

Computational Physics

Topic 01 : Exploratory Data Analysis

Lecture 01 : Top X pandas commands

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Outline

- Reading data formats
- Computing descriptive statistics
- Processing data by filtering and grouping

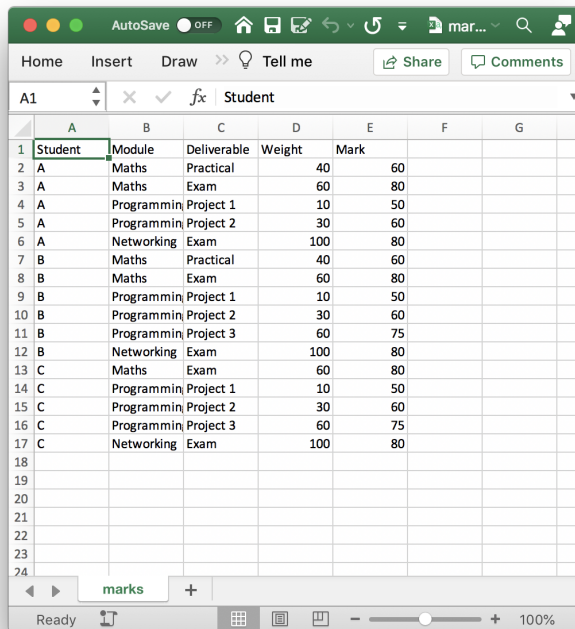
Part I

Introduction

Minimal Dataset

To better understand the various pandas operations we are going to use a tiny* dataset based on (fictional) student results. (marks.csv)

➤ In Excel ...



	A	B	C	D	E	F	G
	Student	Module	Deliverable	Weight	Mark		
1	A	Maths	Practical	40	60		
2	A	Maths	Exam	60	80		
3	A	Programming	Project 1	10	50		
4	A	Programming	Project 2	30	60		
5	A	Networking	Exam	100	80		
6	B	Maths	Practical	40	60		
7	B	Maths	Exam	60	80		
8	B	Programming	Project 1	10	50		
9	B	Programming	Project 2	30	60		
10	B	Programming	Project 3	60	75		
11	B	Networking	Exam	100	80		
12	C	Maths	Exam	60	80		
13	C	Programming	Project 1	10	50		
14	C	Programming	Project 2	30	60		
15	C	Programming	Project 3	60	75		
16	C	Networking	Exam	100	80		

➤ ...or database schema ...

Students

Name ... Other fields

Modules

Name ... Other fields

Deliverables

Name Weight ... Other fields

Grades

Student Module Deliverable Mark

➤ ...like to know ...

- Student performance — weighted mark on each module, missing deliverables etc.
- Module performance — number of attempts and average mark.
- Deliverable performance — number of attempts and average mark, predictor of overall module grade, etc.

*Dataset is small enough that you can verify operation results by hand.

Termonology

```
df.head(1000)
```

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

- A **DataFrame** is a table of data values.
 - `df = pd.read_csv("marks.csv")`
- A **Series** is a list of data values — typically columns in a dataframe. We can access an individual column using
 - `df.Deliverable` (dot notation)
 - `df["Deliverable"]` (dict notation)
 - `df.iloc[:,2]` (numpy, index notation)
- The **index** is a special column whose values can be used to access rows — rather using row number.
 - The default index is equal to the row number.

Part II

Input and Output

Reading data from a CSV file

Pandas supports a huge variety of input/output formats so best approach is to focus on what is needed to process the given data and verify input. Our marks dataset is in CSV format so we start with

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
plt.style.use('seaborn-darkgrid')
```

Always verify input by checking dataset dimensions and looking at some rows,

and input using

```
df = pd.read_csv('marks.csv', sep=',')
print(df.shape)
df.head()
```

```
(16, 5)
[2]:
```

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80

Datatypes

Pandas data types:

- **object** — used for text or mixed numeric and non-numeric values.
- **int64** — integer values,
 - Does not support missing values, so an int column containing at least one missing value will automatically be converted to float.
- **float64** — floating point numbers.
- **bool** — True/False values
- **datetime64** — date and time values
- **category** — Finite (typically small) list of text values

df.dtypes

Student	object
Module	object
Deliverable	object
Weight	int64
Mark	int64
dtype:	object

Regularly verifying datatypes is vital[†] :

- Operations differ based on datatype, eg, '+' concatenate strings but adds numerical values.
- datatype can change based on results, eg, int converts to float due to missing values.

[†]Google "Detecting Excel's gene auto-conversions."

Datatypes — Converting

We will deal with modifying and creating new columns later, but while we are on datatypes, we will look at changing datatypes ...

➤ Using the Series function `astype`

```
df["Weight"] = df["Weight"].astype('float')  
df["Weight"].dtype
```

```
dtype('float64')
```

- New datatype is required argument — `'int'`, `'float'`, `'str'`, `'object'`, `'category'`, etc.
- Simple, but fragile if data conversion is possible.

➤ or using pandas function `to_numeric`

```
df["Weight"] = pd.to_numeric(df["Weight"])  
df["Weight"].dtype
```

```
dtype('float64')
```

- More powerful, can specify what to do in cases where the conversion fails etc
- Have functions `to_numeric`, `to_datetime`, and `to_timedelta`.

Missing Values

Identifying and dealing with missing values is critical step in data preparation. What should you do? delete rows containing missing values? or impute then?

Here we will just look at identifying missing values.

`df.isna()`

	Student	Module	Deliverable	Weight	Mark
0	False	False	False	False	False
1	False	False	False	False	False
2	False	False	False	False	False
3	False	False	False	False	False
4	False	False	False	False	False
5	False	False	False	False	False
6	False	False	False	False	False
7	False	False	False	False	False
8	False	False	False	False	False
9	False	False	False	False	False
10	False	False	False	False	False
11	False	False	False	False	False
12	False	False	False	False	False
13	False	False	False	False	False
14	False	False	False	False	False
15	False	False	False	False	False

`df.isna().sum()`

Student	0
Module	0
Deliverable	0
Weight	0
Mark	0
dtype: int64	

`df.isna().sum().sum()`

0

- Use dataframe function `fillna` to replace missing values.
- Recall False and True map to 0 and 1 respectively.

Output

Saving dataframe to CSV is straightforward (I rarely include the (default) index when saving datasets).

```
df.to_csv('marks_2.csv', index=False)
```

- CSV has become the default file format in Data Mining application especially for 'informal' datasets.
- Other formats are better for speed and resulting file size and for saving meta data not supported by CSV (such as columns datatypes, category information, etc).

Part III

Filtering

Selecting individual rows/columns results in a series

Columns can be accessed using **dot**, **dict** and **numpy index** notation.

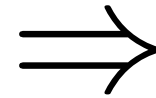
```
df.head(1000)
```

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

```
df.iloc[:,0]
```

```
df['Student']
```

```
df.Student
```



```
Student      A
Module      Maths
Deliverable  Practical
Weight      40
Mark        60
Name: 0, dtype: object
```

```
Student
A
Module
Maths
Deliverable
Practical
Weight
40
Mark
60
Name: 0, dtype: object
```

```
0    A
1    A
2    A
3    A
4    A
5    B
6    B
7    B
8    B
9    B
10   B
11   C
12   C
13   C
14   C
15   C
Name: Student, dtype: object
```

← Access row using numpy index

Head and Tail

Commands `head` and `tail` return the first and last n rows (default $n = 5$) of a dataframe/series.

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.head()`

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80

`df.tail()`

	Student	Module	Deliverable	Weight	Mark
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.head(1)`

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60

`df.tail(1)`

	Student	Module	Deliverable	Weight	Mark
15	C	Networking	Lab Work	100	80

Query — on a single-column criteria

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.query("Student=='A'")`

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80

`df.query("Mark>=70")`

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
1	A	Maths	Exam	60	80
4	A	Networking	Lab Work	100	80
6	B	Maths	Exam	60	80
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

Query — on multiple columns (using python logical operators)

```
df.query("Mark<70 and Module=='Maths'")
```

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
5	B	Maths	Practical	40	60

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60

```
df.query("Mark<70 or Module=='Maths'")
```

Query — on multiple columns (using pandas logical operators)

```
df.query("(Mark<70) & (Module=='Maths'))"
```

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
5	B	Maths	Practical	40	60

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60

```
df.query("(Mark<70) | (Module=='Maths'))"
```


Filtering using loc

Note the square (not round) brackets — think of loc as array indexing not a function call.

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.loc[ROW_SELECTION, COL_SELECTION]`

where row and columns selection can be

- Single values: row number or column name
- An integer list for rows or list of column names
- A boolean list for logical indexing of rows
- A colon to indicate every row/column

`df.loc[df.Module=="Maths", ["Student", "Mark"]]`

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

Student Mark		
0	A	60
1	A	80
5	B	60
6	B	80
11	C	80

More complicated example

I prefer to define row selection criteria, and the column list and order, separately to the `loc` statement.

Student Module Deliverable Weight Mark					
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

Module Student Mark		
2	Programming A	50
3	Programming A	60
7	Programming B	50
8	Programming B	60
12	Programming C	50
13	Programming C	60

```
criteria = ((df.Mark<50) & (df.Module=='Maths')) | ((df.Mark<70) & (df.Module!='Maths'))
columns = ['Module', 'Student', 'Mark']

df.loc[criteria, columns]
```

Sampling

The `sample` function selects a random subset of the dataframe rows.

- Either specify the number of rows (as an integer) or fraction of the data (as a float).
- Can set the seed using `random_state` parameter for reproducible samples.

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.sample(n=3)`

	Student	Module	Deliverable	Weight	Mark
5	B	Maths	Practical	40	60
2	A	Programming	Project 1	10	50
9	B	Programming	Project 3	60	75

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
15	C	Networking	Lab Work	100	80
6	B	Maths	Exam	60	80

	Student	Module	Deliverable	Weight	Mark
10	B	Networking	Project	100	80
1	A	Maths	Exam	60	80
14	C	Programming	Project 3	60	75

Part IV

Sorting

Sorting

A pandas dataframe has two sorting operations:

- `sort_index()` orders rows based on current index.
- `sort_values(COLUMNS)` orders rows based on single column or list of columns.

Two important modifications:

- By default, the sort order is in ascending. Set parameter `ascending=False` to reverse this.
- By default, a new dataframe is returned with desired sort order, set parameter `inplace=True` to update current dataframe instead.

	Student	Module	Deliverable	Weight	Mark
0	A	Maths	Practical	40	60
1	A	Maths	Exam	60	80
2	A	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
4	A	Networking	Lab Work	100	80
5	B	Maths	Practical	40	60
6	B	Maths	Exam	60	80
7	B	Programming	Project 1	10	50
8	B	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
10	B	Networking	Project	100	80
11	C	Maths	Exam	60	80
12	C	Programming	Project 1	10	50
13	C	Programming	Project 2	30	60
14	C	Programming	Project 3	60	75
15	C	Networking	Lab Work	100	80

`df.sort_values(['Module', 'Deliverable'], inplace=True)`

	Student	Module	Deliverable	Weight	Mark
1	A	Maths	Exam	60	80
6	B	Maths	Exam	60	80
11	C	Maths	Exam	60	80
3	A	Programming	Project 2	30	60
8	B	Programming	Project 2	30	60
13	C	Programming	Project 2	30	60
7	B	Programming	Project 1	10	50
12	C	Programming	Project 1	10	50
2	A	Programming	Project 1	10	50
10	B	Networking	Project	100	80
4	A	Networking	Lab Work	100	80
15	C	Networking	Lab Work	100	80
14	C	Programming	Project 3	60	75
9	B	Programming	Project 3	60	75

Part V

Defining New Columns

Defining new columns — row-wise operation

We want to compute the weighted mark for each module for each student. Two steps:

- Create column, `W_Mark`, to store the weighted mark for each deliverable. This is a row by row calculation — only need data in current row to compute the result.
- Create column, `M_Mark`, to store the module mark for each student. This is a group calculation — need all rows for that student and module to compute the result.

	Student	Module	Deliverable	Weight	Mark
1	A	Maths	Exam	60	80
6	B	Maths	Exam	60	80
11	C	Maths	Exam	60	80
0	A	Maths	Practical	40	60
5	B	Maths	Practical	40	60
4	A	Networking	Lab Work	100	
15	C	Networking	Lab Work	100	
10	B	Networking	Project	100	80
2	A	Programming	Project 1	10	50
7	B	Programming	Project 1	10	50
12	C	Programming	Project 1	10	50
3	A	Programming	Project 2	30	60
8	B	Programming	Project 2	30	60
13	C	Programming	Project 2	30	60
9	B	Programming	Project 3	60	75
14	C	Programming	Project 3	60	75

```
df['W_Mark'] = df.Weight * df.Mark // 100
```

Need to use dict notation (not dot notation) when defining a new column.

	Student	Module	Deliverable	Weight	Mark	W_Mark
1	A	Maths	Exam	60	80	48
6	B	Maths	Exam	60	80	48
11	C	Maths	Exam	60	80	48
0	A	Maths	Practical	40	60	24
5	B	Maths	Practical	40	60	24
4	A	Networking	Lab Work	100	80	80
15	C	Networking	Lab Work	100	80	80
10	B	Networking	Project	100	80	80
2	A	Programming	Project 1	10	50	5
7	B	Programming	Project 1	10	50	5
12	C	Programming	Project 1	10	50	5
3	A	Programming	Project 2	30	60	18
8	B	Programming	Project 2	30	60	18
13	C	Programming	Project 2	30	60	18
9	B	Programming	Project 3	60	75	45
14	C	Programming	Project 3	60	75	45

Defining new columns — group aggregate result

I

- Create column, `W_Mark`, to store the weighted mark for each deliverable. This is a row by row calculation — only need data in current row to compute the result.
- Create column, `M_Mark`, to store the module mark for each student. This is a group calculation — need all rows for that student and module to compute the result.

columns to group on output cols

```
df.groupby(['Student', 'Module'])['W_Mark'].sum()
```

aggregate

	Student	Module	Deliverable	Weight	Mark	W_Mark
1	A	Maths	Exam	60	80	48
6	B	Maths	Exam	60	80	48
11	C	Maths	Exam	60	80	48
0	A	Maths	Practical	40	60	24
5	B	Maths	Practical	40	60	24
4	A	Networking	Lab Work	100	80	80
15	C	Networking	Lab Work	100	80	80
10	B	Networking	Project	100	80	80
2	A	Programming	Project 1	10	50	5
7	B	Programming	Project 1	10	50	5
12	C	Programming	Project 1	10	50	5
3	A	Programming	Project 2	30	60	18
8	B	Programming	Project 2	30	60	18
13	C	Programming	Project 2	30	60	18
9	B	Programming	Project 3	60	75	45
14	C	Programming	Project 3	60	75	45

Result has multi-level index, need to use `reset_index` to revert to default index

		W_Mark
Student Module		
A	Maths	72
	Networking	80
	Programming	23
B	Maths	72
	Networking	80
	Programming	68
C	Maths	48
	Networking	80
	Programming	68

Defining new columns — group aggregate result

II

columns to group on

output cols

```
df.groupby(['Student', 'Module'])[['W_Mark']].sum().reset_index()
```

aggregate

	Student	Module	Deliverable	Weight	Mark	W_Mark
1	A	Maths	Exam	60	80	48
6	B	Maths	Exam	60	80	48
11	C	Maths	Exam	60	80	48
0	A	Maths	Practical	40	60	24
5	B	Maths	Practical	40	60	24
4	A	Networking	Lab Work	100	80	80
15	C	Networking	Lab Work	100	80	80
10	B	Networking	Project	100	80	80
2	A	Programming	Project 1	10	50	5
7	B	Programming	Project 1	10	50	5
12	C	Programming	Project 1	10	50	5
3	A	Programming	Project 2	30	60	18
8	B	Programming	Project 2	30	60	18
13	C	Programming	Project 2	30	60	18
9	B	Programming	Project 3	60	75	45
14	C	Programming	Project 3	60	75	45

This is the required result and we can save this to a new dataframe. However, we often want to put this into our original dataframe as an extra column. Only problem we have is different rows so can't just assign to a new column — need to use transform function.

	Student	Module	W_Mark
0	A	Maths	72
1	A	Networking	80
2	A	Programming	23
3	B	Maths	72
4	B	Networking	80
5	B	Programming	68
6	C	Maths	48
7	C	Networking	80
8	C	Programming	68

Defining new columns — group aggregate result

III

columns to group on

output cols

```
df['M_Mark'] = df.groupby(['Student', 'Module'])['W_Mark'].transform(sum)
```

aggregate

	Student	Module	Deliverable	Weight	Mark	W_Mark
1	A	Maths	Exam	60	80	48
6	B	Maths	Exam	60	80	48
11	C	Maths	Exam	60	80	48
0	A	Maths	Practical	40	60	24
5	B	Maths	Practical	40	60	24
4	A	Networking	Lab Work	100	80	80
15	C	Networking	Lab Work	100	80	80
10	B	Networking	Project	100	80	80
2	A	Programming	Project 1	10	50	5
7	B	Programming	Project 1	10	50	5
12	C	Programming	Project 1	10	50	5
3	A	Programming	Project 2	30	60	18
8	B	Programming	Project 2	30	60	18
13	C	Programming	Project 2	30	60	18
9	B	Programming	Project 3	60	75	45
14	C	Programming	Project 3	60	75	45

	Student	Module	W_Mark
0	A	Maths	72
1	A	Networking	80
2	A	Programming	23
3	B	Maths	72
4	B	Networking	80
5	B	Programming	68
6	C	Maths	48
7	C	Networking	80
8	C	Programming	68

	Student	Module	Deliverable	Weight	Mark	W_Mark	M_Mark
1	A	Maths	Exam	60	80	48	72
6	B	Maths	Exam	60	80	48	72
11	C	Maths	Exam	60	80	48	48
0	A	Maths	Practical	40	60	24	72
5	B	Maths	Practical	40	60	24	72
4	A	Networking	Lab Work	100	80	80	80
15	C	Networking	Lab Work	100	80	80	80
10	B	Networking	Project	100	80	80	80
2	A	Programming	Project 1	10	50	5	23
7	B	Programming	Project 1	10	50	5	68
12	C	Programming	Project 1	10	50	5	68
3	A	Programming	Project 2	30	60	18	23
8	B	Programming	Project 2	30	60	18	68
13	C	Programming	Project 2	30	60	18	68
9	B	Programming	Project 3	60	75	45	68
14	C	Programming	Project 3	60	75	45	68

The transform broadcasts the result for each group over every row in that group.

Part VI

Review Exercises

Review Exercises

Generate the following reports:

- ① Number of deliverables by each student.
- ② List and rank deliverables by grade.
- ③ Top 2 deliverables (by grade).
- ④ Top 2 module (by average grade).
- ⑤ Top 2 modules (by minimum grade).
- ⑥ Modules (by minimum grade).

(value_counts, or groupby and count)

(sort_values, rank)

Harder exercises (new functions)

- ① List which students missed which deliverables.

(pivot, melt)