dm22s1

Topic 04 : Exploratory Data Analysis

Part 01 : Exploratory Data Analysis

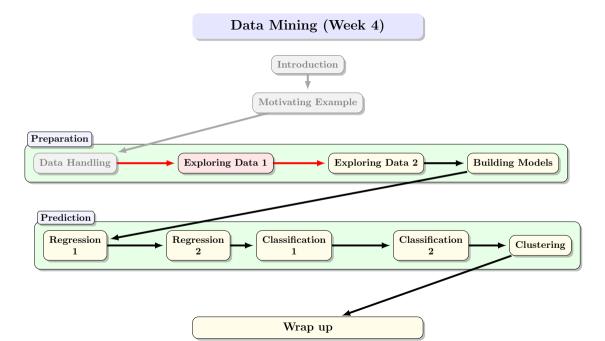
Dr Bernard Butler

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Autumn Semester, 2022

Outline

- EDA Process
- Datasets = Tips, Titanic and Algae Blooms



Exploratory Data Analysis — Summary

- 1. Introduction
- 1.1 Example Datasets
- 1.2 Before we start ...

- First Pass Load Dataset and Initial Clear
- 2.1 dtypes
- 2.2 Missing Values

Acknowledgment

A big thanks to Dr Kieran Murphy, who provided many of the slides for today's lecture.



Introduction

Exploratory Data Analysis (EDA)

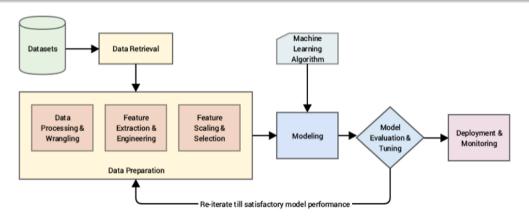
Aim

To understand and summarise a dataset to ensure that the features which are feed to machine learning algorithms are refined and that the results are valid and can correctly interpreted.

Benefits

- Develop insight about the dataset and understanding of the underlying structure.
- Extract important parameters and relationships that hold between them.
- Test underlying assumptions.
- Identify issues that affect model performance outliers, missing values.

Data Pipeline



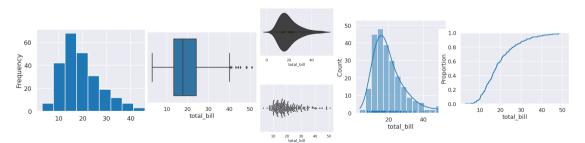
- Data preparation is the core of the data mining pipeline (typical estimates >50% of the time/effort).
- EDA is the data processing and wrangling.
- EDA informs the feature extraction, engineering, transformation and selection.

The Bad News — 'The curse of choice'

What questions to ask?

Dataset global questions: How many features? How many observations? What is the data type of each feature? Any null values? ... Feature specific questions: What is the distribution of each variable? Do there appear to be outliers? What features are related? ... Missing value questions: Are null value a result of the way data was recorded? Can we drop the rows with null values without it significantly affecting your analysis? Can we justify filling in the missing values with the mean or median for that variable? If the data is time-series data, can we fill the missing values with interpolation? Are there so many missing values for a variable that we should drop that variable from the dataset? ... Outlier questions: Why are outliers present? Do the outliers represent real observations (i.e. not errors)? Should we exclude these observations? If not, should we winsorise the values? ... Correlations/Relationships questions: Which variables are most correlated with your target variable? (If applicable) Is there multicollinearity? (Two features that have a correlation > 0.8) How will this affect your model? Do you have variables that represent the same information? Can one be dropped? ...

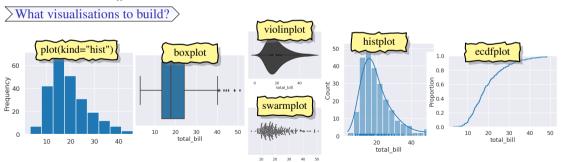
What visualisations to build?



The Bad News — 'The curse of choice'

What questions to ask?

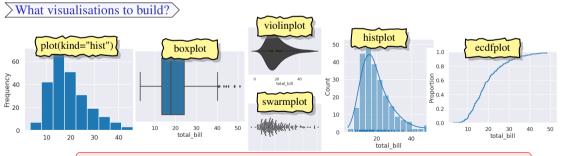
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What questions to ask?

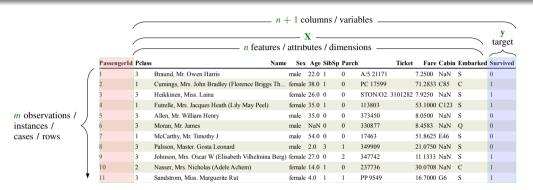
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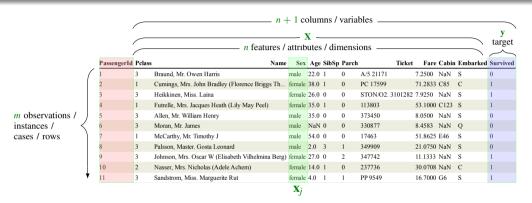
Have a plan, be selective, understand strengths/weaknesses of metrics/visualisations

PassengerId	Pclass	Nan	ne Se	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked	Survived
1	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S	0
2	1	Cumings, Mrs. John Bradley (Florence Briggs Th.	female	38.0	1	0	PC 17599	71.2833	C85	C	1
3	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S	1
4	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S	1
5	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S	0
6	3	Moran, Mr. James	male	NaN	0	0	330877	8.4583	NaN	Q	0
7	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	51.8625	E46	S	0
8	3	Palsson, Master. Gosta Leonard	male	2.0	3	1	349909	21.0750	NaN	S	0
9	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Ber	g) female	27.0	0	2	347742	11.1333	NaN	S	1
10	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30.0708	NaN	C	1
11	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16.7000	G6	S	1

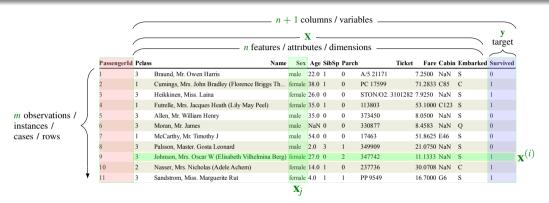
- A labeled dataset consists of m rows $\times (n+1)$ columns / variables
- Use bold to represent vectors and matrices
- Use subscripts to indicate particular feature / attribute / column
- Use superscript in parenthesis to indicate particular observation / instance/ case / row
- So $x_i^{(i)}$ (or $x_{i,j}$) is the *i*-th observation in the *j*-th feature



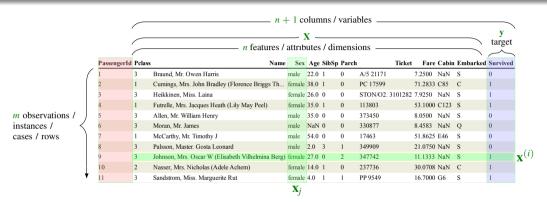
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Example Datasets

We will use a few datasets today to illustrate the various features:

Tips

- Small dataset of total bills, and tips for different servers with gender, day, time and group size.
- Clean, no missing values, some outliers.
- Task: exploratory data analysis

Titanic

- Classic dataset with passenger information for the Titanic's fatal voyage, and whether they survived.
- Has missing values and information rich text fields (Name, ticket number).
- Task: classification predict whether a passenger survived.

Algae Blooms

- Water quality study where samples were taken from different rivers over time.
- Recorded levels of (seven) chemical substances and population of (six) algae species and other information on the sample conditions.
- Task: regression predict algae population level (7 separate populations).

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4
5	25.29	4.71	Male	No	Sun	Dinner	4
6	8.77	2.00	Male	No	Sun	Dinner	2
7	26.88	3.12	Male	No	Sun	Dinner	4
8	15.04	1.96	Male	No	Sun	Dinner	2
9	14.78	3.23	Male	No	Sun	Dinner	2

No target column, so mainly just an exploratory data analysis problem. But questions of interest:

- How do factors sex, smoker, day, time, or size affect tip / percentage tip?
- Does size vary with day, time, smoker?

But some questions don't make sense

 What is the relationship between sex and smoker? — why should they be related?

This is the downside of automatic EDA tools such as pandas—profiling — you will drowned in statistics / charts.

Algae Blooms dataset

												_		
_	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_P <mark>D4</mark>	mean_Chlor	a1	a2	a
0	winter	small	medium	8.00	9.8	60.800	6.238	578.00000	105.00000	170.00000	50.000	0.0	0.0	0.0
1	spring	small	medium	8.35	8.0	57.750	1.288	370.00000	428.75000	558.75000	1.300	1.4	7.6	4.8
2	autumn	small	medium	8.10	11.4	40.020	5.330	346.66699	125.66700	187.05701	15.600	3.3	53.6	1.9
3	spring	small	medium	8.07	4.8	77.364	2.302	98.18200	61.18200	138.70000	1.400	3.1	41.0	18
4	autumn	small	medium	8.06	9.0	55.350	10.416	233.70000	58.22200	97.58000	10.500	9.2	2.9	7.5
5	winter	small	high	8.25	13.1	65.750	9.248	430.00000	18.25000	56.66700	28.400	15.1	14.6	1.4
6	summer	small	high	8.15	10.3	73.250	1.535	110.00000	61.25000	111.75000	3.200	2.4	1.2	3.2
7	autumn	small	high	8.05	10.6	59.067	4.990	205.66701	44.66700	77.43400	6.900	18.2	1.6	0.0
8	winter	small	medium	8.70	3.4	21.950	0.886	102.75000	36.30000	71.00000	5.544	25.4	5.4	2.5
9	winter	Н	ow well	can we p	redict the	e (7) diffe	rent algae po	opulation lev	els using wat	er sample ir	nformation?	7.0	0.0	0.0
10	spring	small	high	7.70	10.2	8.000	1.527	21.57100	12.75000	20.75000	0.800	1 6.6	0.0	0.0
11	summer	small	high	7.45	11.7	8.690	1.588	18.42900	10.66700	19.00000	0.600	32.1	0.0	0.0
12	winter	small	high	7.74	9.6	5.000	1.223	27.28600	12.00000	17.00000	41.000	43.5	0.0	2.1
13	summer	small	high	7.72	11.8	6.300	1.470	8.00000	16.00000	15.00000	0.500	31.1	1.0	3.4
14	winter	small	high	7.90	9.6	3.000	1.448	46.20000	13.00000	61.60000	0.300	52.2	5.0	7.8
15	autumn	small	high	7.55	11.5	4.700	1.320	14.75000	4.25000	98.25000	1.100	69.9	0.0	1.7
16	winter	small	high	7.78	12.0	7.000	1.420	34.33300	18.66700	50.00000	1.100	46.2	0.0	0.0
17	spring	small	high	7.61	9.8	7.000	1.443	31.33300	20.00000	57.83300	0.400	31.8	0.0	3.1
18	summer	small	high	7.35	10.4	7.000	1.718	49.00000	41.50000	61.50000	0.800	50.6	0.0	9.9
19	spring	small	medium	7.79	3.2	64.000	2.822	8777.59961	564.59998	771.59998	4.500	0.0	0.0	0.0
														12

Titanic dataset

	Passenge	rId Sur	vived 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
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4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S
5	6	0	3	Moran, Mr. James	male	NaN	0	0	330877	8.4583	NaN	Q
6	7	0	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	51.8625	E46	S
7	8	0	3	Palsson, Master. Gosta Leonard	male	2.0	3	1	349909	21.0750	NaN	S
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Berg)	female	27.0	0	2	347742	11.1333	NaN	S
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30.0708	NaN	С
10	11	1	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16.7000	G6	S
11	12	~~	Jow well can	we predict a passenger's s	urvival	ucino	inform	nation a	t time of den	ortura?	~1 03	S
12	13	لم	iow well call	Henry			Illioin		A/5. 2151		NaN	S
10	- 4 4	^		Andersson, Mr. Anders	,	000		_	0.45000	04.0550		13 0

Before we start ... Loading libraries

We start by loading in the core data science modules...

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

matplotlib is an excellent visualisation library but some plots needs additional configuration. seaborn sits above matplotlib and has a collection of visualisations optimised for statistical analysis. . . .

```
import seaborn as sns
```

Next, we import some statistical modules ...

```
import scipy.stats as stats
import statsmodels.api as sm
import pingouin as pg
```

scipy.stats has a large number of distributions, parametric and nonparametric statistical tests, and descriptive statistics.
statsmodels is more focused on estimating statistical models.

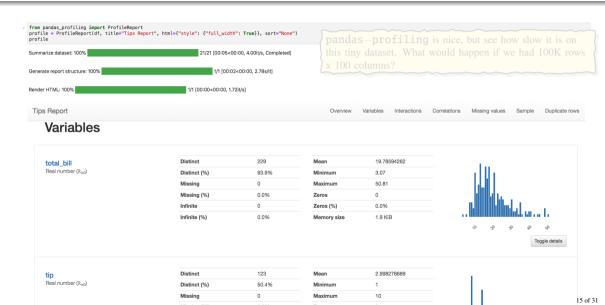
Finally we set options ...

statsmodels is more focused on estimating statistical models.

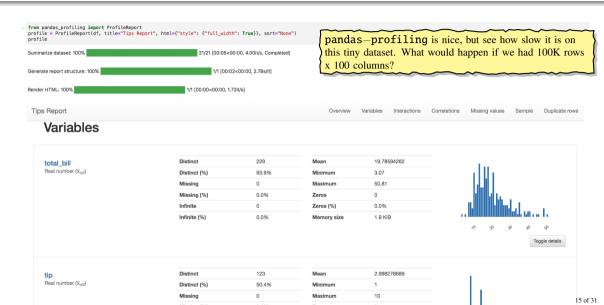
pingouin overlaps with bits of scipy.stats and statsmodels but generates more details and nicer visualisations.

```
plt.style.use("seaborn-darkgrid")
```

Before we start ... auto EDA using pandas—profiling



Before we start ... auto EDA using pandas—profiling



Well, almost zero code....

```
import pandas as pd
import dtale

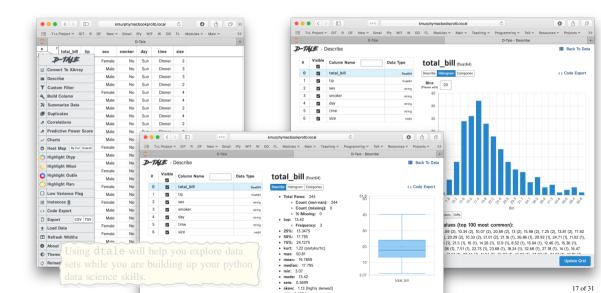
# Read the Tips data into a dataframe, check it looks OK

df = pd.read_csv('tips.csv')

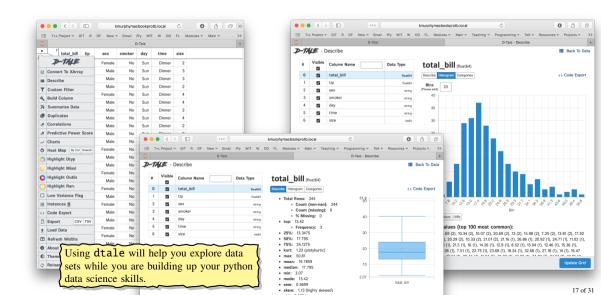
df.head()

# Run dtale to visualize the structure of the dataframe
dtale.show(df)
```

Before we start ... zero-code EDA using dtale



Before we start ... zero-code EDA using dtale



First Pass — Load Dataset and Initial Clean

- Load dataset
- Check variables names
- Verify variable types
- Identify (and possibly address) missing values

Tips — Load

```
df = pd.read_csv("tips.csv")
print(df.shape)
df.head(10) (244, 7)
```

total_bill	tip	sex	smoker	day	time	size
0 16.99	1.01	Female	No	Sun	Dinner	2
1 10.34	1.66	Male	No	Sun	Dinner	3
2 21.01	3.50	Male	No	Sun	Dinner	3
3 23.68	3.31	Male	No	Sun	Dinner	2
4 24.59	3.61	Female	No	Sun	Dinner	4
5 25.29	4.71	Male	No	Sun	Dinner	4
6 8.77	2.00	Male	No	Sun	Dinner	2
7 26.88	3.12	Male	No	Sun	Dinner	4
8 15.04	1.96	Male	No	Sun	Dinner	2
9 14.78	3.23	Male	No	Sun	Dinner	2

df.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
    Column
              Non-Null Count Dtype
    total bill 244 non-null float64
    tip
              244 non-null float64
    sex
              244 non-null
                            object
    smoker
              244 non-null object
    day
              244 non-null
                            object
              244 non-null
                            object
    time
    size
              244 non-null int 64
dtypes: float64(2), int64(1), object(4)
memory usage: 13.5+ KB
```

Tips — Load

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df = pd.read_csv("tips.csv")
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	total_bill	tip	sex	smoker	day	time	size
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<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
    Column
              Non-Null Count Dtvpe
    total bill 244 non—null
                            float64
    tip
              244 non-null float64
    sex
              244 non-null
                            object
    smoker
              244 non-null object
    day
              244 non-null
                           object
              244 non-null
                            object
    time
    size
              244 non-null int 64
dtypes: float64(2), int64(1), object(4)
memory usage: 13.5+ KB
```

Issue: categorical data treated as object (string).

Tips — Fix Data Types

```
df.sex.unique()
                                                       df.smoker.unique()
array(['Female', 'Male'], dtype=object)
                                                      array(['No', 'Yes'], dtype=object)
df.sex = pd.Categorical(df.sex)
                                                       df.smoker = pd.Categorical(df.smoker)
                                                       df.smoker.unique()
df.sex.unique()
['Female', 'Male']
                                                      ['No', 'Yes']
Categories (2, object): ['Female', 'Male']
                                                      Categories (2. object): ['No', 'Yes']
df.day.unique()
array(['Sun', 'Sat', 'Thur', 'Fri'], dtype=object)
df.dav = pd.Categorical(df.dav, categories=['Thur', 'Fri', 'Sun', 'Sat'], ordered=True)
df.day.unique()
['Sun', 'Sat', 'Thur', 'Fri']
Categories (4, object): ['Thur' < 'Fri' < 'Sun' < 'Sat']</pre>
```

Tips — fix datatypes

```
df.time = pd.Categorical(df.time, categories=['Lunch', 'Dinner'], ordered=True) df.time.unique()
```

```
['Dinner', 'Lunch']
Categories (2, object): ['Lunch' < 'Dinner']</pre>
```

df.info()

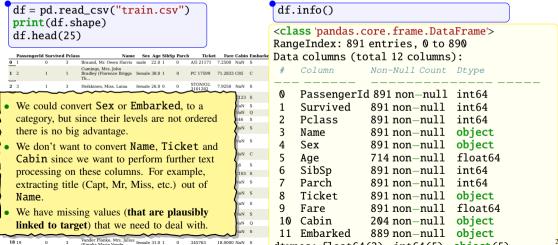
Converting to category will:

- Simplify visualisation (order can be preserved).
- Reduce memory usage (not that big a deal for us).
- Speed up I/O (depending on file format).
- ⇒ Convert to category is a bigger deal for features where the levels have an order.

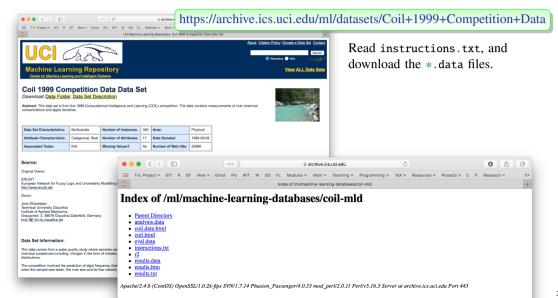
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RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
              Non-Null Count Dtype
    Column
    total bill 244 non-null float64
    tip
              244 non-null float64
    sex
              244 non-null
                           category
    smoker
              244 non-null
                           category
    dav
              244 non-null
                           category
    time
              244 non-null
                           category
    size
              244 non-null int64
dtypes: category(4), float64(2), int64(1)
memory usage: 7.4 KB
```

Titanic — load

- Dataset is split into two parts:
 - train.csv 891 rows with Survived column, used in EDA and model training.
 - test.csv 418 rows without the Survived column, used in competition scoring.



$Algae_Blooms - load$



Pandas function pd.read_table, is a more general function than read_csv.

```
df = pd.read_table('src/Analysis.txt')
print(df.shape)
df.head()
(199, 1)
```

winter small medium 8.00000 9.80000 60.80000 6.23800 578.00000 105.00000 170.00000 50.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

- **0** spring small medium 8.35000 ...
- ${\color{red} 1}$ autumn small medium 8.10000 1...
- $\mathbf{2} \text{ spring small medium } 8.07000 \dots$
- $\bf 3$ autumn small medium $8.06000\ldots$
- 4 winter small high 8.25000 13....

Two problems, first row was treated as column headers, and we need to specify the character(s) used to separate columns



- Now, notice that the number of data row changed from 199 to 200 since the first row is now counted as a data row. And now we are using default columns names.
- The "\s+" matches one or more spaces. This is an example of a regex.
- We need to name the columns.

Algae_Blooms — load (3rd attempt)

Season Size Speed max_pH min_O2 mean_Cl mean_NO3 mean_NH4 mean_oPO4 mean_PO4 mean_Chlor a1 a2 a3

 0
 winter
 small medium 8.00000
 9.80000
 60.80000
 6.23800

 1
 spring
 small medium 8.35000
 8.00000
 57.75000
 1.28800

 2
 autumn
 small medium 8.10000
 11.40000
 40.02000
 5.33000

 3
 spring
 small medium 8.07000
 4.80000
 77.36400
 2.30200

 4
 autumn
 small medium 8.06000
 9.00000
 55.35000
 10.41600

Dataframe looks a bit better, but why are numeric columns converted as **object**?
Reading instructions.txt we see that missing values are indicated by XXXXXXX.

<class 'pandas.core.frame.DataFrame'> RangeIndex: 200 entries, 0 to 199 Data columns (total 18 columns): Column Non-Null Count Dtvpe 200 non-null object Season Size 200 non-null object object Speed 200 non-null max_pH 200 non-null object min O2 200 non-null object mean_Cl 200 non-null object 200 non-null object mean NO3 mean NH4 200 non-null object mean oPO4 200 non-null object 26 of 31

Algae_Blooms — load (4th attempt)

```
Season Size Speed max pH min O2 mean Cl mean NO3 mean NH4 mean oPO4 mean PO4 mean Chlor a1 a2 a3 a
0 winter
        small medium 8.00
                           9.8
                                   60.800
                                           6.238
                                                       <class 'pandas.core.frame.DataFrame'>
1 spring small medium 8.35
                           8.0
                                   57.750
                                           1.288
                                                       RangeIndex: 200 entries, 0 to 199
2 autumn small medium 8.10
                           11.4
                                   40.020
                                           5.330
                                                       Data columns (total 18 columns):
3 spring small medium 8.07
                           4.8
                                   77.364
                                           2.302
                                                                        Non-Null Count Dtype
                                                            Column
4 autumn small medium 8.06
                                   55 350
                                           10 416
                           9.0
                                                                        200 non-null
                                                                                         object
                                                            Season
                                                            Size
                                                                        200 non-null
                                                                                         object
```

Now some variables have missing values

Also we should convert Season, Size and Speed to category and ensure the levels are ordered.

```
200 non-null
                         object
Speed
max_pH
           199 non-null
                         float64
min O2
           198 non-null
                         float64
mean Cl
           190 non-null
                         float64
           198 non-null
                         float64
mean NO3
mean NH4
           198 non-null
                         float64
mean oPO4
           198 non-null
                         float64
                                       27 of 31
```

The three categorical variables have levels with a natural order \Rightarrow convert to category and specify order:

```
df.Season = pd.Categorical(df.Season, categories=['spring', 'summer', 'autumn', 'winter'], ordered=Tr
print(df.Season.unique())
```

```
['winter', 'spring', 'autumn', 'summer']
Categories (4, object): ['spring' < 'summer' < 'autumn' < 'winter']</pre>
```

```
df.Size = pd.Categorical(df.Size, categories=['small', 'medium', 'large'], ordered=True)
print(df.Size.unique())
```

```
['small', 'medium', 'large']
Categories (3, object): ['small' < 'medium' < 'large']</pre>
```

df.Speed = pd.Categorical(df.Speed, categories=['low', 'medium', 'high'], ordered=True)
print(df.Speed.unique())

```
['medium', 'high', 'low']
Categories (3, object): ['low' < 'medium' < 'high']</pre>
```

Which columns have missing values?

Which rows have missing values? How many NAs per row?

Which columns have missing values?

df.isna().sum()

Season Size Speed max_pH min O2 mean Cl 10 mean_NO3 mean NH4 mean_oPO4 mean PO4 12 mean Chlor a 1 a2 a3 a4 a5 a6 а7

Which rows have missing values? How many NAs per row?

Which columns have missing values?

df.isna().sum()

Season Size Speed max_pH min O2 mean Cl 10 mean_NO3 mean_NH4 mean_oPO4 mean PO4 12 mean Chlor a 1 a2 a3 a4 a5 a6 а7

Which rows have missing values? How many NAs per row?

df.isna().sum(axis=1).value_counts()

184 0 dtvpe: int64

Which columns have missing values?

df.isna().sum()

Season Size Speed max_pH min O2 mean_Cl 10 mean_NO3 mean_NH4 mean_oPO4 mean PO4 12 mean Chlor a 1 a2 a3 a4 a5 a6 а7

- Two columns (features) account for 22 NAs, but cannot just drop them as will lose a lot of information.
- Two rows (observations) account for 12 NAs \Rightarrow remove.
- Removing other rows with a NA will result in a los of 14 rows (7% of the data), instead will impute later.

Which rows have missing values? How many NAs per row?

df.isna().sum(axis=1).value_counts()

```
184
0
dtvpe: int64
```

Which columns have missing values?

df.isna().sum()

Season Size Speed max_pH min O2 mean_Cl 10 $mean_NO3$ mean NH4 mean_oPO4

mean PO4 12 mean Chlor a 1

a2 a3 a4

a 5 a6 а7

Two columns (features) account for 22 NAs, but cannot just drop them as will lose a lot of information.

- Two rows (observations) account for 12 NAs \Rightarrow remove.
- Removing other rows with a NA will result in a los of 14 rows (7% of the data), instead will impute later.

Which rows have missing values? How many NAs per row?

df.isna().sum(axis=1).value_counts()

184 0 dtype: int64

Rows / Cols to drop?

df.loc[df.isna().sum(axis=1)==6]

NaN

NaN

Season Size Speed max pH min O2 mean Cl mean NO3 mean NH4 mean oPO4 mean PO4 mean Chlor 61 summer small medium 6.4 NaN NaN NaN NaN NaN 14.0 NaN

198 winter large medium 8.0 7.6 NaN NaN NaN df = df.loc(df.isna().sum(axis=1)<61.copv()

print(df.shape) (198, 18) NaN

Tips

✓ Loaded data, corrected dtypes (categorical with order levels)

After Loading and Initial Clean — Where are we?

- Sanitised column names not needed, but note column name size shadows pandas dataframe function size \Rightarrow so use df["size"] instead of df.size.
- ✓ No missing values

>Titanic >

- ✓ Loaded data no conversion of dtypes needed (but if you don't plots/crosstab order won't agree)
- ✓ Sanitised column names not needed.
- Missing values in Age (177/891=20%), Cabin (687/891=77%), and Embarked (2/891=0.2%).
 - A feature with 77% missing values should be considered for deletion, but what if the presence of a missing value actually tells us something? \Rightarrow convert to a boolean feature.

Algae Blooms

- ✓ Loaded data, corrected dtypes (categorical with ordered levels)
- Sanitised column names.
- Missing values
 - Removed two rows with 6 NA each, accounted for 12/33=36% of the missing values.
 - Remaining, 21 NAs are concentrated in mean_CL (8) and mean_Chlor (10). EDA will suggest options.

After Loading and Initial Clean — Where are we?

Next we might

- Save result of initial clean:
 - To either a CSV (if we don't mind losing dtype metadata)

```
df.to_csv('data/Analysis.csv', index=False)
```

• To (say) pickle format (to keep dtype metadata)

```
df.to_pickle('data/Analysis.pkl')
```

Later can read dataframe back in using

```
df = pd.read_pickle('data/Analysis.pkl')
print(df.shape)
df.head(1)
```

• If the dataset is large (>100K rows), save a (reproducible) sample of the dataset for later EDA to speed up calculations (especially visualisations).

```
df.sample(frac=.25, random_state=42).to_pickle('data/Analysis_sample.pkl')
```