(MSc) Data Mining

Topic 02 : Exploratory Data Analysis

Part 01 : Exploratory Data Analysis

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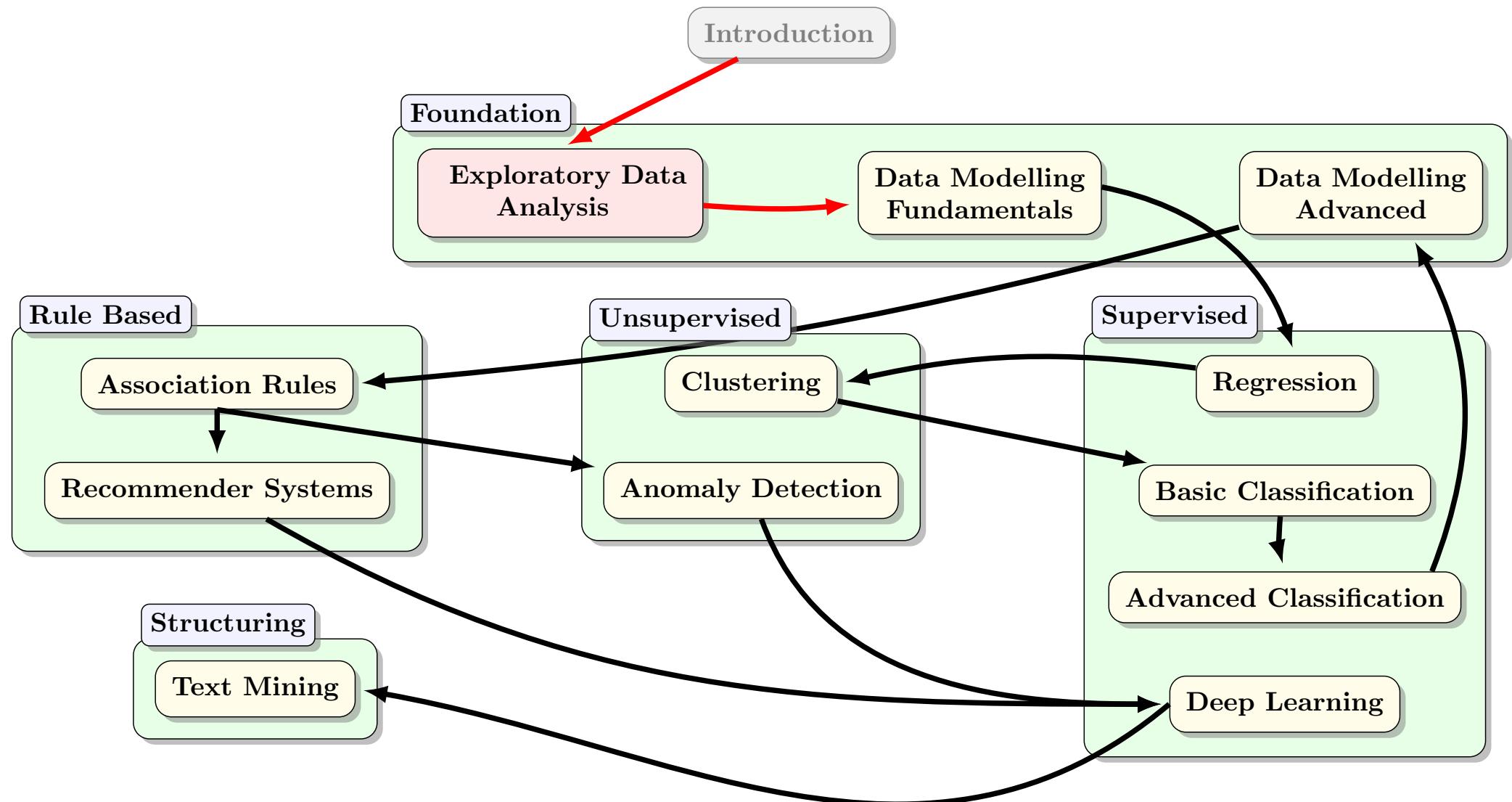
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Outline

- EDA Process
- Datasets — Tips, Titanic and Algae Blooms
- Identifying and resolving issues (missing value, outliers)
- Generating ToDo list for Feature Engineering/Transformation/Selection

Data Mining (Week 2)

Introduction

Foundation

- Exploratory Data Analysis
- Data Modelling Fundamentals
- Data Modelling Advanced

Rule Based

- Association Rules
- Recommender Systems

Unsupervised

- Clustering
- Anomaly Detection

Supervised

- Regression
- Basic Classification
- Advanced Classification
- Deep Learning

Structuring

- Text Mining

Exploratory Data Analysis — Summary

Introduction

Exploratory Data Analysis (EDA)
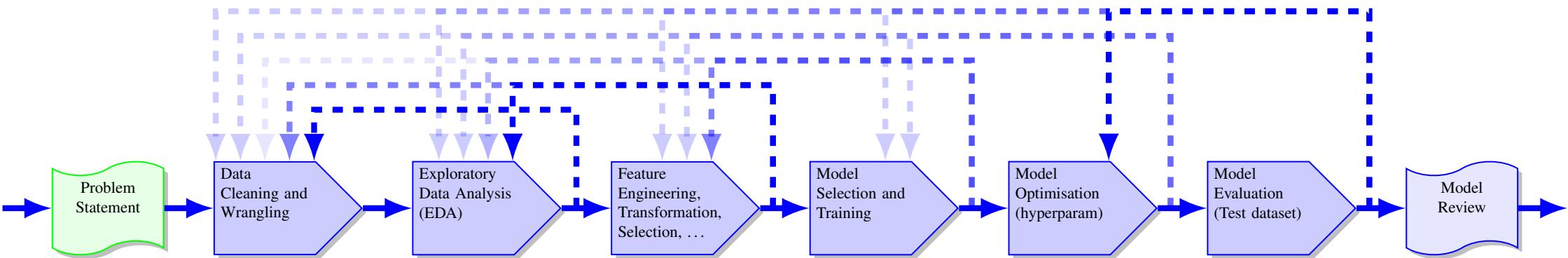
> Aim

To understand and summarise a dataset with the aim that issues are discovered, relevant relations between features and the target and between features are identified, in order to inform the subsequent training of machine learning models.

> 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 Mining Workflow

Problem Statement → Data Cleaning and Wrangling → Exploratory Data Analysis (EDA) → Feature Engineering, Transformation, Selection, ... → Model Selection and Training → Model Optimisation (hyperparam) → Model Evaluation (Test dataset) → Model Review
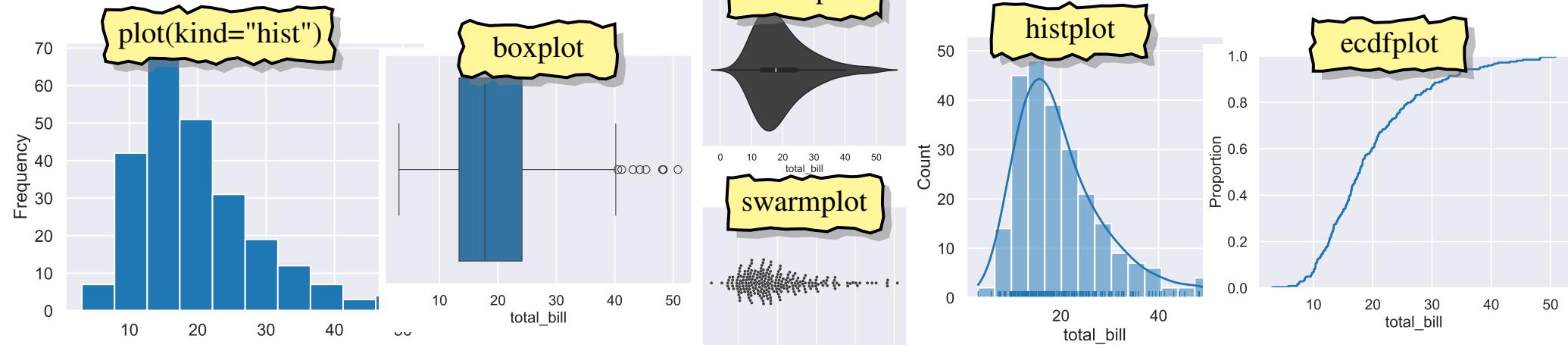
- Data pre-precessing (Data Cleaning + EDA + Feature Engineering) is the core of the data mining pipeline (typical estimates >50% of the time/effort).
- Decision made during earlier steps in the workflow impact on later steps.
  - Better data cleaning simplifies EDA.
  - EDA informs the feature extraction, engineering, transformation and selection.
  - Better features simplify model selection and training.
- Workflow is iterative — based on issues found (or better understanding of the data) we often need to revisit earlier steps in the workflow.

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?

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

Terminology / Notation

$n + 1$ columns / variables

$\mathbf{X}$

$\mathbf{y}$
target

n features / attributes / dimensions

PassengerId	Pclass	Name	Sex	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 Berg)	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

m observations / instances / cases / rows

$\mathbf{x}^{(i)}$

$\mathbf{X}_j$

- 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 .... $\mathbf{x}_j$
- Use superscript in parenthesis to indicate particular observation / instance/ case / row .... $\mathbf{x}^{(i)}$
- So $x_j^{(i)}$ (or $x_{i,j}$) is the i-th observation in the j-th feature .... $x_j^{(i)}$

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).

`Tips` dataset

	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 drown in statistics / charts.

Algae Blooms dataset

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1	a2	a3	a4	a5	a6	a7
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	0.0	34.2	8.3	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	1.9	6.7	0.0	2.1
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	0.0	0.0	0.0	9.7
3	spring	small	medium	8.07	4.8	77.364	2.302	98.18200	61.18200	138.70000	1.400	3.1	41.0	18.9	0.0	1.4	0.0	1.4
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	0.0	7.5	4.1	1.0
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	0.0	22.5	12.6	2.9
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	3.9	5.8	6.8	0.0
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	0.0	5.5	8.7	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	0.0	0.0	0.0	0.0
9	winter	sm													0.0	0.0	1.7
10	spring	small	high	7.70	10.2	8.000	1.527	21.57100	12.75000	20.75000	0.800	16.6	0.0	0.0	0.0	1.2	0.0	6.0
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	0.0	0.0	0.0	1.5
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	0.0	1.2	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	0.0	1.9	0.0	4.1
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	0.0	4.0	0.0	0.0
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	0.0	0.0	0.0	0.0
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	1.2	0.0	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	4.8	7.7	1.4	7.2
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	4.3	3.6	8.2	2.2
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	44.6	0.0	0.0	1.4

How well can we predict the (7) different algae population levels using water sample information?

`Titanic` dataset

	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
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	C
10	11	1	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16.7000	G6	S
11	12	1									C103	S
12	13	0									NaN	S
13	14	0	3	Andersson, Mr. Anders Johan	male	39.0	1	5	347082	31.2750	NaN	S
14	15	0	3	Vestrom, Miss. Hulda Amanda Adolfina	female	14.0	0	0	350406	7.8542	NaN	S
15	16	1	2	Hewlett, Mrs. (Mary D Kingcome)	female	55.0	0	0	248706	16.0000	NaN	S
16	17	0	3	Rice, Master. Eugene	male	2.0	4	1	382652	29.1250	NaN	Q
17	18	1	2	Williams, Mr. Charles Eugene	male	NaN	0	0	244373	13.0000	NaN	S
18	19	0	3	Vander Planke, Mrs. Julius (Emelia Maria Vande...	female	31.0	1	0	345763	18.0000	NaN	S
19	20	1	3	Masselmani, Mrs. Fatima	female	NaN	0	0	2649	7.2250	NaN	C
20	21	0	2	Fynney, Mr. Joseph J	male	35.0	0	0	239865	26.0000	NaN	S
21	22	1	2	Beesley, Mr. Lawrence	male	34.0	0	0	248698	13.0000	D56	S
22	23	1	3	McGowan, Miss. Anna "Annie"	female	15.0	0	0	330923	8.0292	NaN	Q
23	24	1	1	Sloper, Mr. William Thompson	male	28.0	0	0	113788	35.5000	A6	S

How well can we predict a passenger's survival using information at time of departure?

Before we start . . . Loading libraries

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

```
1  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. . . .

```
2  import seaborn as sns
```

Next, we import some statistical modules . . .

```
3  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.
pingouin overlaps with bits of scipy.stats and statsmodels but generates more details and nicer visualisations.

Finally we set options . . .

```
4  sns.set_style('darkgrid')
   pd.set_option('display.max_columns', None)
   pd.set_option('display.width', 1000)
```

Before we start . . . auto EDA using `pandas-profiling`

```python
from pandas_profiling import ProfileReport
profile = ProfileReport(df, title="Tips Report", html={"style": {"full_width": True}})
profile
```
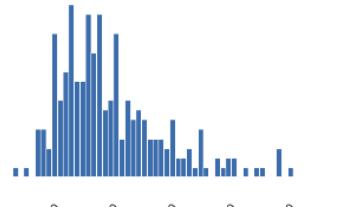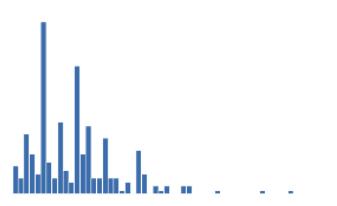
Summarize dataset: 100% ████████████████████ 20/20 [00:03<00:00, 3.95it/s, Completed]

Generate report structure: 100% █████████ 1/1 [00:03<00:00, 3.03s/it]

Render HTML: 100% ███████████ 1/1 [00:00<00:00, 1.47it/s]

> `pandas-profiling` is nice, but see how slow it is on this tiny dataset. What would happen if we had 100K rows x 100 columns?

Tips Report

Overview   Variables   Interactions   Correlations   Missing values   Sample   Duplicate rows

Variables
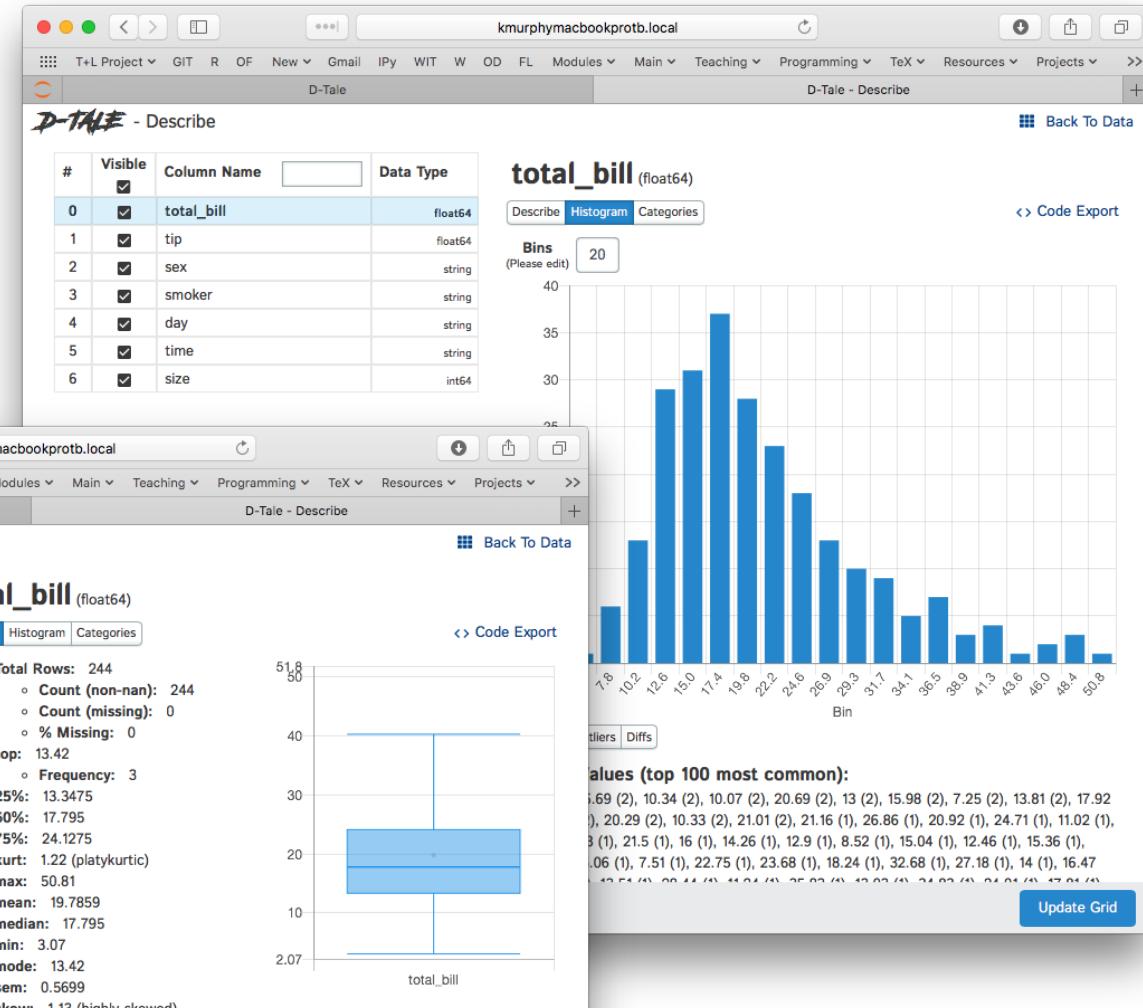
total_bill
Real number ($\mathbb{R}_{\geq 0}$)

HIGH CORRELATION
HIGH CORRELATION
HIGH CORRELATION
HIGH CORRELATION

Distinct	229	Minimum	3.07
Distinct (%)	93.9%	Maximum	50.81
Missing	0	Zeros	0
Missing (%)	0.0%	Zeros (%)	0.0%
Infinite	0	Negative	0
Infinite (%)	0.0%	Negative (%)	0.0%
Mean	19.78594262	Memory size	2.0 KiB

Toggle details

tip
Real number ($\mathbb{R}_{\geq 0}$)

HIGH CORRELATION
HIGH CORRELATION
HIGH CORRELATION
HIGH CORRELATION

Distinct	123	Minimum	1
Distinct (%)	50.4%	Maximum	10
Missing	0	Zeros	0
Missing (%)	0.0%	Zeros (%)	0.0%
Infinite	0	Negative	0
Infinite (%)	0.0%	Negative (%)	0.0%
Mean	2.998278689	Memory size	2.0 KiB

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

Using `dtale` will help you explore data sets while you are building up your python data science skills.

First Pass — Load Dataset and Initial Clean

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

Tips — Load

5
```
df = pd.read_csv("data/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

6
```
df.info()
```

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

Issue: categorical data treated as object (string).

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Tips — Fix Data Types I

7
```
df.sex.unique()
```
```
array(['Female', 'Male'], dtype=object)
```
8
```
df.sex = pd.Categorical(df.sex)
df.sex.unique()
```
```
['Female', 'Male']
Categories (2, object): ['Female', 'Male']
```

9
```
df.smoker.unique()
```
```
array(['No', 'Yes'], dtype=object)
```
10
```
df.smoker = pd.Categorical(df.smoker)
df.smoker.unique()
```
```
['No', 'Yes']
Categories (2, object): ['No', 'Yes']
```

11
```
df.day.unique()
```
```
array(['Sun', 'Sat', 'Thur', 'Fri'], dtype=object)
```
12
```
df.day = pd.Categorical(df.day, categories=['Thur', 'Fri','Sat', 'Sun'], ordered=True)
df.day.unique()
```
```
['Sun', 'Sat', 'Thur', 'Fri']
Categories (4, object): ['Thur' < 'Fri' < 'Sat' < 'Sun']
```

Tips — Fix Data Types   II

¹³

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

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

¹⁴
```
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).

⇒ Converting to category is a bigger deal for features where the levels have an order.

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
 #   Column      Non-Null Count   Dtype
---  ------      --------------   -----
 0   total_bill  244 non-null     float64
 1   tip         244 non-null     float64
 2   sex         244 non-null     category
 3   smoker      244 non-null     category
 4   day         244 non-null     category
 5   time        244 non-null     category
 6   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.

15
```
df = pd.read_csv("data/train.csv")
print(df.shape)
df.head(25)
```

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

- We could convert `Sex` or `Embarked`, to a category, but since their levels are not ordered there is no big advantage.
- We don't want to convert `Name`, `Ticket` and `Cabin` since we want to perform further text processing on these columns. For example, extracting title (Capt, Mr, Miss, etc.) out of `Name`.
- We have missing values (**that are plausibly linked to target**) — we need to deal with this.

16
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 891 entries, 0 to 890
Data columns (total 12 columns):
 #   Column       Non-Null Count   Dtype
---  -------      --------------   -----
 0   PassengerId  891 non-null     int64
 1   Survived     891 non-null     int64
 2   Pclass       891 non-null     int64
 3   Name         891 non-null     object
 4   Sex          891 non-null     object
 5   Age          714 non-null     float64
 6   SibSp        891 non-null     int64
 7   Parch        891 non-null     int64
 8   Ticket       891 non-null     object
 9   Fare         891 non-null     float64
 10  Cabin        204 non-null     object
 11  Embarked     889 non-null     object
dtypes: float64(2), int64(5), object(5)
memory usage: 83.7+ KB
```

`Algae_Blooms` – Load   I

https://archive.ics.uci.edu/ml/datasets/Coil+1999+Competition+Data

Coil 1999 Competition Data
Donated on 9/8/1999

This data set is from the 1999 Computational Intelligence and Learning (COIL) competition. The data contains measurements of river chemical concentrations and algae densities.

Dataset Characteristics	Subject Area	Associated Tasks
Multivariate	Physics and Chemistry	-
Feature Type	**# Instances**	**# Features**
Categorical, Real	340	-

Dataset Information ⌃

Additional Information
This data comes from a water quality study where samples were taken from sites on different European rivers of a period of approximately one year. These samples were analyzed for various chemical substances including: nitrogen in the form of nitrates, nitrites and ammonia, phosphate, pH, oxygen, chloride. In parallel, algae samples were collected to determine the ...
SHOW MORE ⌄

Has Missing Values?
No

Variables Table ⌃

Variable Name	Role	Type	Demographic	Description	Units	Missing Values
						no
						no
						no

DOWNLOAD

CITE

DOI
10.24432/C59W45

License
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This allows for the sharing and adaptation of the datasets for any purpose, provided that the appropriate credit is given.

Click on `Download` to download an archive of the dataset and move the files in archive into your subfolder `data` of your `Algae_Blooms` folder in your `datasets` folder.

The UCI repo has recently undergone a significant update, and one consequence of this change is that this dataset has been cleaned and now contains the data in `csv` format.
In the following slides we will work with the original `analysis.txt` (see lab) dataset to illustrate typical import issues.

`Algae_Blooms` — Load (1st attempt) II

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

```
17 df = pd.read_table('data/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 34.20000 8.30000 0.00000
0 spring small medium 8.35000 ...
1 autumn small medium 8.10000 1...
2 spring small medium 8.07000 ...
3 autumn small medium 8.06000 ...
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.

`Algae_Blooms` — Load (2nd attempt) III

18

```
df = pd.read_table('data/analysis.txt', sep=r'\s+', header=None)
print(df.shape)                                              (200, 18)
df.head()
```

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	winter	small	medium	8.00000	9.80000	60.80000	6.23800	578.00000	105.00000	170.00000	50.00000	0.0	0.0	0.0	0.0	34.2	8.3	0.0
1	spring	small	medium	8.35000	8.00000	57.75000	1.28800	370.00000	428.75000	558.75000	1.30000	1.4	7.6	4.8	1.9	6.7	0.0	2.1
2	autumn	small	medium	8.10000	11.40000	40.02000	5.33000	346.66699	125.66700	187.05701	15.60000	3.3	53.6	1.9	0.0	0.0	0.0	9.7
3	spring	small	medium	8.07000	4.80000	77.36400	2.30200	98.18200	61.18200	138.70000	1.40000	3.1	41.0	18.9	0.0	1.4	0.0	1.4
4	autumn	small	medium	8.06000	9.00000	55.35000	10.41600	233.70000	58.22200	97.58000	10.50000	9.2	2.9	7.5	0.0	7.5	4.1	1.0

- Now, notice that the number of data rows changed from 199 to 200 since the first row is now treated as a data row (and not headers). Also, now we are using default columns names.
- The r"\s+" matches one or more spaces. This is an example of a regex.
- We need to name the columns.

`Algae_Blooms` — Load (3rd attempt)   IV

19

```python
names = ('Season','Size','Speed','max_pH','min_O2','mean_Cl', 'mean_NO3', 'mean_NH4', 'mean_oPO4',
         'mean_PO4', 'mean_Chlor', 'a1', 'a2', 'a3', 'a4', 'a5', 'a6', 'a7')

df = pd.read_table('data/analysis.txt', sep=r'\s+', names=names)
print(df.shape)
df.head()
```

(200, 18)

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1	a2	a3	a4	a5	a6	a7
0	winter	small	medium	8.00000	9.80000	60.80000	6.23800	578.00000	105.00000	170.00000	50.00000	0.0	0.0	0.0	0.0	34.2	8.3	0.0
1	spring	small	medium	8.35000	8.00000	57.75000	1.28800	370.0000										
2	autumn	small	medium	8.10000	11.40000	40.02000	5.33000	346.6669										7
3	spring	small	medium	8.07000	4.80000	77.36400	2.30200	98.1820										4
4	autumn	small	medium	8.06000	9.00000	55.35000	10.41600	233.7000										

> 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   Dtype
___  _____      _____   _____
 0   Season      200 non-null     object
 1   Size        200 non-null     object
 2   Speed       200 non-null     object
 3   max_pH      200 non-null     object
 4   min_O2      200 non-null     object
 5   mean_Cl     200 non-null     object
 6   mean_NO3    200 non-null     object
 7   mean_NH4    200 non-null     object
 8   mean_oPO4   200 non-null     object
 9   mean_PO4    200 non-null     object
 10  mean_Chlor  200 non-null     object
 11  a1          200 non-null     float64
 12  a2          200 non-null     float64
```

`Algae_Blooms` — Load (4th attempt)   V

20

```python
names = ('Season','Size','Speed','max_pH','min_O2','mean_Cl', 'mean_NO3', 'mean_NH4', 'mean_oPO4',
         'mean_PO4', 'mean_Chlor', 'a1', 'a2', 'a3', 'a4', 'a5', 'a6', 'a7')

df = pd.read_table('data/analysis.txt', sep=r'\s+', names=names, na_values='XXXXXXX')
print(df.shape)
df.head()
```

`(200, 18)`

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1	a2	a3	a4	a5	a6	a7
0	winter	small	medium	8.00	9.8	60.800	6.238	578.00000	105.000	170.00000	50.0	0.0	0.0	0.0	0.0	34.2	8.3	0.0
1	spring	small	medium	8.35	8.0	57.750	1.288	370.0000										
2	autumn	small	medium	8.10	11.4	40.020	5.330	346.6669										7
3	spring	small	medium	8.07	4.8	77.364	2.302	98.18200										4
4	autumn	small	medium	8.06	9.0	55.350	10.416	233.7000										

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 200 entries, 0 to 199
Data columns (total 18 columns):
 #   Column       Non-Null Count   Dtype
___  _____       _____   _____
 0   Season       200 non-null     object
 1   Size         200 non-null     object
 2   Speed        200 non-null     object
 3   max_pH       199 non-null     float64
 4   min_O2       198 non-null     float64
 5   mean_Cl      190 non-null     float64
 6   mean_NO3     198 non-null     float64
 7   mean_NH4     198 non-null     float64
 8   mean_oPO4    198 non-null     float64
 9   mean_PO4     198 non-null     float64
 10  mean_Chlor   188 non-null     float64
 11  a1           200 non-null     float64
 12  a2           200 non-null     float64
```

Now some variables have missing values

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

`Algae_Blooms` — Fix Data Types   II

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']
```

```
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']
```

```
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']
```

`Algae_Blooms` — Identification of Missing Values (NA)

1 Which columns have missing values?

24 ● `df.isna().sum()`

```
Season        0
Size          0
Speed         0
max_pH        1
min_O2        2
mean_Cl      10
mean_NO3      2
mean_NH4      2
mean_oPO4     2
mean_PO4      2
mean_Chlor   12
a1            0
a2            0
a3            0
a4            0
a5            0
a6            0
a7            0
dtype: int64
```

- 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 loss of 14 rows (7% of the data), instead will impute later.

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

25 ● `df.isna().sum(axis=1).value_counts()`

```
0    184
1      7
2      7
6      2
Name: count, dtype: int64
```

4 Rows / ~~Cols~~ to drop?

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

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1	a2	a3	a4
61	summer	small	medium	6.4	NaN	NaN	NaN	NaN	NaN	14.0	NaN	19.4	0.0	0.0	2.0
198	winter	large	medium	8.0	7.6	NaN	NaN	NaN	NaN	NaN	NaN	0.0	12.5	3.7	1.0

27 ●
```
df = df.loc[df.isna().sum(axis=1)<6].copy()
print(df.shape)
```
`(198, 18)`

After Loading and Initial Clean — Where are we? I

> Tips

✔ Loaded data, corrected dtypes (categorical with order levels).

✔ Sanitised column names — not needed, but note column name `size` shadows pandas dataframe function `size` ⇒ so we need to 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? ⇒ 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?   II

Next we might

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

    28
    ```python
    df.to_csv('output/analysis.csv', index=False)
    ```

    - To save as, say feather (or pickle) format (in order to keep `dtype` metadata)

    29
    ```python
    df.to_feather('output/analysis.feather')
    ```

    Later can read dataframe back in using

    30
    ```python
    df = pd.read_feather('output/analysis.feather')
    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).

    31
    ```python
    df.sample(frac=.25, random_state=42).to_pickle('output/analysis_sample.pkl')
    ```
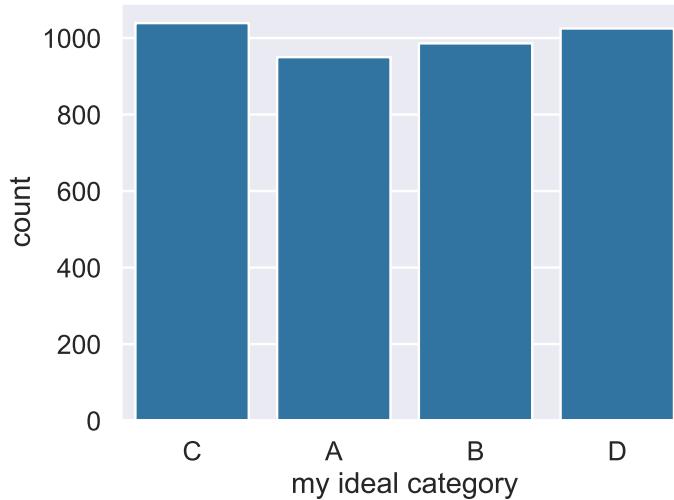
A Selection of Statistical Visualisations and Metrics

Relationship to Target

	Feature	Categorical	Numerical
Categorical	`nunique, unique, describe, value_counts,` ... `countplot,` ...	`crosstab,` ... `countplot,` ...	`boxplot,` ... `catplot, boxplot,` ...
Numerical	`describe,` ... `histplot, boxplot, displot, qqplot,` ...	`groupby+describe,` ... `catplot, boxplot,` ...	`correlations,` ... `lmplot,` ...

Categorical Variable

The Ideal
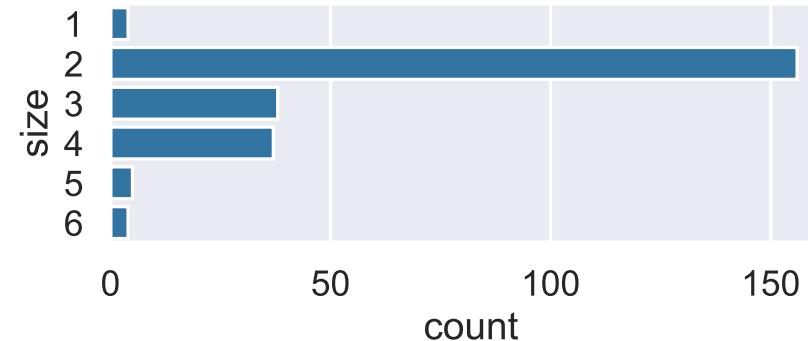
- Each level equally likely.
- Not too many levels: 2–12(ish).

Tools

- `nunique`, `unique`, `value_counts`.

Reality

Tips

32 ●
```
sns.countplot(y="size", data=df)
```


- If `size` was the target, then most models will train towards the majority class (`size=2`).
- If `size` was a feature, then quality of predictor could vary greatly depending on the feature categorical level.
- Consider merge/drop rare category levels.

- `sns.countplot` — shows the counts of observations in each categorical level using bars.

Categorical Variable — Relationship with (Categorical) Target

feature   target   Titanic
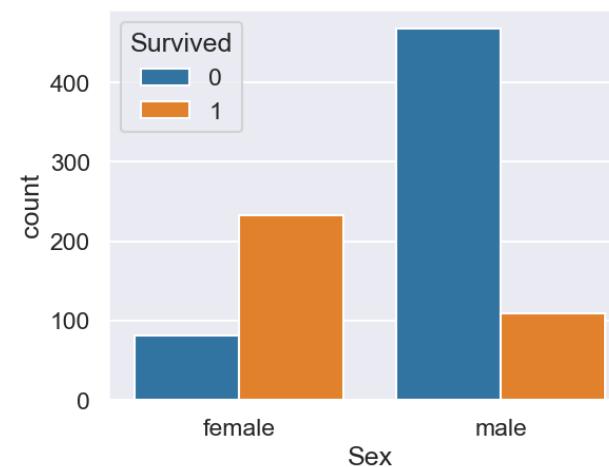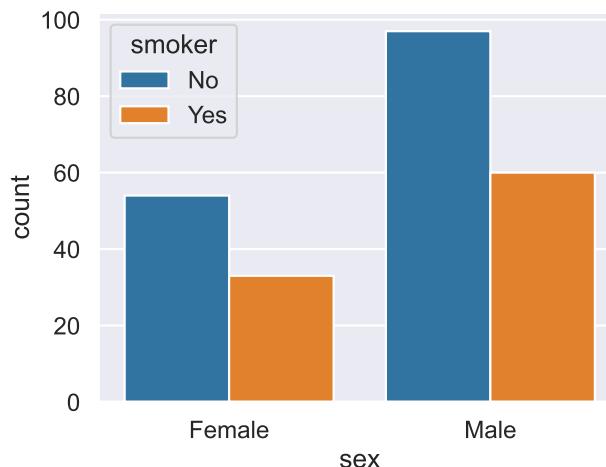
33 ●
```python
sns.countplot(x="Sex", hue="Survived", data=df)
```


34 ●
```python
pd.crosstab(columns=df.Sex, index=df.Survived, margins=True, normalize='columns') \
    .style.format("{:.2%}").background_gradient(cmap='summer_r')
```

sex	Female	Male	All
smoker			
No	62.07%	61.78%	61.89%
Yes	37.93%	38.22%	38.11%

No relationship between `sex` and `smoker`
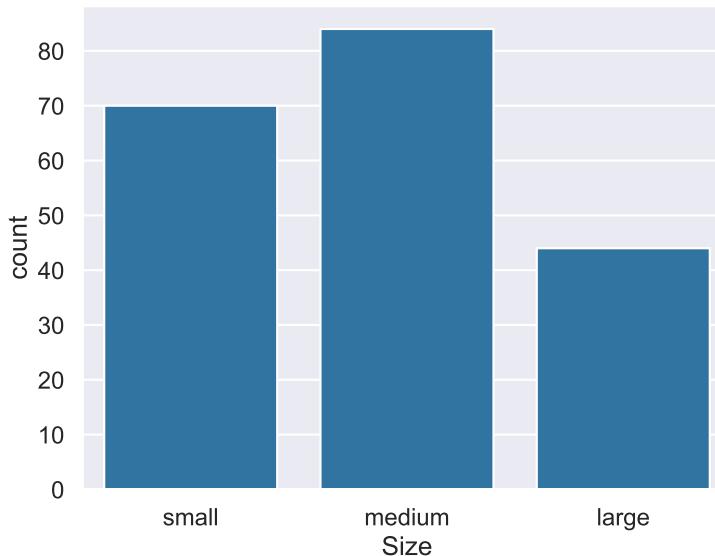
Sex	female	male	All
Survived			
0	25.80%	81.11%	61.62%
1	74.20%	18.89%	38.38%

Strong relationship between `Sex` and `Survived`

Categorical Variable — Relationship with (Numerical) Target   I

35 `sns.countplot(x="Size", data=df)`

36 `sns.catplot(x="Size", y="a4", data=df, kind='bar')`
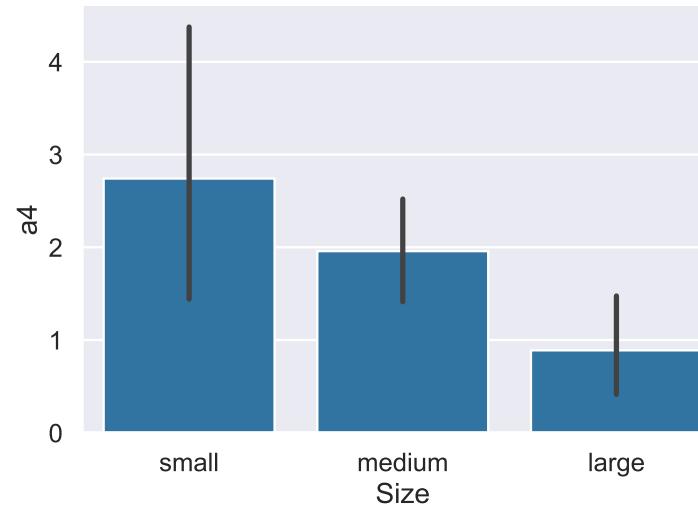
- Shows the counts of observations in each categorical level using bar (height/width).
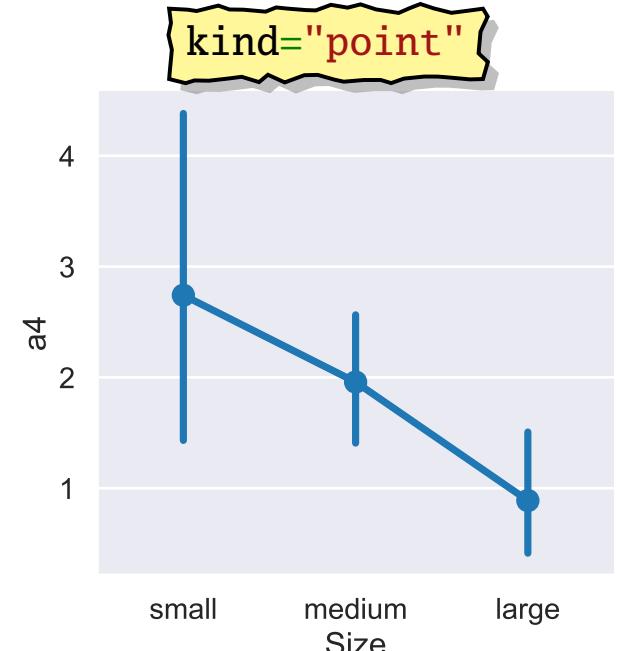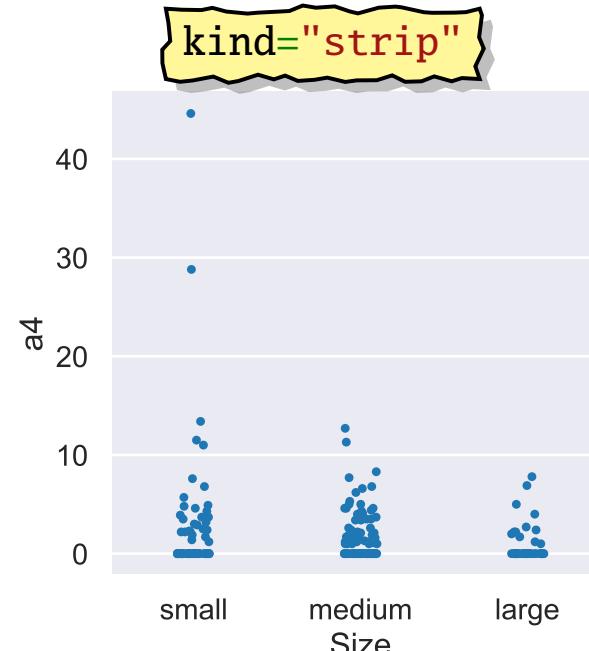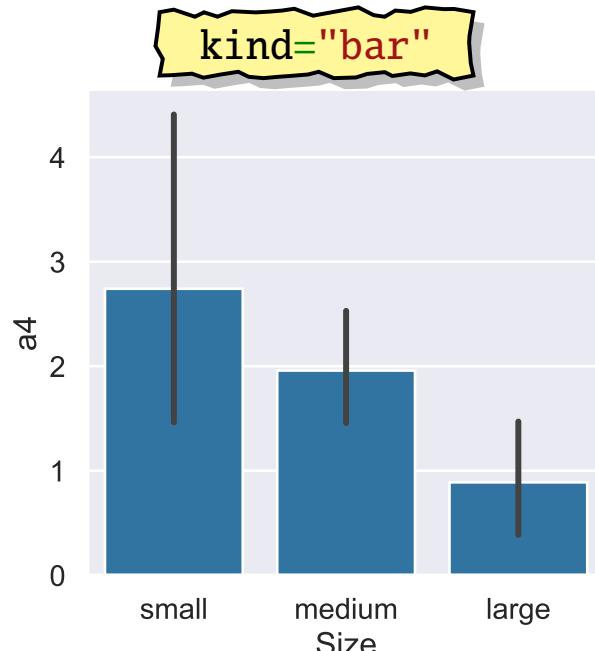
- Shows the average level (mean) and uncertainty (std) of the numerical target (a4) in each categorical level of the categorical variable.
- Vertical bar shows 95% confidence interval.

Is it usable?

Is it useful?
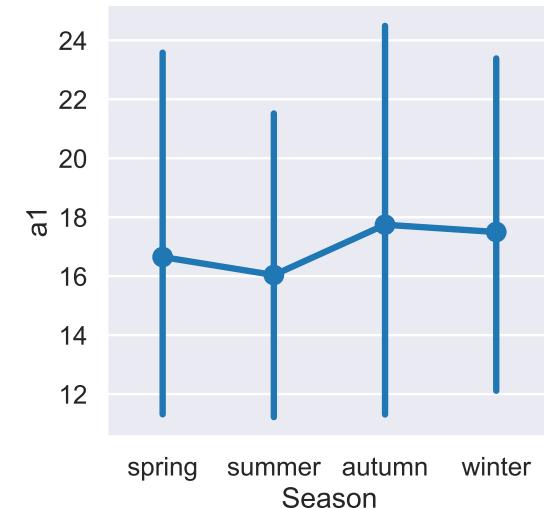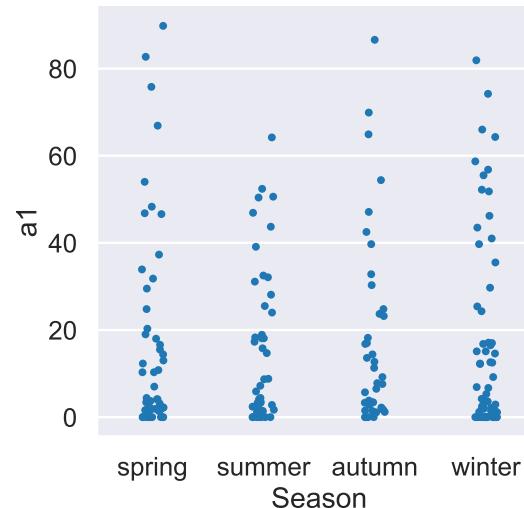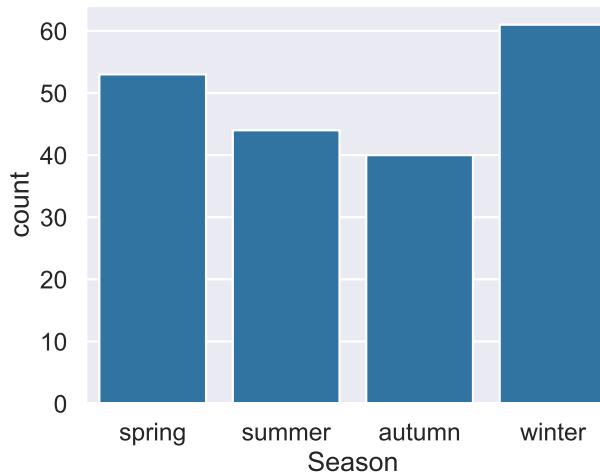
Categorical Variable — Relationship with (Numerical) Target   II

The option `kind` in `catplot` can be:

- `bar` and `point` show essentially the same information, but `point` is more compact when comparing multiple categorical features to a continuous target on the same plot.
- `strip` shows individual observations — useful (as in this case) to show that the larger uncertainty in `Size="small"` observations is mainly due to two outliers.

Example — Dataset: `Algae Blooms`, Feature: `Season`, Target: `a1`
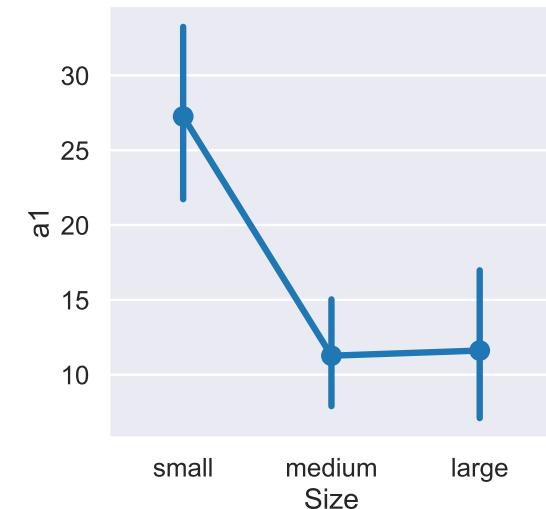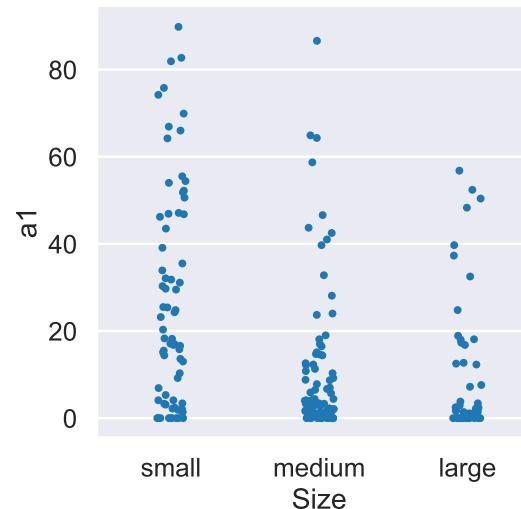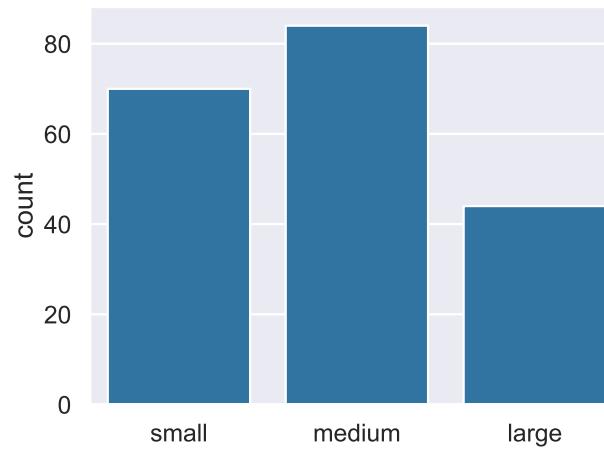
37 ●
```
df.groupby("Season",observed=False)["a1"].agg(["mean","count","std"])
```

Season	mean $\bar{x}$	count n	std σ
spring	16.649057	53	23.093786
summer	16.038636	44	17.920798
autumn	17.745000	40	21.611203
winter	17.498361	61	22.568256

- Countplot shows no issues with feature `Season` — all levels approximately equally represented.
- Catplots show slightly less spread in `a1` for `Season="summer"` observations. (`strip` shows smaller range, `point` shows smaller standard deviation).
⇒ Mean levels of `a1` for different levels of `Season` are well within the 95% confidence intervals ($\bar{x} \pm \sigma 1.96/\sqrt{n}$), so no/weak relationship between categorical feature and numerical target.

Example — Dataset: `Algae Blooms`, Feature: `Size`, Target: `a1`

38

```
df.groupby("Size",observed=True)["a1"].agg(["min","max","mean","count","std"])
```

	min	max	mean	count	std
Size			$\bar{x}$	n	σ
small	0.0	89.8	27.255714	70	24.895426
medium	0.0	86.6	11.267857	84	17.163124
large	0.0	56.8	11.611364	44	16.556123

- Countplot shows no issues with feature `Size`.
- Catplot (**point**) shows that levels of `a1` are higher for `Size="small"` observations.
- ⇒ Confidence interval for `Size="small"` observations do not overlap with CI for other levels, so significant relationship between categorical feature and numerical target.
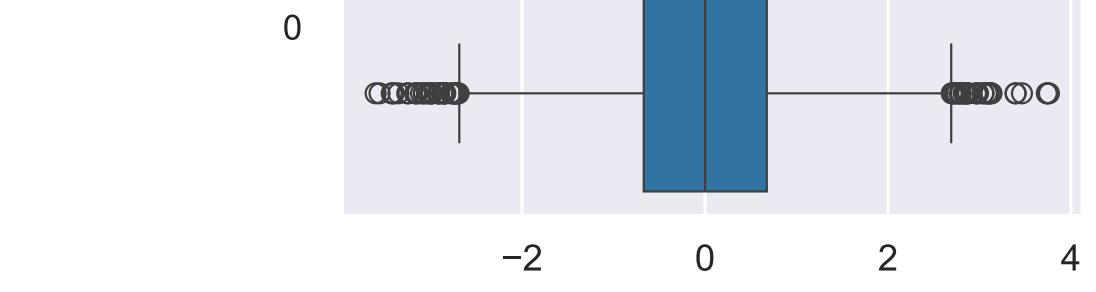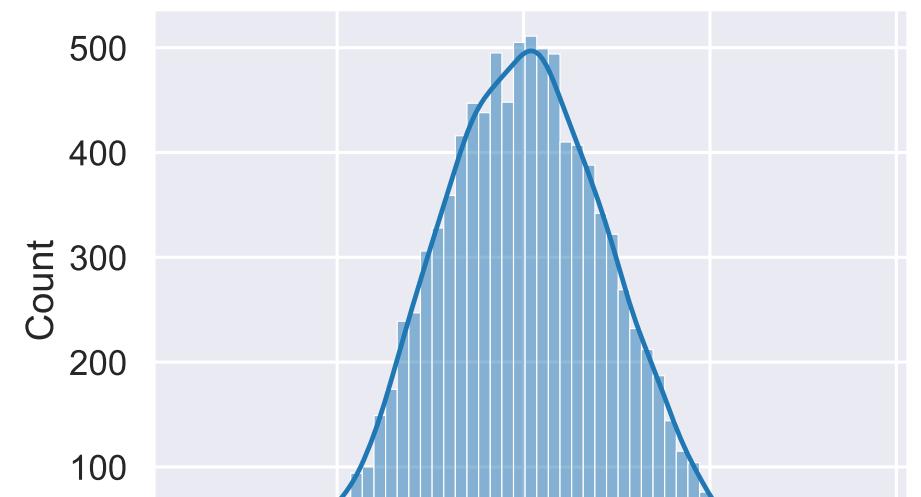
Numerical Variable

Things here are more complicated as a numerical variable could follow many different distributions. Here we look at data following the standard normal distribution. To start we generate 10,000 values and put in to new DataFrame, df2.

40 ·
```python
sns.histplot(x="x", data=df2, kde=True)
```
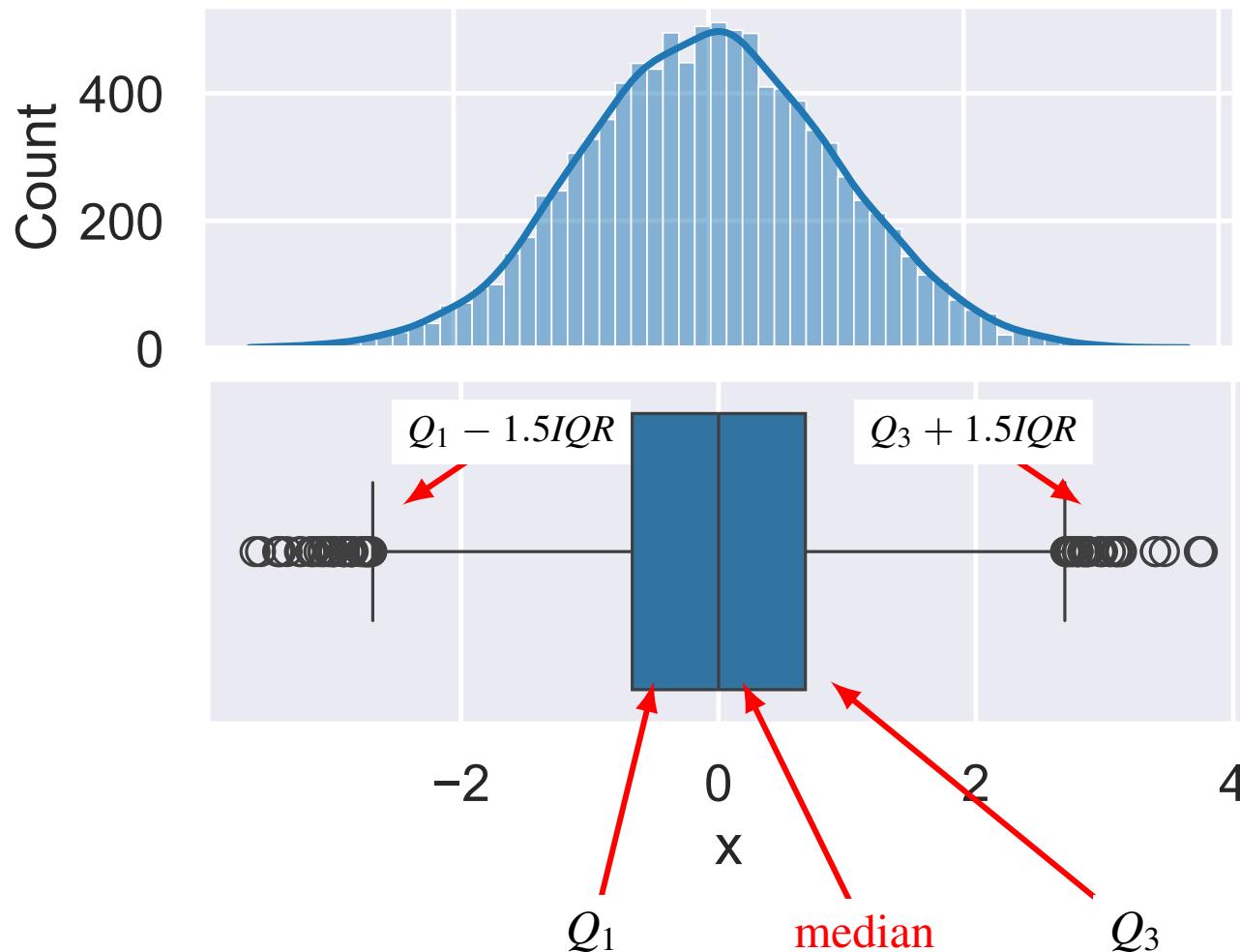
39 ·
```python
rv = stats.norm()
data = rv.rvs(size=10_000)
df2 = pd.DataFrame(data, columns=["x"])
df2.head(5)
```

	x
0	-1.829158
1	1.928193
2	-0.133119
3	1.016313
4	2.122524

41 ·
```python
sns.boxplot(x="x", data=df2)
```

Histplot (Histogram) and Boxplot
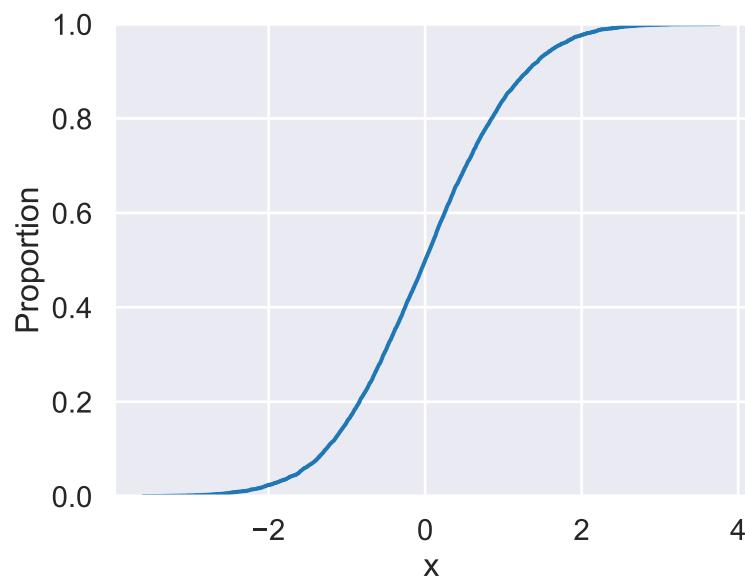
- Histogram is useful in depicting location, spread and shape.

- Curve, is estimate of shape given infinite data and infinite number of bins.

- Boxplots also depicts location, spread and shape, but uses median for estimate of centre, and quartiles for spread.

- Half the data is within the box, data points outside the whiskers (lines) are possible outliers, denoted by circles.

Cumulative Plot and QQ-Plot
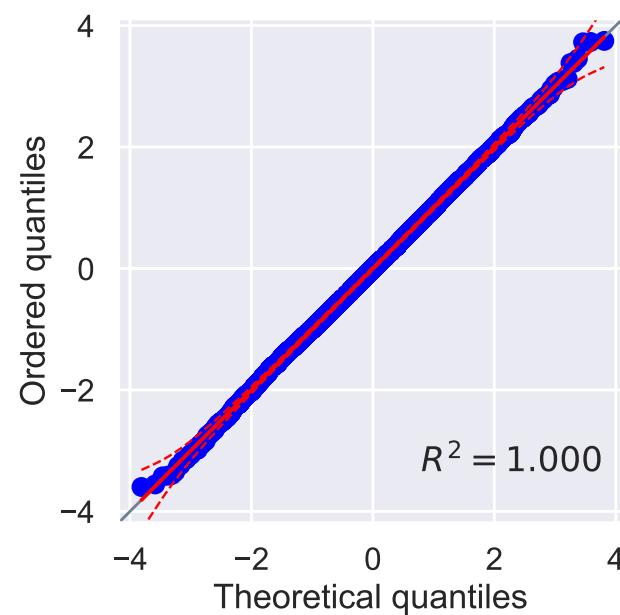
```
sns.ecdfplot(data=df2, x="x")
```

```
import pingouin as pg
```


$R^2 = 1.000$

- Represents the proportion of observations less than or equal to given value.
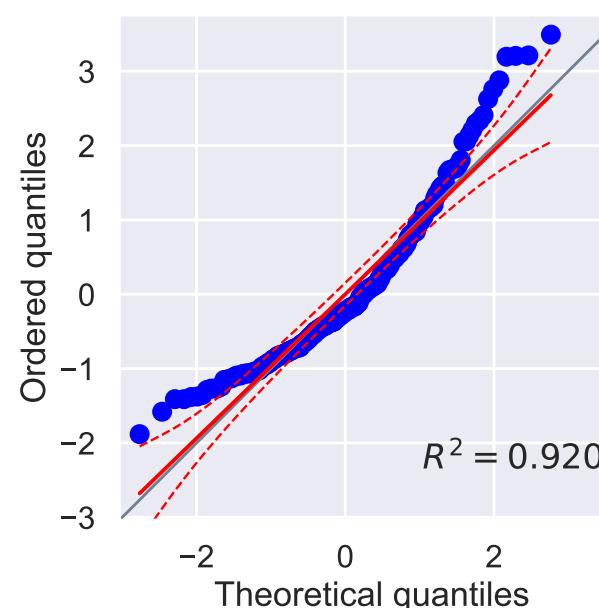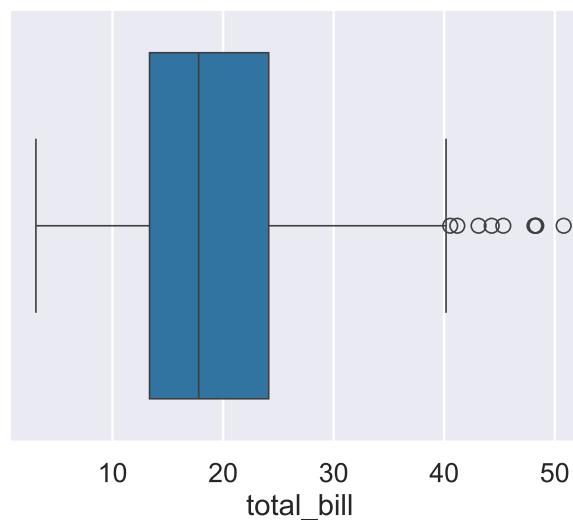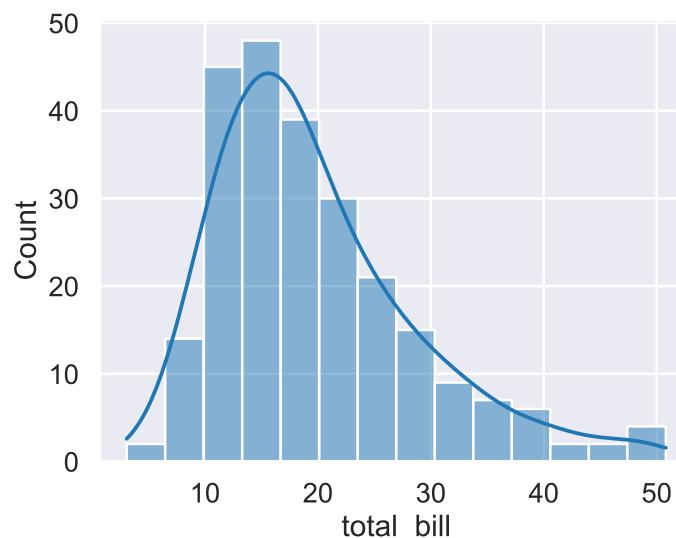
- Plot of observed quantiles against theoretical (assuming normal) quantiles. If both sets of quantiles came from the same distribution, we should see the points forming a line that's roughly straight.

# Example — Dataset: `Tips`, Feature: `total_bill`
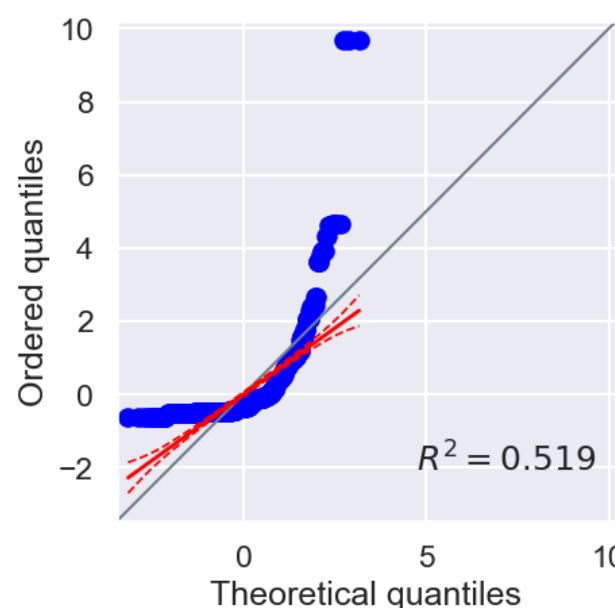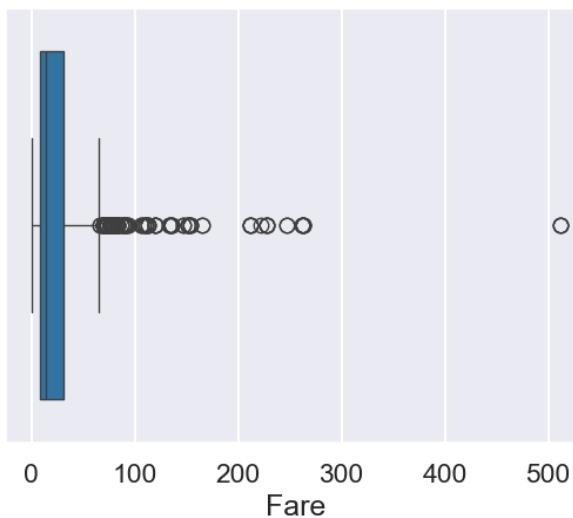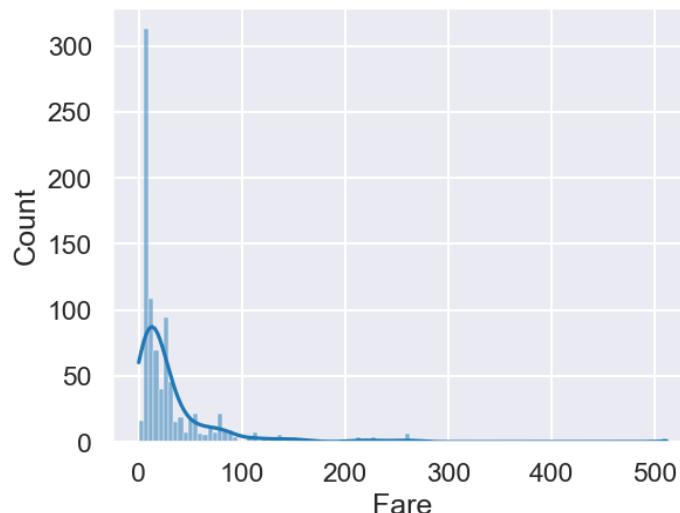

```
df.total_bill.describe()
```

```
count    244.000000
mean      19.785943
std        8.902412
min        3.070000
25%       13.347500
50%       17.795000
75%       24.127500
max       50.810000
Name: total_bill, dtype: float
```

$R^2 = 0.920$

- Data is bell curve shaped, but right skewed (data is more spread out to the right).
- Outliners to the right.
- QQ-Plot indicate that data is not normal, but we could transform it to be more closer to normal.

Example — Dataset: `Titanic`, Feature: `Fare`
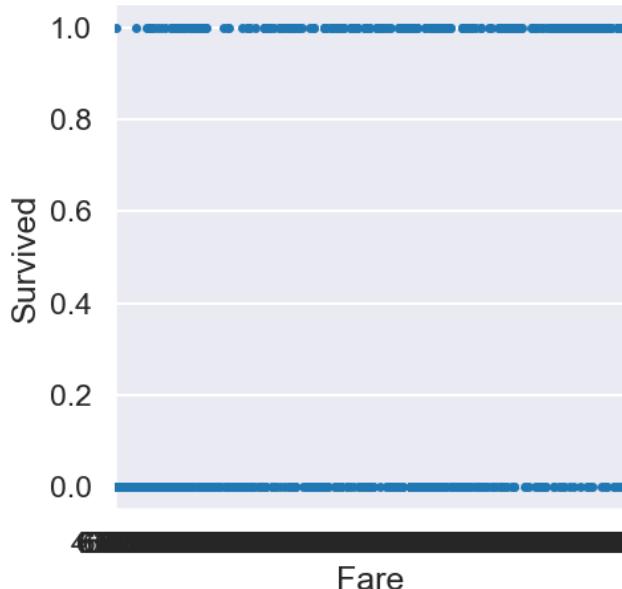

```
df.Fare.describe()
```

```
count    891.000000
mean      32.204208
std       49.693429
min        0.000000
25%        7.910400
50%       14.454200
75%       31.000000
max      512.329200
Name: Fare, dtype: float64
```

$R^2 = 0.519$
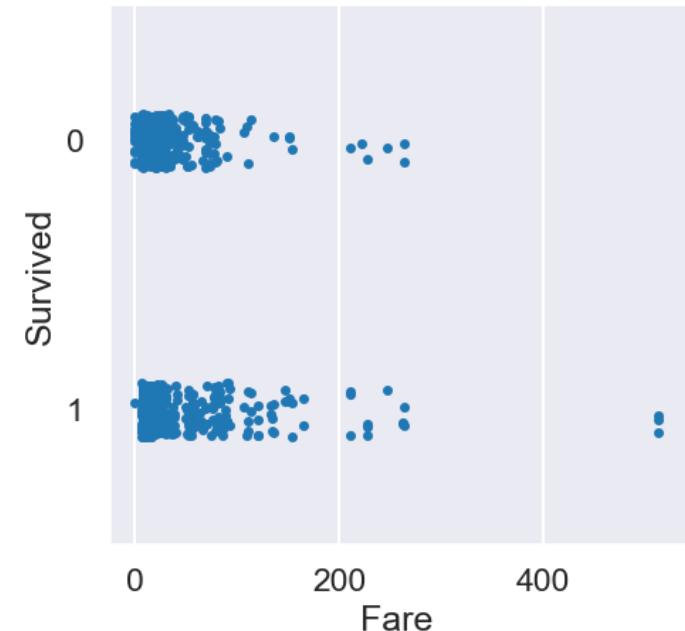
- This variable is more skewed and dominated by its outliers which need to be resolved.

Warning —- Plot Output Depends on Data Assumptions

[46]
```
df = pd.read_csv("data/train.csv")
sns.catplot(data=df, x="Fare", y="Survived")
```

[47]
```
df = pd.read_csv("data/train.csv")
df.Survived = df.Survived.astype(str)
sns.catplot(data=df, x="Fare", y="Survived")
```


- seaborn tries to infer the correct graph based on the data values/type, but it does not always get it correct.
- Survived stores 0 and 1 and has dtype int.
- Converting to a Categorical with numeric levels is not enough.
- astype(str) converts 0 and 1 to "0" and "1" works.
- or append option orient='h'

[48]
```
df = pd.read_csv("data/train.csv")
df.Survived = pd.Categorical(df.Survived)
sns.catplot(data=df, x="Fare", y="Survived")
```

Second Pass — Individual Features and Target

- Categorical vs numerical target

- Categorical vs numerical features
- Identify (and possibly address) issues   } Is it usable?

- Relationship to target.   } Is it useful?

Dataset: `Titanic`, Target: `Survived`
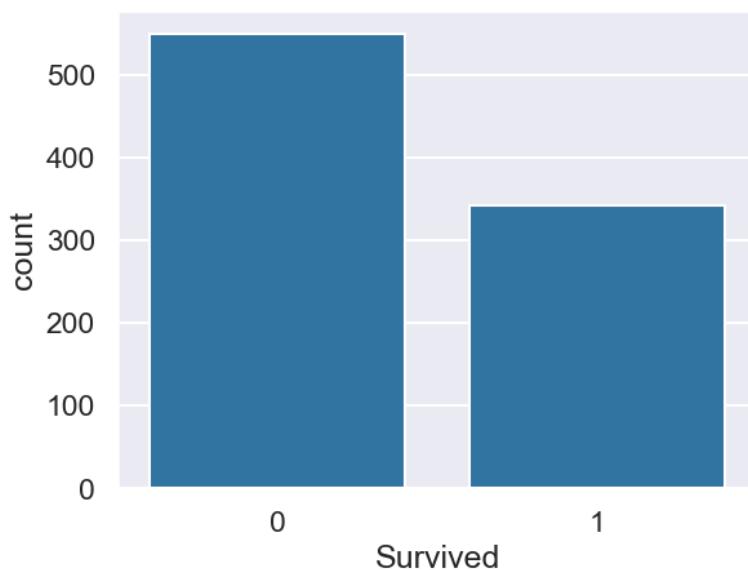
49 `df.Survived.value_counts(normalize=True, dropna=False)`

```
Survived
0    0.616162
1    0.383838
Name: proportion, dtype: float64
```

50 `sns.countplot(x="Survived", data=df)`

51 `df.Survived.unique()`

```
[0, 1]
Categories (2, int64): [0, 1]
```

52 `df.Survived.describe()`

```
count     891
unique      2
top         0
freq      549
Name: Survived, dtype: int64
```

- Simplest classification problem (two classes) with both classes nearly equal frequency.
- In a unbalanced classification problem where the minority class occurs about 20% or lower, models can focus too much on the majority class.

44 of 66

Dataset: `Algae Blooms`, Target: `a1,..., a7`

53
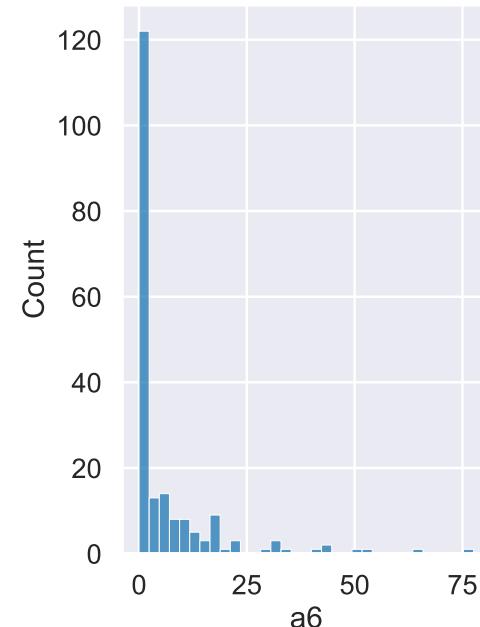
```python
targets = [c for c in df.columns if c[0]=="a"]
targets
```

['a1', 'a2', 'a3', 'a4', 'a5', 'a6', 'a7']

54

```python
df[targets].describe()
```

55

```python
plt.figure(figsize=(4,6))
sns.histplot(x="a6", data=df)
```

	a1	a2	a3	a4	a5	a6	a7
count	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000
mean	16.996465	7.470707	4.334343	1.997475	5.115657	6.004545	2.487374
std	21.421713	11.065461	6.976788	4.439205	7.511846	11.711053	5.181536
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	1.525000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
50%	6.950000	3.000000	1.550000	0.000000	2.000000	0.000000	1.000000
75%	24.800000	11.275000	4.975000	2.400000	7.500000	6.975000	2.400000
max	89.800000	72.600000	42.800000	44.600000	44.400000	77.600000	31.600000

All distributions are heavily skewed to the right, many with outliers (see next slide). All of the zero measurements are probably due to population levels too low to be measured.

Dataset: `Algae Blooms`, Target: `a1,...,  a7`

56
```python
fig, axs = plt.subplots(1, 7, figsize=(24,6))
for k, c in enumerate(targets):
    sns.boxplot(data=df, y=c, color="lightblue", ax=axs[k])
    axs[k].set_xlabel(c)
```


The outliers are likely to be true measurements, but their presence can heavily influence the model training — common strategy is to fit two models (one with the case with target outliers and one without) to assess impact of outliers.

Individual Features
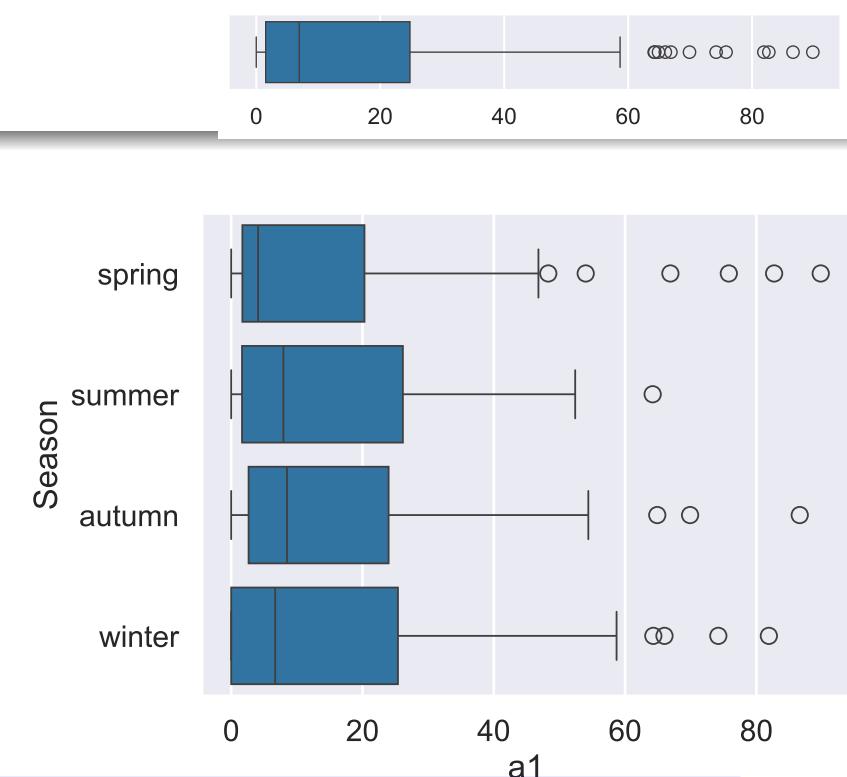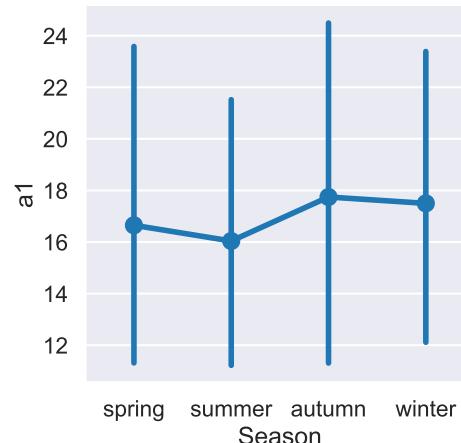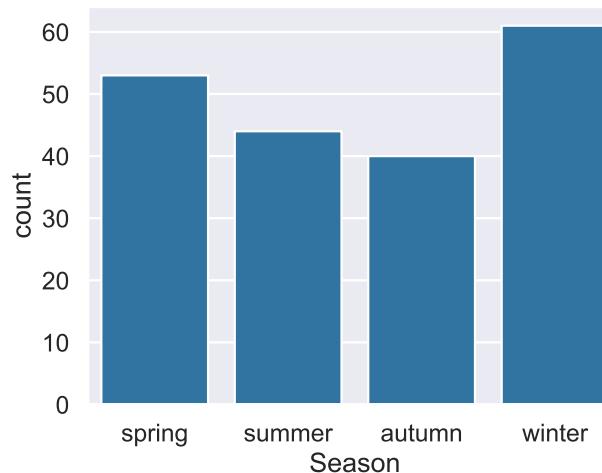
To keep this EDA overview more manageable we will focus on the `Algae Blooms` data set ...

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1	a2	a3	a4	a5	a6	a7
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	0.0	34.2	8.3	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	1.9	6.7	0.0	2.1
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	0.0	0.0	0.0	9.7
3	spring	small	medium	8.07	4.8	77.364	2.302	98.18200	61.18200	138.70000	1.400	3.1	41.0	18.9	0.0	1.4	0.0	1.4

> Sneak perview

- Three categorical variables `Season`, `Size`, and `Speed`.
  - No missing values
  - No high cardinality, and reasonable balanced.
- Eight numerical variables `max_pH`, ..., `mean_Chlor`
- Missing values present
- Some variables heavily skewed — might need to transform.
- Possibility of features being interrelated — multicollinearity — try principal component analysis.

Dataset: `Algae Blooms`, Feature: `Season`, Target: `a1`
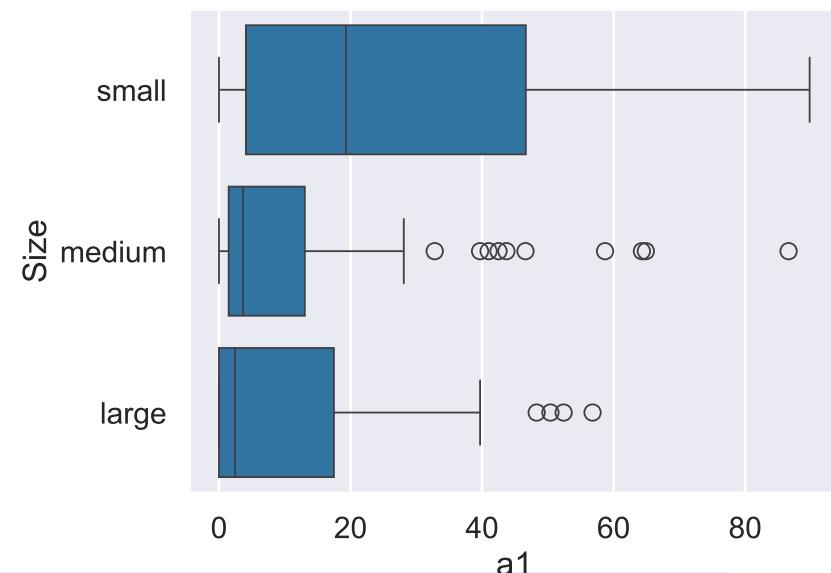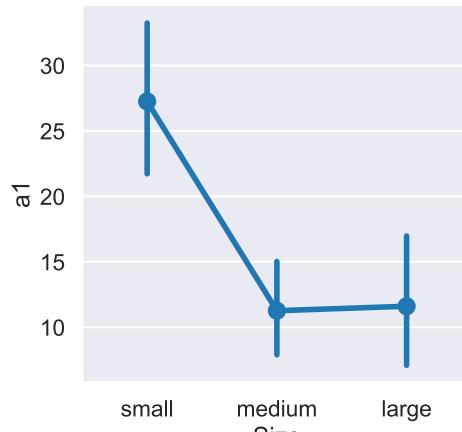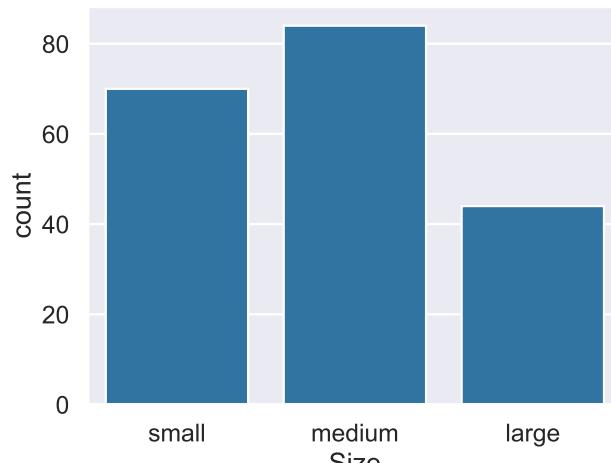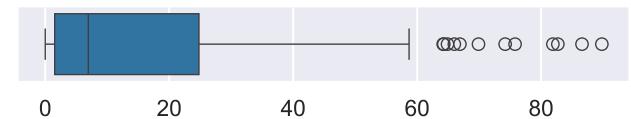
57 `df.groupby("Season",observed=True)["a1"].agg(["min","max","mean","count","std"])`

	min	max	mean	count	std
Season			$\bar{x}$	n	σ
spring	0.0	89.8	16.649057	53	23.093786
summer	0.0	64.2	16.038636	44	17.920798
autumn	0.0	86.6	17.745000	40	21.611203
winter	0.0	81.9	17.498361	61	22.568256

- Countplot shows no issues with feature `Season` — all levels approximately equally represented.
- Catplots show slightly less spread in `a1` for `Season="summer"` observations.
- No/weak relationship between `Season` feature and `a1` target.

Dataset: `Algae Blooms`, Feature: `Size`, Target: `a1`
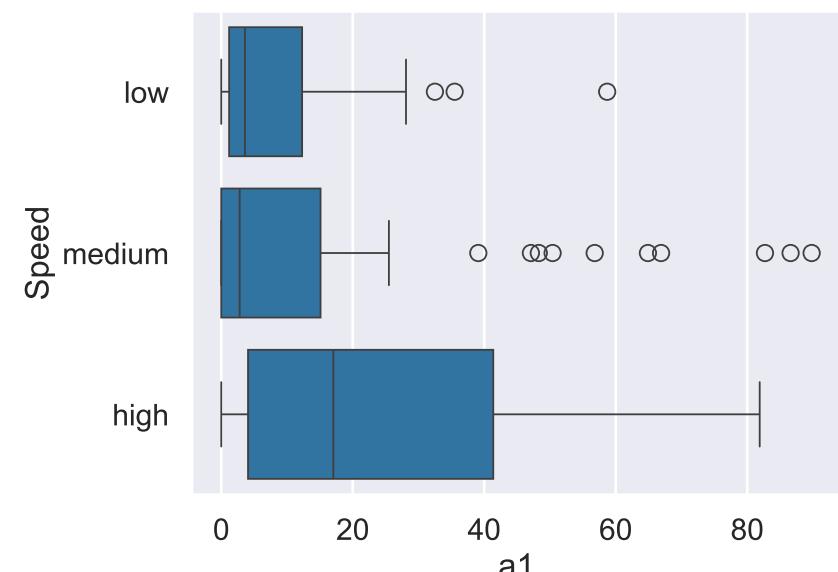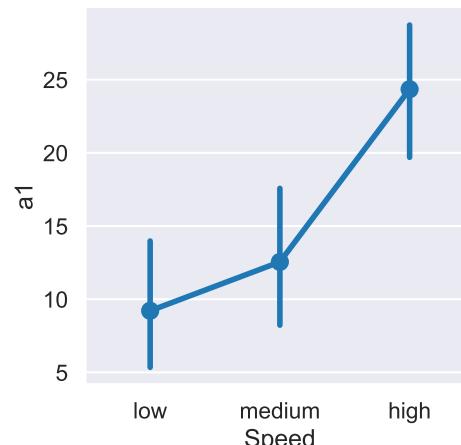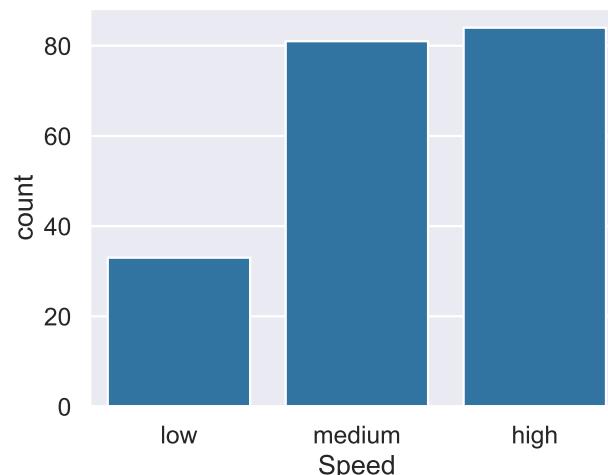
58

```
df.groupby("Size",observed=True)["a1"].agg(["min","max","mean","count","std"])
```

Size	min	max	mean $\bar{x}$	count n	std σ
small	0.0	89.8	27.255714	70	24.895426
medium	0.0	86.6	11.267857	84	17.163124
large	0.0	56.8	11.611364	44	16.556123

- Countplot shows no issues with feature `Size`.
- `Size`=`"small"` rivers have higher frequencies of `a1` alga ((point) catplot), and observed frequencies for small rivers is much more widespread across the domain of frequencies than for other types of rivers (boxplot).

Dataset: `Algae Blooms`, Feature: `Speed`, Target: `a1`
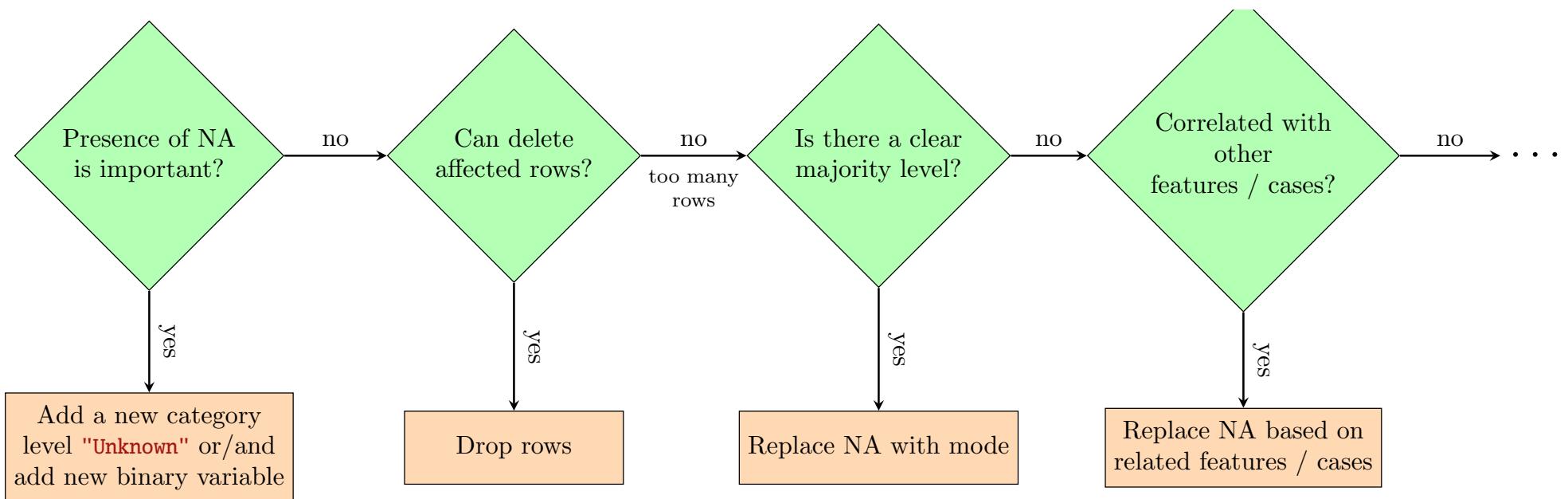

```
df.groupby("Speed",observed=True)["a1"].agg(["min","max","mean","count","std"])
```

	min	max	mean	count	std
Speed			$\bar{x}$	n	σ
low	0.0	58.7	9.209091	33	13.164758
medium	0.0	89.8	12.548148	81	21.146986
high	0.0	81.9	24.345238	84	22.209123

- Countplot shows no issues with feature `Speed`.
- `Speed="high"` rivers have larger average population of `a1` alga ((point) catplot), and observed population level are more widespread than for other types of rivers (boxplot).

Categorical Variables — Dealing with Missing Values

```
           Presence of NA        no      Can delete        no       Is there a clear      no      Correlated with      no    . . .
           is important?                 affected rows?   too many    majority level?               other
                                                          rows                                      features / cases?

                │ yes                         │ yes                       │ yes                         │ yes

        Add a new category            Drop rows              Replace NA with mode          Replace NA based on
        level "Unknown" or/and                                                             related features / cases
        add new binary variable
```
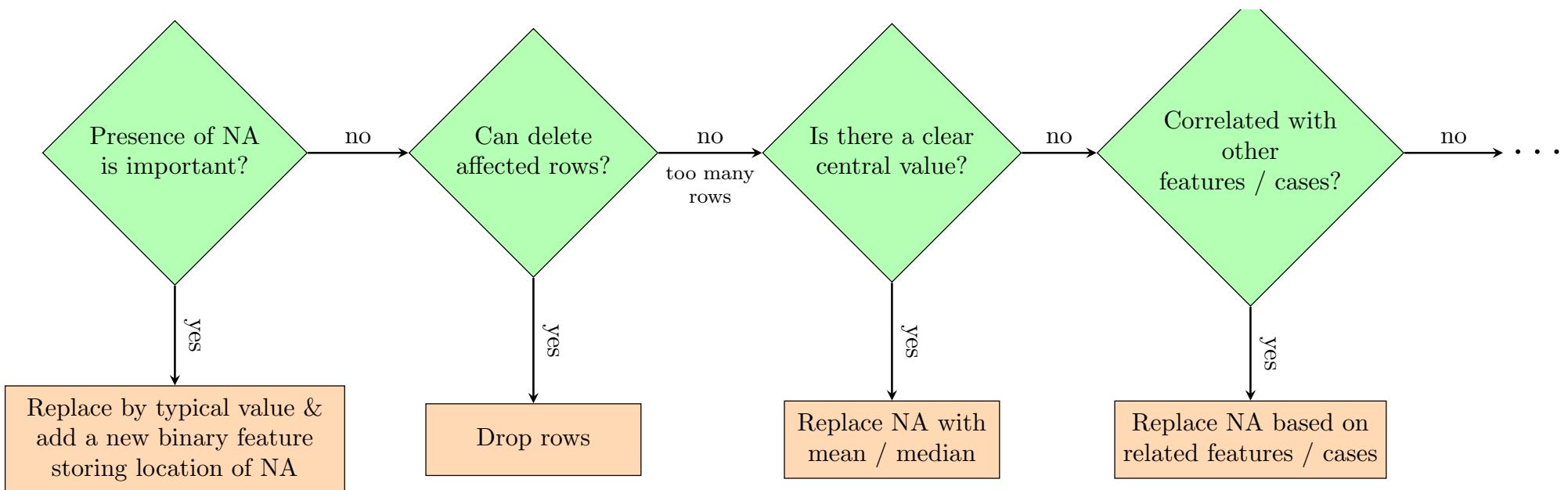
In terms of our three datasets, only `Titanic` has missing values in categorical features:

- Location of `cabin`'s missing values are important (1st class passengers were most likely to have a cabin) so add new category level `"Unknown"`.

- Replace `Embarked`'s 2 missing values with mode (`"S"`, 644/891=72%).
  Note: Use `df.Embarked.value_counts(dropna=False)` to include missing values in count tables.

Numerical Variables — Dealing with Missing Values

```
Presence of NA          no      Can delete              no      Is there a clear        no      Correlated with         no    . . .
is important?       ─────────►   affected rows?      ─────────►  central value?      ─────────►  other               ──────►
                                                  too many                                       features / cases?
                                                    rows
     │ yes                            │ yes                          │ yes                           │ yes
     ▼                                ▼                              ▼                               ▼
Replace by typical value &                                     Replace NA with                Replace NA based on
add a new binary feature            Drop rows                  mean / median                  related features / cases
storing location of NA
```
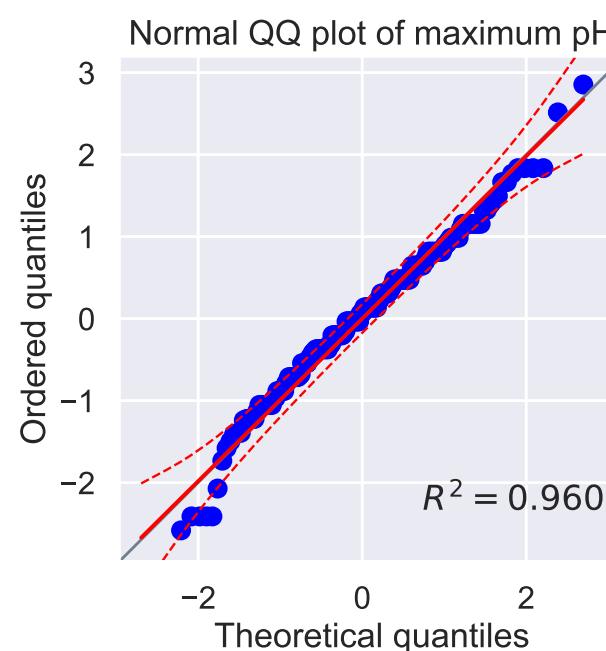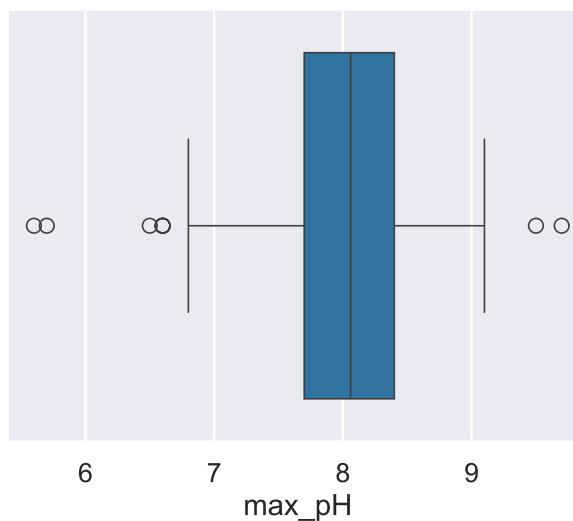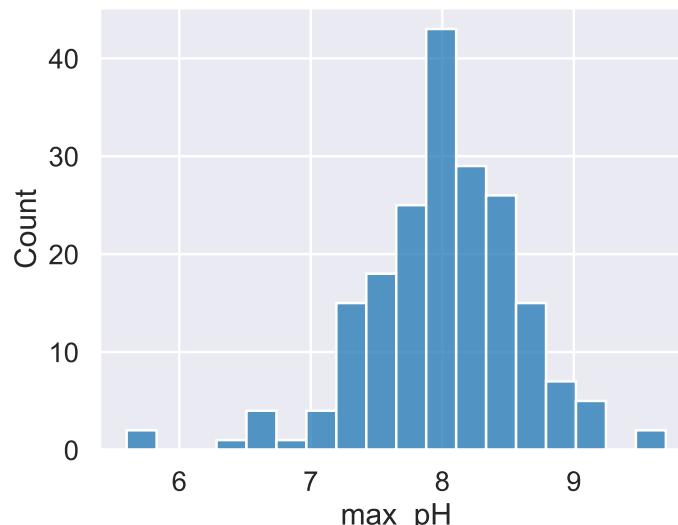
In terms of our three datasets:

- In `Titanic`, feature `Fare` appears to have no missing values, but has 15 zero entries. Are these missing values? or free tickets due to age? . . .

- In `Algae Blooms`, some of the 8 numeric features have NAs . . . next few slides.

Dataset: `Algae Blooms`, Feature: `max_pH`


```
60
df.max_pH.isna().sum()
```

`np.i`

```
count    197.000000
mean       8.019975
std        0.590169
min        5.600000
25%        7.700000
50%        8.060000
75%        8.400000
max        9.700000
Name: max_pH, dtype: float64
```

Normal QQ plot of maximum pH

$R^2 = 0.960$

- Data is relatively normal — minor issue with (left) outliers.
⇒ Will replace (single) NA by mean

```
61
df.max_pH.fillna(df.max_pH.mean(), inplace=True)
```
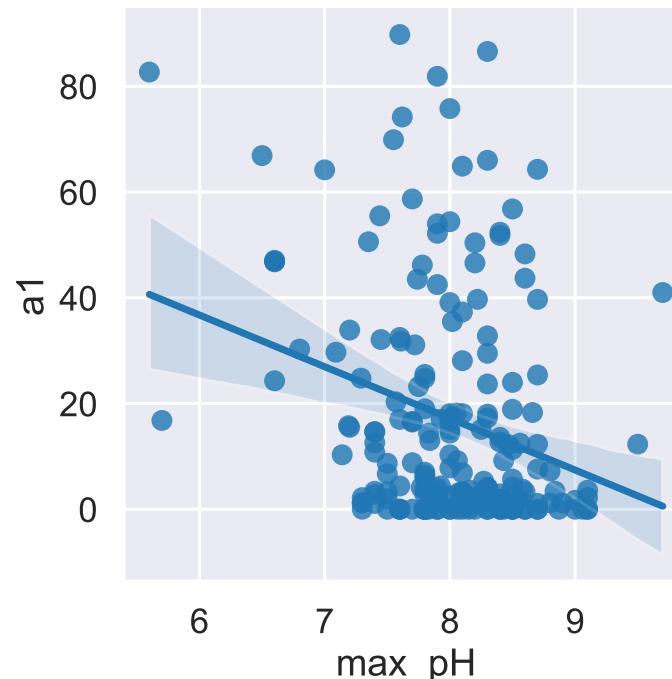
Dataset: `Algae Blooms`, Feature: `max_pH`, Target: `a1`

Is there a relationship between feature `max_pH` and target `a1`?

62 `df[["max_pH", "a1"]].corr()`

63 `sns.lmplot(x="max_pH", y="a1", data=df)`

	max_pH	a1
max_pH	1.000000	-0.268539
a1	-0.268539	1.000000
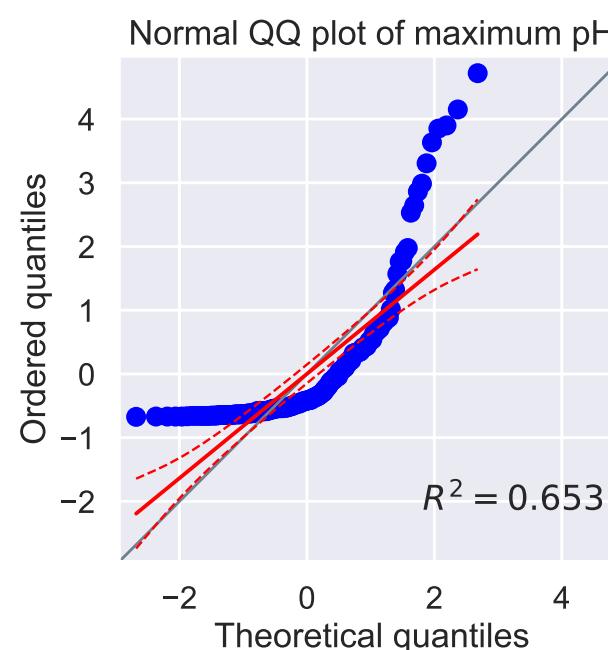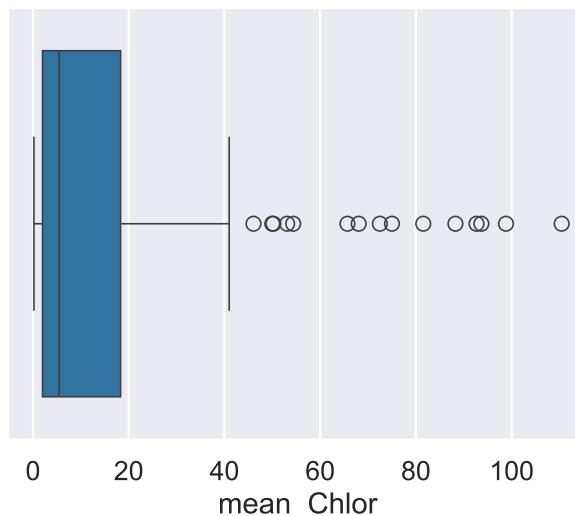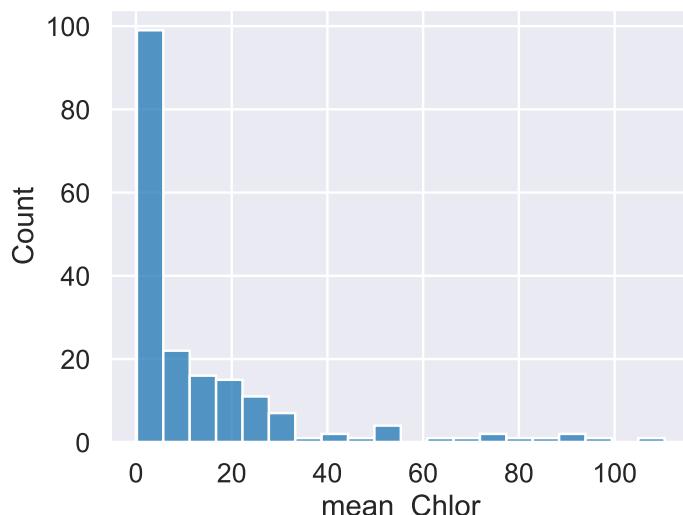
(Pearson's) Correlation coefficient, r, measures the strength of a **linear** relationship between two numerical variables.
- near zero means no/weak linear relationship.
- near ± 1 zero means strong linear relationship.
- sign indicates direction.

- Correlation coefficient, $r = -0.27$, shows (at most) a weak negative linear relationship.
- No obvious relationship visible in scatter plot.

Dataset: `Algae Blooms`, Feature: `mean_Chlor`

Normal QQ plot of maximum pH

$R^2 = 0.653$

```
64 df.mean_Chlor.isna().sum()
                                    np.i
```

```
count     188.000000
mean       13.971197
std        20.495920
min         0.200000
25%         2.000000
50%         5.475000
75%        18.307500
max       110.456000
Name: mean_Chlor, dtype: float
```

- Data is not normal, heavily skewed to the right $\Rightarrow$ mean is a poor representative of the central location.

$\Rightarrow$ Will replace (single) NA by median

```
65 df.mean_Chlor.fillna(df.mean_Chlor.median(), inplace=True)
```

After Target and Individual Feature Pass — Where are we?   I

> Tips

- Reviewed each feature — location, spread, shape, issues.
- No missing values
- `total_bill`, and `total_tip` have possible outliers.

> Titanic

- Reviewed each feature — location, spread, shape, issues.
- Generated ToDo list for for cleaning, feature extraction
    - Identified features that appear to be related to the target.
    - Feature `age` has missing values.
    - Feature `Fare`
        - has 15 measurements with value 0 — decide missing value or not.
        - distribution has large outliers and is skewed — remove/fix outliers and transform.
    - Feature `Name` has could be used to obtain new feature `Title`.
    - . . .

> Algae Blooms

- Reviewed each feature — location, spread, shape, issues.
- Imputed missing values using feature distributions (mean/median).
- Identified features that appear to be related to the target.

Aside: Steps needed to create new feature `Title` from feature `Name`

```
df = pd.read_csv('assets/train.csv')
df.head()
```
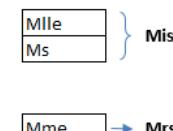
	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28		
				Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.925		
				Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
				Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S

1 Have a (text) feature representing the passenger's name.

Title	Count
Capt	1
Col	4
Don	1
Dona	1
Dr	8
Jonkheer	1
Lady	1
Major	2
Master	61
Miss	260
Mlle	2
Mme	1
Mr	757
Mrs	197
Ms	2
Rev	8
Sir	1
the Countess	1

2 Rare categories can be merged under a single label – 'Dona', 'Lady', 'the Countess', 'Capt', 'Col', etc. .
Duplicate/redundant categories can be merged – the titles 'Mlle', and 'Ms' and can be merged under 'Miss'. 'Mme' can be merged with 'Mrs'.

Capt	
Col	
Don	
Dona	
Dr	rare_title
Jonkheer	
Lady	
Major	
Rev	
Sir	
the Countess	

Mlle	Miss
Ms	

Mme	→ Mrs

3 New categorical feature with 5 unique values

Master	Miss	Mr	Mrs	rare_title
61	264	757	198	29

Third Pass — Relationships Between Features (and Target)

- Correlations

Correlations — Relationship Between two Variables

⟩Pearson's correlation coefficient,*r*⟩

is a measure of linear correlation between two variables. Its value lies between -1 and +1, -1 indicating total negative linear correlation, 0 indicating no linear correlation and 1 indicating total positive linear correlation.

⟩Spearman's rank correlation coefficient, ρ⟩

is a measure of monotonic correlation between two variables, and is therefore better in catching nonlinear monotonic correlations than Pearson's *r*. Its value also lies between -1 and +1, with values near zero indicating no monotonic relation.

⟩Kendall rank correlation coefficient, τ⟩

measures ordinal association between two variables. Its value lies between -1 and +1 with values near zero indicating no relation.

⟩Phi-k, ϕk⟩
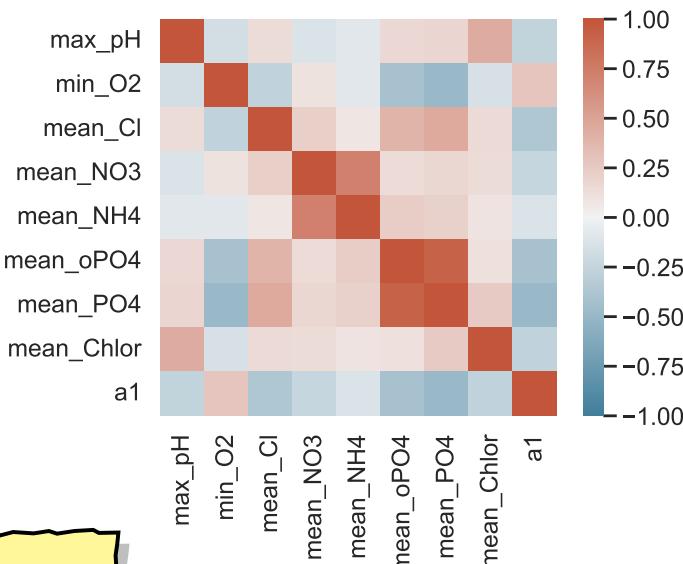
is a new and practical correlation coefficient that works consistently between categorical, ordinal and interval variables, captures non-linear dependency and reverts to the Pearson correlation coefficient in case of a bivariate normal input distribution. Its value also lies between 0 and +1, with values near zero indicating no relation.

Pearson's Correlation Coefficient — Dataset: `Algae Blooms`

66
```python
columns = df.columns[3:12]
corr = df[columns].corr()
corr
```

67
```python
cmap = sns.diverging_palette(230, 20, as_cmap=True)
sns.heatmap(corr, square=True, vmin=-1, vmax=1, cmap=cmap)
plt.show()
```

|	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1
max_pH	1.000000	-0.167981	0.136369	-0.130762	-0.093521	0.158769	0.179885	0.445864	-0.268539
min_O2	-0.167981	1.000000	-0.278333	0.099444	-0.087478	-0.416163	-0.487486	-0.153265	0.285564
mean_Cl	0.136369	-0.278333	1.000000	0.225041	0.071913	0.391054	0.457449	0.149856	-0.371171
mean_NO3	-0.130762	0.099444	0.225041	1.000000	0.721444	0.144588	0.168601	0.139679	-0.241211
mean_NH4	-0.093521	-0.087478	0.071913	0.721444	1.000000	0.227237	0.208180	0.088947	-0.132656
mean_oPO4	0.158769	-0.416163	0.391054	0.144588	0.227237	1.000000	0.914365	0.115621	-0.417358
mean_PO4	0.179885	-0.487486	0.457449	0.168601	0.208180	0.914365	1.000000	0.253621	-0.487023
mean_Chlor	0.445864	-0.153265	0.149856	0.139679	0.088947	0.115621	0.253621	1.000000	-0.277987
a1	-0.268539	0.285564	-0.371171	-0.241211	-0.132656	-0.417358	-0.487023	-0.277987	1.000000
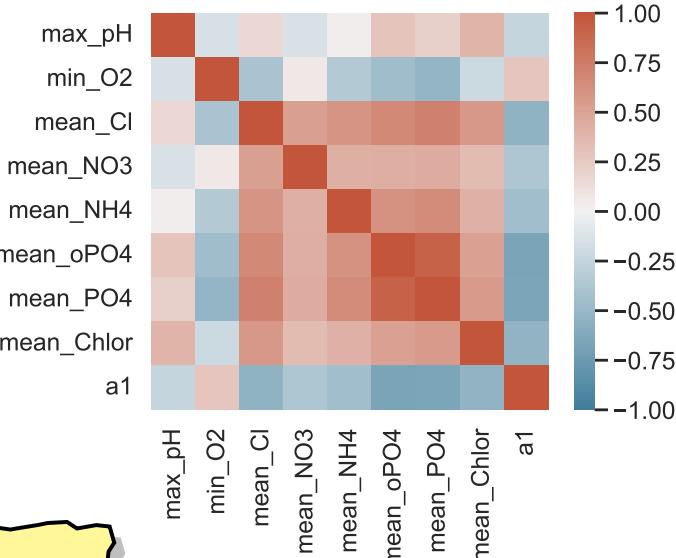
- Categorical variables are not included.
- Suggests best predictors for `a1` are `mean_PO4`, `mean_oPO4`, and `meanCl`.
- `mean_PO4` and `mean_oPO4` are highly correlated (0.91) — could use values of one to estimate missing values of the other.

Spearman's Rank Correlation Coefficient — Dataset: `Algae Blooms`

```python
columns = df.columns[3:12]
corr = df[columns].corr(method='spearman')
corr
```

```python
cmap = sns.diverging_palette(230, 20, as_cmap=Tr
sns.heatmap(corr, square=True, vmin=-1, vmax=1,
plt.show()
```

|	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1
max_pH	1.000000	-0.148676	0.159079	-0.145182	0.026160	0.290245	0.214569	0.394813	-0.247787
min_O2	-0.148676	1.000000	-0.405142	0.057610	-0.348226	-0.457805	-0.519786	-0.217714	0.283418
mean_Cl	0.159079	-0.405142	1.000000	0.530374	0.592052	0.670399	0.713479	0.564915	-0.546845
mean_NO3	-0.145182	0.057610	0.530374	1.000000	0.425010	0.432303	0.451272	0.346805	-0.382403
mean_NH4	0.026160	-0.348226	0.592052	0.425010	1.000000	0.603157	0.646690	0.406656	-0.449194
mean_oPO4	0.290245	-0.457805	0.670399	0.432303	0.603157	1.000000	0.914921	0.510930	-0.671019
mean_PO4	0.214569	-0.519786	0.713479	0.451272	0.646690	0.914921	1.000000	0.554167	-0.656670
mean_Chlor	0.394813	-0.217714	0.564915	0.346805	0.406656	0.510930	0.554167	1.000000	-0.537823
a1	-0.247787	0.283418	-0.546845	-0.382403	-0.449194	-0.671019	-0.656670	-0.537823	1.000000
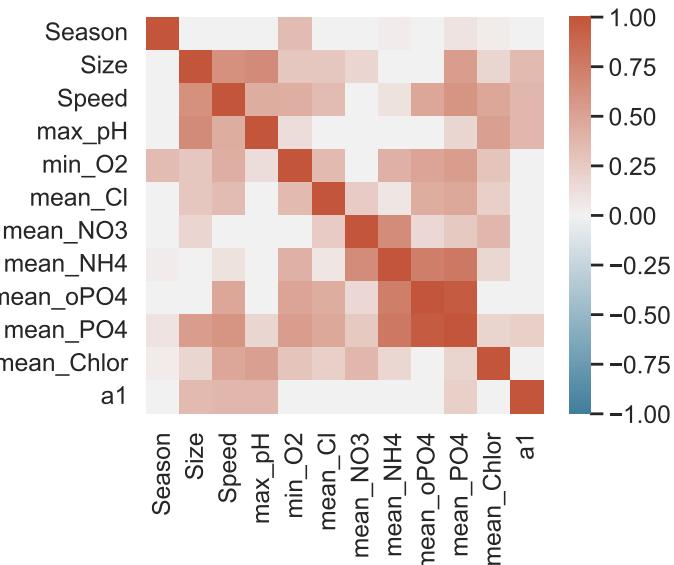
- Now best predictors for `a1` also include `mean_Chlor` and `mean_NH4`.

Phik Correlation Coefficient — Dataset: `Algae Blooms`

```python
import phik
columns = df.columns[:12]
corr = df[columns].phik_matrix()
corr
```

```python
cmap = sns.diverging_palette(230, 20, as_cmap=Tr
sns.heatmap(corr, square=True, vmin=-1, vmax=1,
plt.show()
```

|	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO3	mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a1
Season	1.000000	0.000000	0.000000	0.000000	0.343496	0.000000	0.000000	0.034202	0.000000	0.093199	0.045361	0.000000
Size	0.000000	1.000000	0.620101	0.655207	0.270013	0.268198	0.182410	0.000000	0.000000	0.531635	0.173516	0.353390
Speed	0.000000	0.620101	1.000000	0.445096	0.437356	0.339237	0.000000	0.101348	0.483298	0.594480	0.479735	0.369374
max_pH	0.000000	0.655207	0.445096	1.000000	0.125231	0.000000	0.000000	0.000000	0.000000	0.175105	0.528134	0.372031
min_O2	0.343496	0.270013	0.437356	0.125231	1.000000	0.353196	0.000000	0.416999	0.492457	0.535996	0.296376	0.000000
mean_Cl	0.000000	0.268198	0.339237	0.000000	0.353196	1.000000	0.243887	0.073692	0.443047	0.472824	0.225583	0.000000
mean_NO3	0.000000	0.182410	0.000000	0.000000	0.000000	0.243887	1.000000	0.642789	0.158463	0.259915	0.368142	0.000000
mean_NH4	0.034202	0.000000	0.101348	0.000000	0.416999	0.073692	0.642789	1.000000	0.734681	0.776197	0.167533	0.000000
mean_oPO4	0.000000	0.000000	0.483298	0.000000	0.492457	0.443047	0.158463	0.734681	1.000000	0.954601	0.000000	0.000000
mean_PO4	0.093199	0.531635	0.594480	0.175105	0.535996	0.472824	0.259915	0.776197	0.954601	1.000000	0.192920	0.221308
mean_Chlor	0.045361	0.173516	0.479735	0.528134	0.296376	0.225583	0.368142	0.167533	0.000000	0.192920	1.000000	0.000000
a1	0.000000	0.353390	0.369374	0.372031	0.000000	0.000000	0.000000	0.000000	0.000000	0.221308	0.000000	1.000000
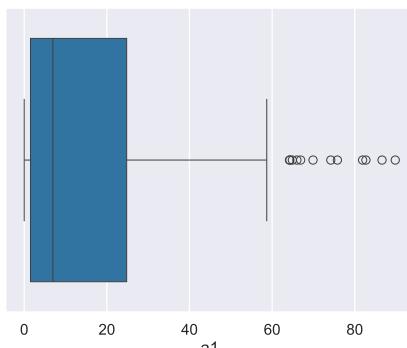
- Now include categorical variables — `Season` is not related, but `Size` and `Speed` are.

Multi-Relation Plots
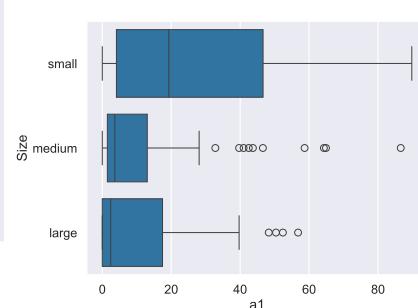

```
sns.boxplot(x="a1", data=df)
```
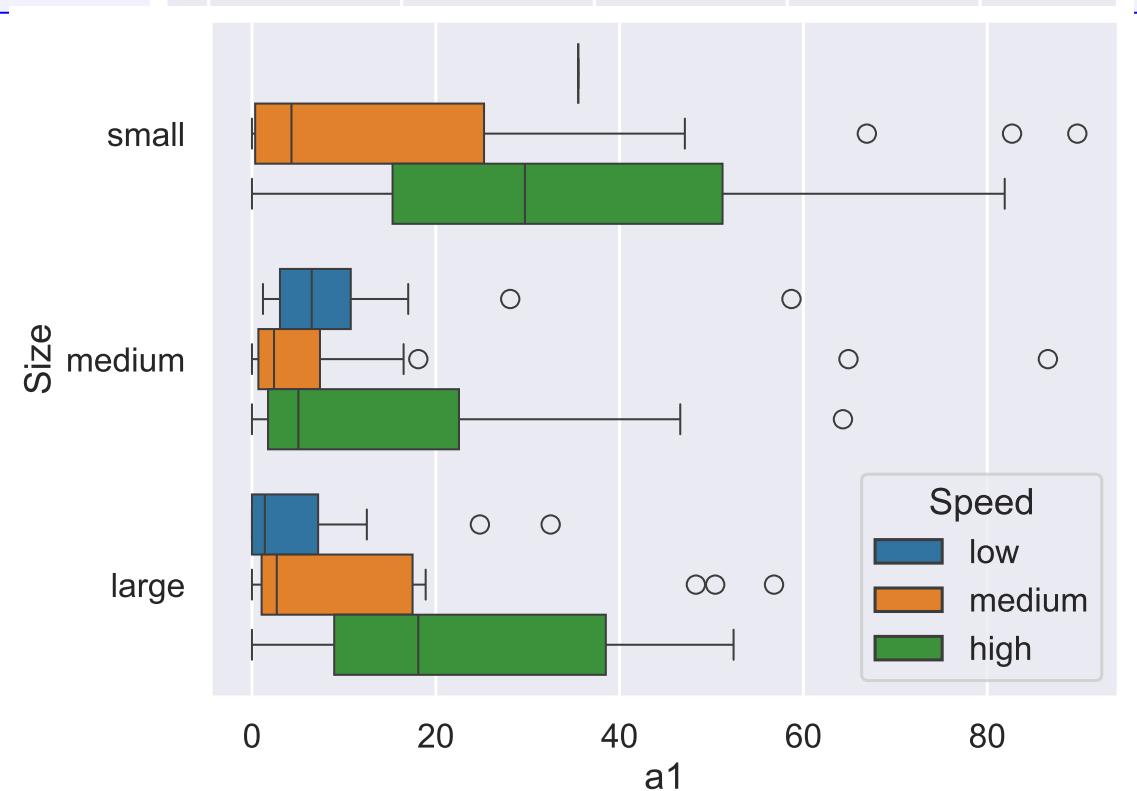
```
sns.boxplot(x="a1", y="Size", data=df)
```

```
sns.boxplot(x="a1", y="Size", hue="Speed", data=df)
```

- If have n features, then have $n(n-1)$ possible visualisations — gets a bit crazy.

After Third Pass — Where are we?

- Reviewed each feature — location, spread, shape, issues.

- Identified any correlation among features and with target.

- Located and resolved missing values.

- Generated list of possible feature engineering tasks.

Resources

Resources

> Guides

- 1 hour, Youtube on generating seaborn plots — excellent (but has wrong on interpretation of box plot)

  `https://www.youtube.com/watch?v=6GUZXDef2U0&t=1363s`

> Articles on Exploratory Data Analysis

- Titanic Survival Dataset Part 1/2: Exploratory Data Analysis (9 min read)

  `https://www.kaggle.com/mcromao/titanic-exploratory-data-analysis`

- Titanic - Exploratory Data Analysis

  `https://becominghuman.ai/`

  `titanic-survival-dataset-part-1-2-exploratory-data-analysis-5b98f7917913`

- When Should You Delete Outliers from a Data Set?

  `https://humansofdata.atlan.com/2018/03/when-delete-outliers-dataset`