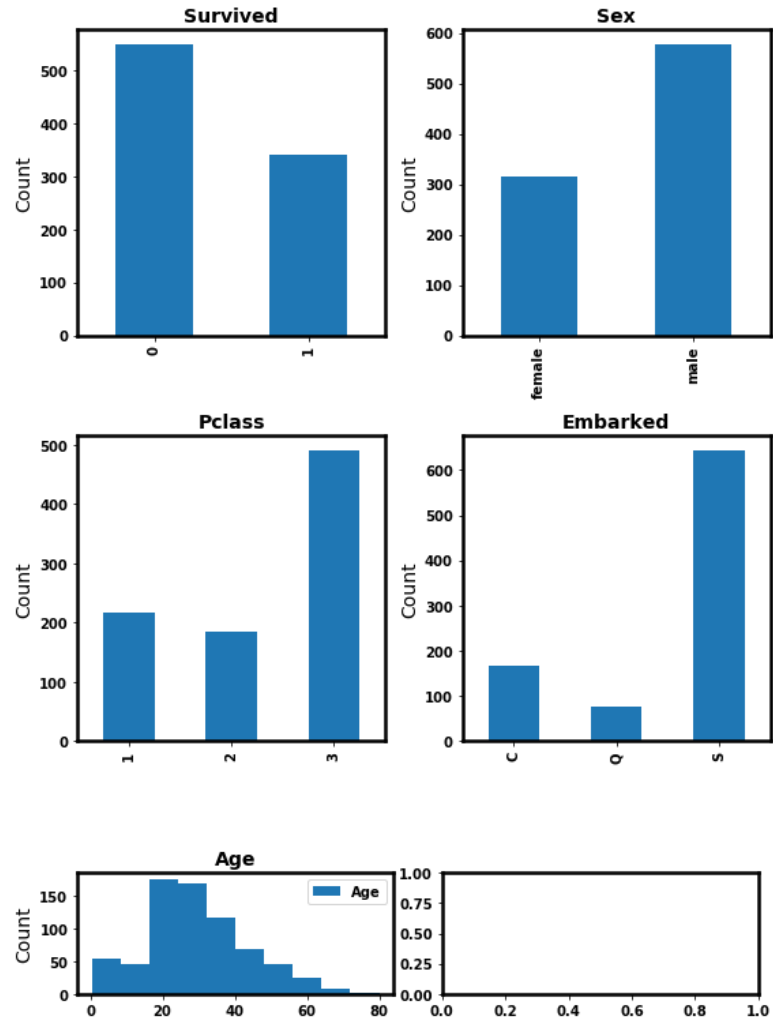
- hence, the Positive examples may influence Θ more than the Negative

Eliminating this potential source of bias in optimization will be the topic of a future module.

We've looked at the distributions as normalized (fractions of total).

We can also look at them un-normalized, or absolute count

```
In [13]: clh.plot_attrs(train_data, [ "Survived", "Sex", "Pclass", "Embarked" ], attr_type="Cat", plot=True, normalize=False)
clh.plot_attrs(train_data, [ "Age" ], attr_type="Num", normalize=False)
```



Conditional survival probability (condition on single attribute)

Let's explore whether there is a relationship between the target (Survived) and single features

- This might tell us whether the feature has some predictive value
 - If the distribution of the target is different for each value of the feature
 - The feature may have an association with the target

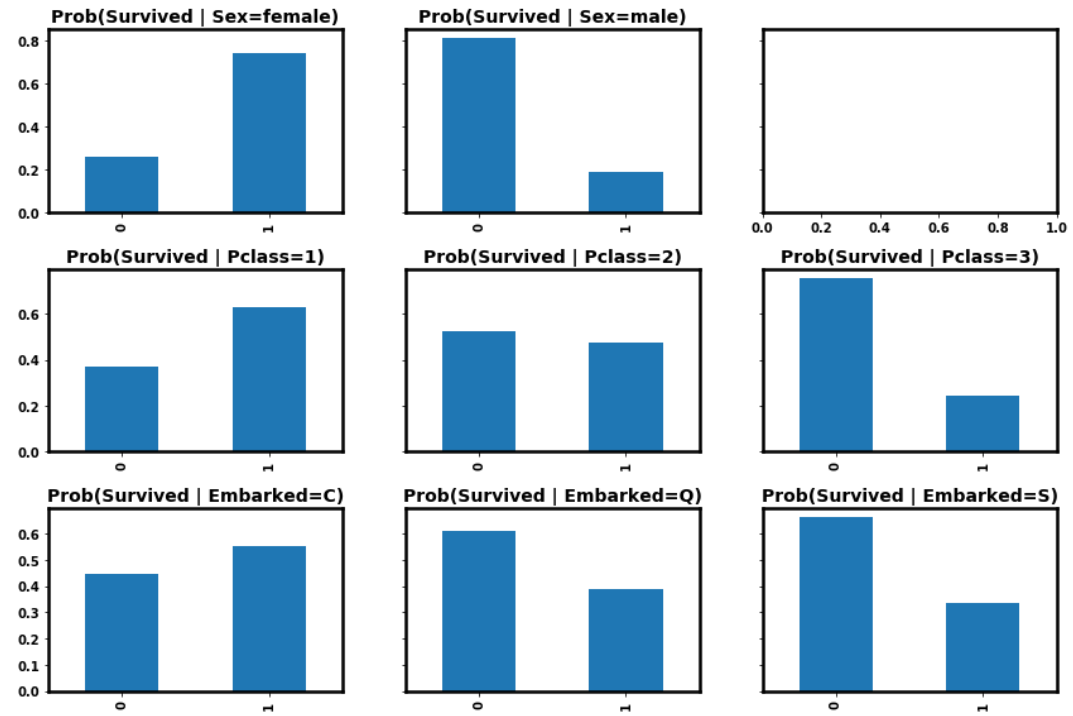
```
In [14]: fig, axs = clh.plot_conds(train_data, [ ("Survived", { "Sex": "female"}),
                                                ("Survived", { "Sex": "male"}),
                                                None,
                                                ("Survived", { "Pclass": 1}),
                                                ("Survived", { "Pclass": 2}),
                                                ("Survived", { "Pclass": 3}),

                                                ("Survived", { "Embarked": "C"}),
                                                ("Survived", { "Embarked": "Q"}),
                                                ("Survived", { "Embarked": "S"})
                                                ],
                                share_y="row",
                                normalize="False"
                                )

# In case the figure is truncated in this slide, we will re-display it in the next (without the code)
plt.close(fig)
```

```
In [15]: # Display the figure again, in it's own slide, so it is not truncated
fig
```

Out[15]:



Interesting !

- Women are 3 times as likely to survive
- NOT being in the lowest Class doubles or triples your survival probability
- Embarking at Cherbourg increased your probability of surviving
 - WHY ? Is there a correlation between Class and point of embarkation maybe ?

Preview: There may also be lessons here for dealing with missing data

Conditional survival probability (condition on multiple attributes)

- Having examined possible associations between the target and single features
- We now examine a possible association to pairs of features
- A single feature alone may not separate the data into different target values
- But combinations of features might

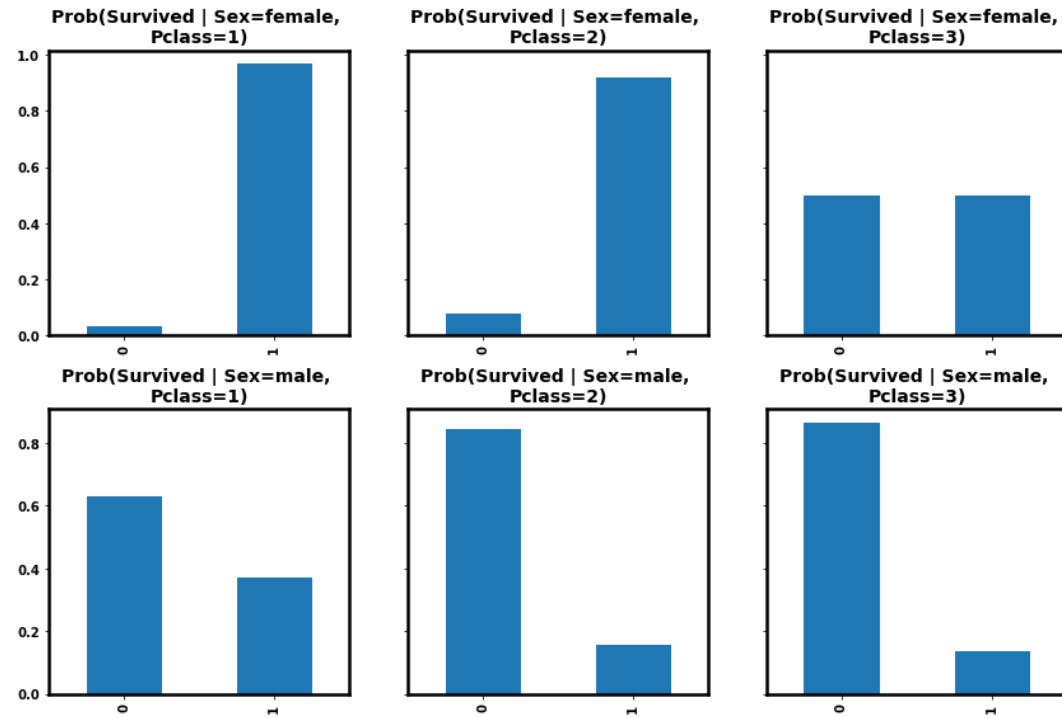
```
In [16]: fig, axs = clh.plot_conds(train_data, [
        ( "Survived", { "Sex": "female", "Pclass": 1}),
        ( "Survived", { "Sex": "female", "Pclass": 2}),
        ( "Survived", { "Sex": "female", "Pclass": 3}),

        ( "Survived", { "Sex": "male", "Pclass": 1}),
        ( "Survived", { "Sex": "male", "Pclass": 2}),
        ( "Survived", { "Sex": "male", "Pclass": 3}),
        ],
        share_y="row"
    )

# In case the figure is truncated in this slide, we will re-display it in the ne
xt (without the code)
plt.close(fig)
```

```
In [17]: # Display the figure again, in it's own slide, so it is not truncated
fig
```

Out[17]:



Remember our original theory that being Female *unconditionally* increased chances of Survive ?

- We can see now see that this was only true *conditionally* for Classes 1 and 2

This suggests that some *feature engineering* (creating *synthetic features* from the raw features) may increase accuracy of the prediction of Survive

- create a synthetic $\text{PClass} \neq 3$ feature
- use it in a *compound* feature: $(\text{PClass} \neq 3)$ and $(\text{Sex} = \text{Female})$

The creation of synthetic features is also called *transformation*.

Creating such a compound feature will be the topic of a subsequent module.

For now: we will limit ourselves to raw features.

Age

We have not yet looked at whether the `Age` feature may help us predict `Survive/Not Survive`.

Since there are too many discrete ages, we will look at the probability of `Survive` conditioned on `Age` buckets.

- each bucket has an `Age` range of 15 years
- lower age in bucket is denoted by `AgeBucket` attribute

```
In [18]: train_data_augmented = train_data.copy()
train_data_augmented["AgeBucket"] = train_data["Age"] // 15 * 15
train_data_augmented[["AgeBucket", "Survived"]].groupby(['AgeBucket']).mean()
```

Out[18]:

Survived	
AgeBucket	
0.0	0.576923
15.0	0.362745
30.0	0.423256
45.0	0.404494
60.0	0.240000
75.0	1.000000

Wow ! Children below the age of 15 (bucket 0.0) had a much better chance of survival.

(And it doesn't pay to be old when disaster strikes!)

Another thing becomes apparent through the bucketing:

- the relationship between Age and Survive is **not linear**
 - probability of Survive in Age range 15-30 is *lower* than adjacent buckets

We would be hard pressed to see this using Age as a continuous variable

Note that the Linear Regression equation

$$\mathbf{y} = \Theta^T \mathbf{x}$$

implies a *linear relationship* between target \mathbf{y} and each feature Θ_j

- An example with feature value $2 * \mathbf{x}_j$ has twice the impact on \mathbf{y} as an example with feature value \mathbf{x}_j .

So using the raw Age feature in prediction is probably not a great idea.

A better idea would be to use

- synthetic feature AgeBucket
- as a *categorical* variable
 - True/False: an example is in each bucket

Again:

- we will see how to properly encode categorical features in a subsequent module
- for now: we will stick with the raw feature Age

Embarked

The Embarked attribute tells us where the passenger boarded:

- C=Cherbourg, Q=Queenstown, S=Southampton.

Could this be a predictor of Survived ?

Or perhaps

- there is a correlation between Embarked and PClass
 - First Class passengers may have boarded at one location; Third Class in another
 - in which case Embarked would not provide any information in addition to PClass

We don't know the answer

- but these are questions well worth exploring in the Exploratory Data Analysis step.

Cabin

Might the Cabin location be associated with Survival ?

Note that the front of the ship went down first.

- Worst cabins (pink, Third class) were dispersed between front and back
- Best cabins (white, First class) were dispersed between above/below deck
- Mid cabins(yellow, Second Class) were *not* near front of ship



Aside: Using Pandas for partitioning the data

Aside: How does `pd.groupby()` work ?

If you examine our modules to see how we are partitioning the data

- You will see how useful the Pandas `groupby` method is
- For those who know SQL: this is similar to grouping in database queries
- For those who want to know how `groupby` works, this section explains
 - Feel free to skip it `

The Pandas Split-Apply-Combine pattern is very powerful

- This is very SQL-like, for those who have used databases
- Below is some simpler Pandas code to show exactly how it works

```

In [19]: # Partition by the attribute "Sex"
males    = train_data[ train_data["Sex"] == "male"]
females  = train_data[ train_data["Sex"] == "female"]

# Aggregate within each group: count,mean.  n.b., only doing this for the "Survived" column
count_males, count_females = males.shape[0], females.shape[0]
survival_males, survival_females = males["Survived"].mean(), females["Survived"].mean()

print( "male\t{c}\t{m:0.4f}".format(c=count_males, m=survival_males) )
print( "female\t{c}\t{m:0.4f}".format(c=count_females, m=survival_females) )

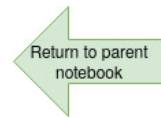
# Or, use the pd.groupby
train_data.groupby("Sex").agg(["mean", "count"])["Survived"]

male      577      0.1889
female    314      0.7420

```

Out[19]:

	mean	count
Sex		
female	0.742038	314
male	0.188908	577



Recipe Step C: Prepare the data

We will follow all the steps for the Prepare the Data step per our Recipe.

But

- We will initially only discuss what we intend to do for each sub-step
- The actual code will be deferred to the end of this section
- We will use a single Pipeline to implement all the steps of Prepare the Data

Recipe C.1: Cleaning

Our initial data exploration revealed some attributes with missing data

- Age
- Cabin
- Embarked

We will address various strategies for dealing with missing data in the module on Data Transformations.

For now, we will take a very simple (and naive) approach

- For numeric attributes: use the median value
- For non-numeric attributes: use the most frequent value

Recipe C.2: Handling non-numeric features/targets

The next step in the Recipe is dealing with non-numeric variables.

- Numericalize (convert to a number) categorical variables

Mechanically: we will use a single Pipeline to accomplish several steps in the Recipe

- Data cleaning
- Converting categorical features
- Transformations

That is, we will implement Cleaning and Numericalization as types of transformers.

Categorical Transformation: Binary variable special case

We will need to transform our categorical features into numbers.

The way to treat categorical values is not obvious and there are many *wrong* ways to do it.

Fortunately, a binary categorical variable is an easy special case.

Again: this will suffice for a first pass

- We will subsequently generalize to non-binary categorical variables.

Which variables are categorical ?

We can (and should) apply *human logic* to answer this question.

But a little code can help:

In [20]: `train_data.info()`

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 891 entries, 0 to 890
Data columns (total 12 columns):
PassengerId    891 non-null int64
Survived        891 non-null int64
Pclass         891 non-null int64
Name           891 non-null object
Sex            891 non-null object
Age            714 non-null float64
SibSp          891 non-null int64
Parch          891 non-null int64
Ticket         891 non-null object
Fare           891 non-null float64
Cabin          204 non-null object
Embarked       889 non-null object
dtypes: float64(2), int64(5), object(5)
memory usage: 83.7+ KB
```

All of the columns described as `object` are non-numerical and hence likely suspects

- Name, Sex, Cabin, Embarked

We will have to numericalize `Sex` as this is the only categorical feature we retain for our initial model.

But, as observed during our first look, some numeric columns are *also* candidates

- Survived
- PassengerId, Pclass

This is where *human logic* comes in:

- Is there an *ordering relationship* among the values for a variable ?
- If not: it may be categorical

Our target `Survived` was given to us as numeric

- The categorical values Survive/Not Survive have been encoded as 1 and 0.

It will turn out that this is an adequate (although not perfect) encoding of a *binary* variable.

So, by luck (or bad encoding) we don't have to convert the categorical `Survived` feature to a binary digit.

Recipe C.3: Transformations

In this step we can

- Transform/filter existing features
- Add new features synthesized from raw features.

The synthetic features suggested by our EDA

- Compound feature for Sex/PClass
- Age Bucket

would be created in the Transformation step.

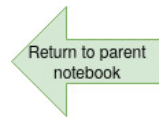
In this introduction: we will only perform the minimal transformations necessary

- missing data imputation
- numericalization

But we will give you a taste for what might be possible.

Recipe C.4: Scaling

For this exercise: no scaling will be performed.



Recipe Step C in practice: a sophisticated pipeline

Now is the time to start coding !

We begin by

- Eliminating training examples that don't have targets
- Removing the target column from the training data
 - To be sure we don't accidentally cheat

```
In [21]: # Remove examples where target is not defined  
train_data = train_data[ train_data["Survived"].notnull() ]  
  
# Separate target from features  
y_train = train_data["Survived"]  
train_data.drop(columns=["Survived"], inplace=True)
```

We recommend using Pipeline s in sklearn

- all transformations are combined into a single Pipeline
- the *same* Pipeline is use to transform
 - training examples
 - test examples

This is not necessary, just good practice.

Our first model will use only *raw* features

- Pclass
- Sex
- Age
- SibSp: passenger's number of "same-level" relatives (Sibling, Spouse)
- Parch: passenger's number of "different-level" relatives (Parent, Child)

The numeric pipeline

We need separate transformations for Numeric and Non-Numeric features

- e.g., missing data imputation differs

The `ColumnTransformer` in `sklearn` allows us to

- create Pipelines
- that are restricted to sets of features

The Pipeline for numeric features

- Selects those attributes identified as numeric (variable num_features)
- Performs Cleaning:
 - Missing data imputation
 - Replacing missing value with median value of the feature

```
In [22]: num_features = ["Age", "SibSp", "Parch", "Fare", "Pclass"]
num_transformers= Pipeline(steps=[ ('imputer', SimpleImputer(strategy='median')) ] )
num_pipeline = ColumnTransformer( transformers=[ ("numeric", num_transformers, num_features) ] )
```

The ColumnTransformer

- Filters the features to those in num_features
- Applies the numeric Pipeline
 - The single transformer SimpleImputer for missing data imputation

Let's see what the numeric pipeline produces.

Note: the result is a NumPy array

- That is the type produced by the final transformer (`SimpleImputer`)

```
In [23]: num_pipeline.fit_transform(train_data)[:num_head]
```

```
Out[23]: array([[22.    ,  1.    ,  0.    ,  7.25   ,  3.    ],
                [38.    ,  1.    ,  0.    , 71.2833,  1.    ],
                [26.    ,  0.    ,  0.    ,  7.925  ,  3.    ],
                [35.    ,  1.    ,  0.    , 53.1    ,  1.    ],
                [35.    ,  0.    ,  0.    ,  8.05   ,  3.    ]])
```

The non-numeric pipeline

The Pipeline for non-numeric features

- Selects those attributes identified as Categorical (variable `cat_features`)
- Performs Cleaning
 - Missing data imputation
 - Replacing missing value with the value of the feature that occurs most often
- Performs Numericalization on feature Sex

One reason for separate numeric/non-numeric Pipelines is that the transformers are not identical

WARNING: I'm doing a little cheating in this code by ignoring all categorical features other than Sex

```
In [24]: cat_features = ["Sex" ]
cat_transformers= Pipeline(steps=[ ('imputer', SimpleImputer(strategy="most_frequent")),
                                   ('sex_encoder', OrdinalEncoder())
                                   ] )
cat_pipeline = ColumnTransformer( transformers=[ ("categorical", cat_transformers, cat_features) ] )
```

Again, the `ColumnTransformer`

- Filters features to those in `cat_features`
- Applies the non-numeric pipeline
 - Transformer for missing data imputation: `SimpleImputer`
 - with a different strategy than the one for numeric features
 - Transformer for Numericalization: `OrdinalEncoder`

One reason for separate numeric and non-numeric pipelines is that they implement different transformations.

Let's see what the non-numeric pipeline produces.


```
In [25]: cat_pipeline.fit_transform(train_data)[:num_head]  
train_data["Sex"].head(num_head)
```

```
Out[25]: array([[1.],  
                [0.],  
                [0.],  
                [0.],  
                [1.]])
```

```
Out[25]: 0      male  
        1      female  
        2      female  
        3      female  
        4      male  
        Name: Sex, dtype: object
```

Combining the numeric and categorical pipelines: **ColumnTransformer**

We have been using `ColumnTransformer` to filter the features before applying each pipeline

We will also use it as a simple way to combine the numeric and non-numeric pipelines.

ColumnTransformer alert:

- Depending on what version of `sklearn` you are using, this may still be considered an "experimental" feature
- If that is the case: you might want to explore FeatureUnion: the "official" way of combining pipelines
 - You must manually select the features of each type
 - Apply the corresponding Pipelines
 - "Glue together" (horizontally) the results of the Pipelines

```
In [26]: preprocess_pipeline = ColumnTransformer(  
    transformers=[ ("numeric", num_transformers, num_features),  
                  ("categorical", cat_transformers, cat_features)  
                ]  
    )
```

Let's look at the result of applying the combined `preprocess_pipeline`

```
In [27]: X_train = preprocess_pipeline.fit_transform(train_data)

X_train.shape
X_train[:num_head]

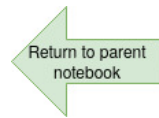
# X_train is now an ndarray, so really can't discern columns, but are in same order as in Feature Union
# so first the num_features, then cat_features
# Can verify this by looking at train_data
all_features = num_features.copy()
all_features.extend(cat_features)
train_data.loc[:, all_features ].head()
```

Out[27]: (891, 6)

```
Out[27]: array([[22.    ,  1.    ,  0.    ,  7.25 ,  3.    ,  1.    ],
               [38.    ,  1.    ,  0.    , 71.2833,  1.    ,  0.    ],
               [26.    ,  0.    ,  0.    ,  7.925 ,  3.    ,  0.    ],
               [35.    ,  1.    ,  0.    , 53.1    ,  1.    ,  0.    ],
               [35.    ,  0.    ,  0.    ,  8.05  ,  3.    ,  1.    ]])
```

Out[27]:

	Age	SibSp	Parch	Fare	Pclass	Sex
0	22.0	1	0	7.2500	3	male
1	38.0	1	0	71.2833	1	female
2	26.0	0	0	7.9250	3	female
3	35.0	1	0	53.1000	1	female
4	35.0	0	0	8.0500	3	male



Recipe Step D: Train a model

OK, we have identified features and now want to predict Survived.

How do we do it ?

Recipe D.1: Select a model

We currently know of two models for the Classification task

- K Nearest Neighbors
- Logistic Regression

We will use Logistic Regression.

To review:

$$s = \Theta^T \mathbf{x}$$

$$\hat{p} = \sigma(s)$$

$$\hat{\mathbf{y}}^{(i)} = \begin{cases} \text{Negative} & \text{if } \hat{p}^{(i)} < 0.5 \\ \text{Positive} & \text{if } \hat{p}^{(i)} \geq 0.5 \end{cases}$$

We will re-visit the choice of threshold 0.5 at a later time.

Varying the threshold is an attempt at balancing the impact of making two different types of incorrect prediction

- False Positive: predicting Positive when the true target is Negative
- False Negative: predicting Negative when the true target is Positive

Depending on your problem, the impact of being incorrect is not the same for both cases.

Step D.2: Fit

The prior steps in the Recipe have led us to this point

- We removed examples for which the target/label `Survived` was not defined
- We dealt with missing values for features
- We transformed the data into numeric form
- We made sure the target was separated from the features

We're ready to fit our chosen model: Logistic Regression.

Logistic Regression classifier

Let's instantiate a `LogisticRegression` object, `sklearn`'s implementation of Logistic Regression.

```
In [28]: # New version of sklearn will give a warning if you don't specify a solver (b/c  
the default solver -- liblinear -- will be replaced in future)  
logistic_clf = linear_model.LogisticRegression(solver='liblinear')
```

More models, more fun ! Same price !

Although we have selected Logistic Regression as our model, there are other models for the Classification task.

It turns out to be just as easy to run *multiple* models as it is one !

So, for pedantic purposes, we will fit *many* models

- To show you how easy it is
- We will not delve deeply into the other models, at least for now

SVM Classifier

We instantiate an object that implements a Support Vector Classifier (SVC):


```
In [29]: from sklearn.svm import SVC  
svm_clf = SVC(gamma="auto")
```

Random Forest Classifier

We instantiate an object that implements a Random Forest Classifier.

```
In [30]: from sklearn.ensemble import RandomForestClassifier  
         forest_clf = RandomForestClassifier(n_estimators=100, random_state=42)
```

Fit the models

We will train all the models at once.

This demonstrates the power of a consistent API:

- Training several models is no more difficult than training one.

Cheating in Cross Validation

There is a very

- subtle
- but easy to fall into

way to "cheat" when using cross-validation (especially in Pipeline s)

The most obvious way to write the code to fit the models is:

```

In [31]: for name, clf in { "Logistic": logistic_clf,
                           "SVM": svm_clf,
                           "Random Forest": forest_clf
                           }.items():

    # Transform the data
    X_train = preprocess_pipeline.fit_transform(train_data)
    _ = clf.fit(X_train, y_train)

    # Cross validation
    scores = cross_val_score(clf, X_train, y_train, cv=10)
    print("Model: {m:s} avg cross val score={s:3.2f}\n".format(m=name, s=scores.
mean()))

    # Fit the model using all training data.
    # cross_val_score does not run the fit on the complete data.
    # It runs a number of fits, each fit being on the data with one fold held o
ut for validation.
    _ = clf.fit(X_train, y_train)

```

Model: Logistic avg cross val score=0.80

Model: SVM avg cross val score=0.71

Model: Random Forest avg cross val score=0.82

This innocuous looking piece of good

- allows information to "leak" from out-of-sample validation examples
- to training

It is "cheating" because information from the "future" (out-of-sample examples) can influence the fit

- this information would not be available at test/prediction time

Can you spot it ?

We will cover this in the module [Using Pipelines to avoid cheating in cross validation](#)
([Prepare data Overview.ipynb#Using-pipelines-to-avoid-cheating-in-cross-validation](#))

Fortunately, `sklearn` makes it easy to perform Cross Validation without peeking into the future.

(Other Machine Learning toolkits may not make it as easy).

- Create a Pipeline with a classifier as the final element
- Use that Pipeline as the "model" for Cross Validation

Here is the proper code:


```

In [32]: for name, clf in { "Logistic": logistic_clf,
                           "SVM": svm_clf,
                           "Random Forest": forest_clf
                           }.items():

    # Combine the transformation pipeline with a final classification step
    model_pipeline = Pipeline(steps=[ ("transform", preprocess_pipeline),
                                      ("classify", clf)
                                      ])

    # Cross validation on the combined pipeline
    scores = cross_val_score(model_pipeline, train_data, y_train, cv=10)
    print("Model: {m:s} avg cross val score={s:3.2f}\n".format(m=name, s=scores.
mean()))

    # Fit the model using all training data.
    # cross_val_score does not run the fit on the complete data.
    # It runs a number of fits, each fit being on the data with one fold held o
ut for validation.
    _ = model_pipeline.fit(train_data, y_train)

```

Model: Logistic avg cross val score=0.80

Model: SVM avg cross val score=0.71

Model: Random Forest avg cross val score=0.82

We observe that

- the Cross Val scores (our proxy for Performance Metric)
- were not heavily affected by the cheating

But, there is no such guarantee.

There is an additional advantage to including the model as the final step of the pipeline

- It makes it easy to consistently apply the same transformation to a test example as to a training example
 - Test examples require Missing data imputation, Numericalization, etc. too
- Prediction is as simple as
 - `model_pipeline.predict(X_test)`

Nested Pipelines

Notice the use of nested Pipelines:

- `model_pipeline` contains Pipeline `preprocess_pipeline` as an element
- `preprocess_pipeline` contains Pipelines `num_transformers` and `cat_transformers` as elements



Recipe D.4: Error analysis

Cross validation gives you a metric, *at an aggregate level*, of how well the model performed out of sample.

You will gain deeper insight into the Classification task by analyzing *individual* predictions.

Go through each out of sample example and determine the predicted class.

- Is there some class for which the predictions are much less successful than others ?
- Is there some identifiable commonality among examples on which mis-prediction occurred ?

This is a signal to improve your model

- Perhaps by adding features that aid prediction for the mis-classified examples or target class

There is some standard terminology for analyzing classification predictions.

For binary classification, to be concrete, let's call the two classes Positive (P) and Negative (N).

Let's create a table

- The row labels correspond to the predicted class
- The column labels correspond to the target (actual) class

In pictures:

	P	N
P	TP	FP
N	FN	TN

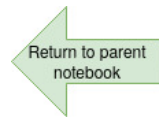
- The entry labeled True Positive (TP) denotes the number of examples
 - that were correctly predicted as Positive
- The entry labeled as False Positive (FP) denotes the number of examples
 - that were incorrectly predicted as Positive
- The entry labeled True Negative (TN) denotes the number of examples
 - that were correctly predicted as Negative
- The entry labeled False Negative denotes the number of examples
 - that were incorrectly predicted as Negative

So

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{TN} + \text{FN}}$$

Examples that are either False Positive (FP) or False Negative (FN) are mis-predictions.

Error Analysis focuses on the examples of either type.



Titanic revisited: OHE features

(Pre-requisite for this section: Review the notebook [Categorical Variables \(Categorical Variables.ipynb\)](#))

Is `Pclass` really a numeric feature just because it was presented to us as a value in $\{1, 2, 3\}$?

We argue that it should be treated as a *categorical* feature

- Any integer ordering we could impose would also impose a magnitude that could affect the math
 - $\{1, 2, 3\}$ versus $\{10, 20, 30\}$

The proper way to deal with categorical variables is with One Hot Encoding.

Let's treat `Pclass` as categorical and refit our model.

- Move `Pclass` from `num_features` to `cat_features`

```
In [33]: print("First model\n\tcategorical features are: {c:s}\n\tnumeric features are:
{n:s}".format(
    c=", ".join(cat_features), n=", ".join(num_features))
)
```

First model

categorical features are: Sex

numeric features are: Age, SibSp, Parch, Fare, Pclass

```
In [34]: num_features = ["Age", "SibSp", "Parch", "Fare" ]
num_transformers= Pipeline(steps=[ ('imputer', SimpleImputer(strategy='median')) ] )
num_pipeline = ColumnTransformer( transformers=[ ("numeric", num_transformers, num_features) ] )

cat_features = ["Sex", "Pclass" ]
cat_transformers= Pipeline(steps=[ ('imputer', SimpleImputer(strategy="most_frequent")),
                                   ('cat_encoder', OneHotEncoder(sparse=False))
                                   ] )
cat_pipeline = ColumnTransformer( transformers=[ ("categorical", cat_transformers, cat_features) ] )

preprocess_pipeline = ColumnTransformer(
    transformers=[ ("numeric", num_transformers, num_features),
                  ("categorical", cat_transformers, cat_features)
                  ]
)
```



```
In [35]: print("Second model\n\tcategorical features are: {c:s}\n\tnumeric features are:
{n:s}".format(
    c=", ".join(cat_features), n=", ".join(num_features))
)
```

Second model

categorical features are: Sex, Pclass

numeric features are: Age, SibSp, Parch, Fare

The `cat_pipeline` now creates 5 indicators whereas the old one created only 1

- The `Sex` attribute is now 2 indicators ("Is Female", "Is Male") rather than the integer 0/1
- The `Pclass` attribute is now 3 indicators ("Is class 1", "Is class 2", "Is class 3")

Let's look at the first couple of training examples after OHE has been applied.

We will show the encoding along with the corresponding class labels.

```
In [36]: # Run the categorial pipeline
cat_ndarray = cat_pipeline.fit_transform(train_data)

# Let's examine the first first rows of the ndarray, and relate them to the same
rows in the DataFrame,
# -- n.b., with the DataFrame, we can see the column names
num_to_see = 7

print(cat_features[0] + ":\n")
cat_ndarray[:num_to_see, :2]

train_data.loc[:, [ cat_features[0] ] ].head(num_to_see)
```

Sex:

```
Out[36]: array([[0., 1.],
               [1., 0.],
               [1., 0.],
               [1., 0.],
               [0., 1.],
               [0., 1.],
               [0., 1.]])
```

Out[36]:

	Sex
0	male
1	female
2	female
3	female
4	male
5	male
6	male

You should see that

- the Male examples (e.g., rows 0, 4) are encoded as vector $[0, 1]$
- the Female examples (e.g., rows 1, 2) are encoded as vector $[1, 0]$

Let's look at the encoding for `Pclass` :

```
In [37]: print(cat_features[1] + ":\n")
cat_ndarray[:num_to_see, -3:]
train_data.loc[:, [cat_features[1]]].head(num_to_see)
```

Pclass:

```
Out[37]: array([[0., 0., 1.],
                [1., 0., 0.],
                [0., 0., 1.],
                [1., 0., 0.],
                [0., 0., 1.],
                [0., 0., 1.],
                [1., 0., 0.]])
```

Out[37]:

	Pclass
0	3
1	1
2	3
3	1
4	3
5	3
6	1

You should see that

- Class 3 (e.g., rows 0, 2) are encoded as $[0, 0, 1]$

Notice that \mathbf{X} now has many more feature columns.

```
In [38]: X_train = preprocess_pipeline.fit_transform(train_data)

# Note: All the columns in untransformed train_data are NOT in X_train, especial
ly the target Survived !
train_data.columns
X_train.shape
X_train
```

```
Out[38]: Index(['PassengerId', 'Pclass', 'Name', 'Sex', 'Age', 'SibSp', 'Parch',
               'Ticket', 'Fare', 'Cabin', 'Embarked'],
              dtype='object')
```

```
Out[38]: (891, 9)
```

```
Out[38]: array([[22., 1., 0., ..., 0., 0., 1.],
               [38., 1., 0., ..., 1., 0., 0.],
               [26., 0., 0., ..., 0., 0., 1.],
               ...,
               [28., 1., 2., ..., 0., 0., 1.],
               [26., 0., 0., ..., 1., 0., 0.],
               [32., 0., 0., ..., 0., 0., 1.]])
```

What effect did the change in treatment of `Pclass` from numeric to OHE have?


```

In [39]: for name, clf in { "Logistic": logistic_clf,
                           "SVM": svm_clf,
                           "Random Forest": forest_clf
                           }.items():

    model_pipeline = Pipeline(steps=[ ("transform", preprocess_pipeline),
                                      ("classify", clf)
                                      ])

    # Cross validation
    scores = cross_val_score(model_pipeline, train_data, y_train, cv=10)
    print("Model: {m:s} avg cross val score={s:3.2f}\n".format(m=name, s=scores.
mean()))

    # Fit the model using all training data.
    # cross_val_score does not run the fit on the complete data.
    # It runs a number of fits, each fit being on the data with one fold held o
ut for validation.
    _ = model_pipeline.fit(train_data, y_train)

```

Model: Logistic avg cross val score=0.79

Model: SVM avg cross val score=0.73

Model: Random Forest avg cross val score=0.81

Not too different across models (hard to even know whether the difference is statistically significant).

- Some models (e.g., Random Forest) are *not sensitive* to encoding of Categorical
- Logistic Regression is potentially sensitive, but it depends on the data
 - Would encoding `Pclass` with integers $\{1000, 2000, 3000\}$ have affected it ?

In [40]: `print("Done")`

Done

