(MSc) Data Mining

Topic 02: Exploratory Data Analysis

Part 01 : Exploratory Data Analysis

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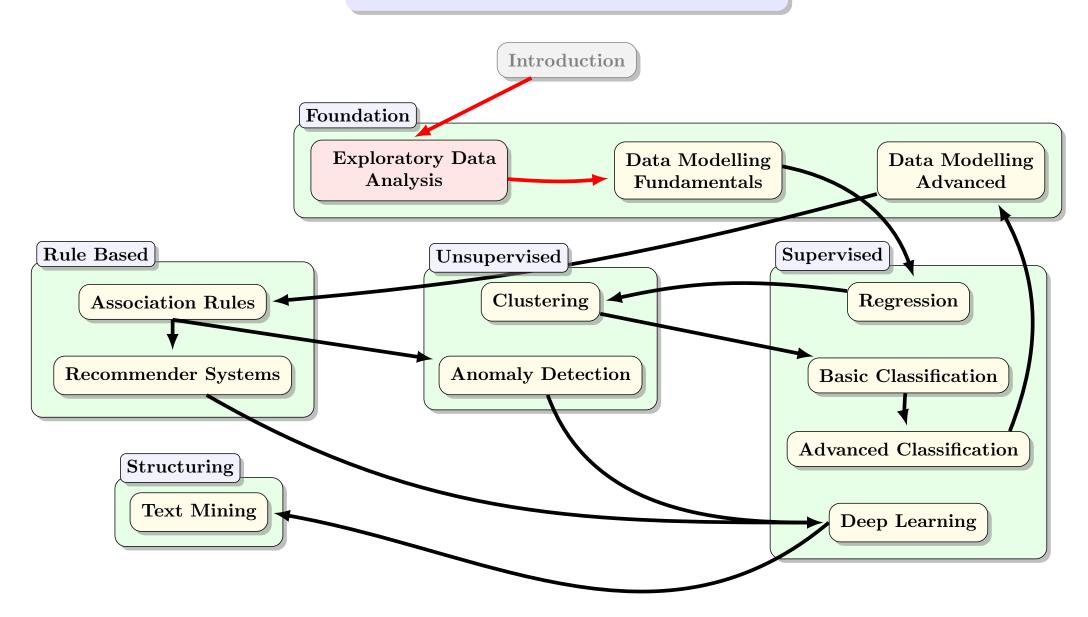
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Spring Semester, 2025

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)



Exploratory Data Analysis — Summary

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Exploratory Data Analysis (EDA)

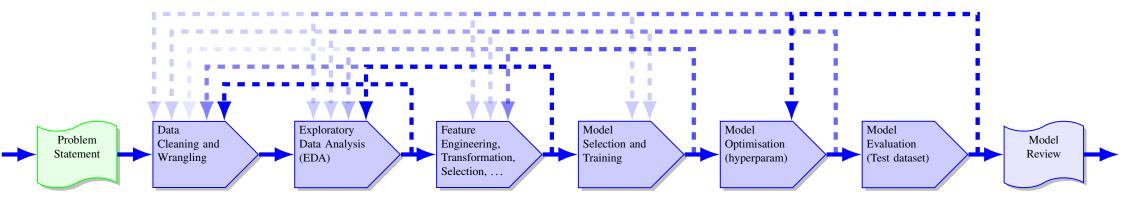
Aim

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

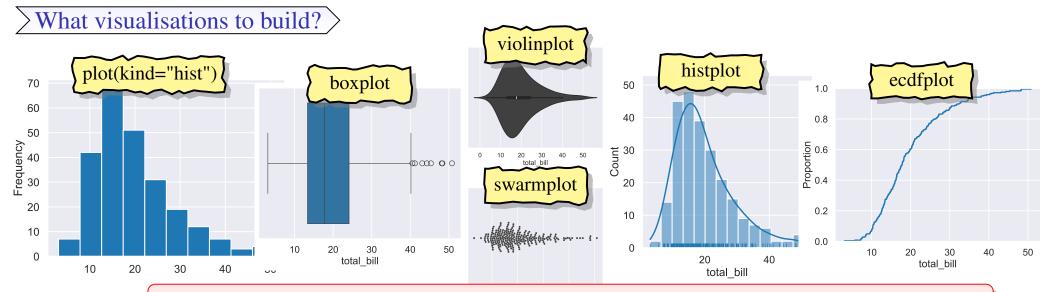


- Data pre-precessing (Data Cleaning + EDA + Feature Engineering) is the core of the data mining pipeline (typical estimates >50% of the time/effort).
- Decision made during earlier steps in the workflow impact on later steps.
 - Better data cleaning simplifies EDA.
 - EDA informs the feature extraction, 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'

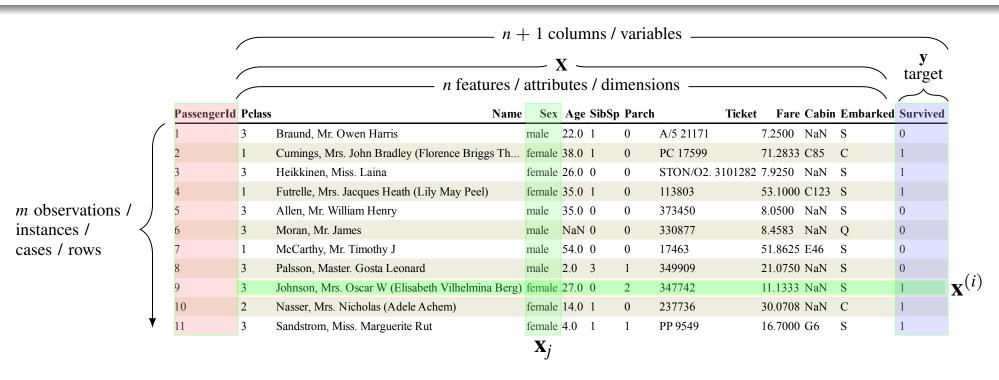
What questions to ask?

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? ...



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

Terminology / Notation



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

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	2 mean_C	Cl mean_	NO3 mean_NH4	mean_oPO4	mean_PO4	mean_Chlor	a 1	a2	a3	a4	a5	a6	a 7
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	sn	How w	vell can	we pre	dict the	(7) diffe	erent algae pop	ulation leve	ls using w	ater sample	info	orma	tion	?	0.0	0.0	1.7
10	spring	small	hìgh	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

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Introduction Example Datasets

Titanic dataset

_	PassengerId	Survived	Pclass	Na	ıme	Sex	Age	SibSp	Parch		Ticket	Fare	Cabin	Embarke
0	1	0	3	Braund, Mr. Owen Harris			22.0		0	A/5 21171		7.2500		S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th					0	PC 17599		71.2833		C
2	3	1	3	Heikkinen, Miss. Laina		male			0	STON/O2. 3				
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	fe	male	35.0	1	0	113803		53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry			35.0		0	373450		8.0500		S
5	6	0	3	Moran, Mr. James	m	ale	NaN	0	0	330877		8.4583	NaN	Q
6	7	0	1	McCarthy, Mr. Timothy J	m	ale	54.0	0	0	17463		51.8625		S
7	8	0	3	Palsson, Master. Gosta Leonard	m	ale	2.0	3	1	349909		21.0750	NaN	S
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Be	erg) fe	male	27.0	0	2	347742		11.1333	NaN	S
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	fe	male	14.0	1	0	237736		30.0708	NaN	С
10	11	1	3	Sandstrom, Miss. Marguerite Rut	fe	male	4.0	1	1	PP 9549		16.7000	G6	S
11	12	1	<u>ب</u>		مبہ	<u> </u>	جمم	<u> </u>	~~	112200	~~	ومعجم	C103	S
12	13	0	How v	well can we predict a passenger's surviv	val u	sing	ınto	rmati	on at	time of de	parture	e?	NaN	S
13	14	0	3	Andersson, Mr. Anders Johan	m	ale	39.0	1	5	347082		31.2750	NaN	S
14	15	0	3	Vestrom, Miss. Hulda Amanda Adolfina	fe	male	14.0	0	0	350406		7.8542	NaN	S
15	16	1	2	Hewlett, Mrs. (Mary D Kingcome)	fe	male	55.0	0	0	248706		16.0000	NaN	S
16	17	0	3	Rice, Master. Eugene	m	ale	2.0	4	1	382652		29.1250	NaN	Q
17	18	1	2	Williams, Mr. Charles Eugene	m	ale	NaN	0	0	244373		13.0000	NaN	S
18	19	0	3	Vander Planke, Mrs. Julius (Emelia Maria Vande	e fe	male	31.0	1	0	345763		18.0000	NaN	S
19	20	1	3	Masselmani, Mrs. Fatima	fe	male	NaN	0	0	2649		7.2250	NaN	C
20	21	0	2	Fynney, Mr. Joseph J	m	ale	35.0	0	0	239865		26.0000	NaN	S 1
21	22	1	2	Beesley, Mr. Lawrence	m	ale	34.0	0	0	248698		13.0000	D56	S
22	23	1	3	McGowan, Miss. Anna "Annie"	fe	male	15.0	0	0	330923		8.0292	NaN	Q
23	24	1	1	Sloper, Mr. William Thompson	m	ale	28.0	0	0	113788		35.5000	A6	S

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. . . .

ates more details and nicer visualisations.

```
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.

pingouin overlaps with bits of scipy.stats and statsmodels but gener-

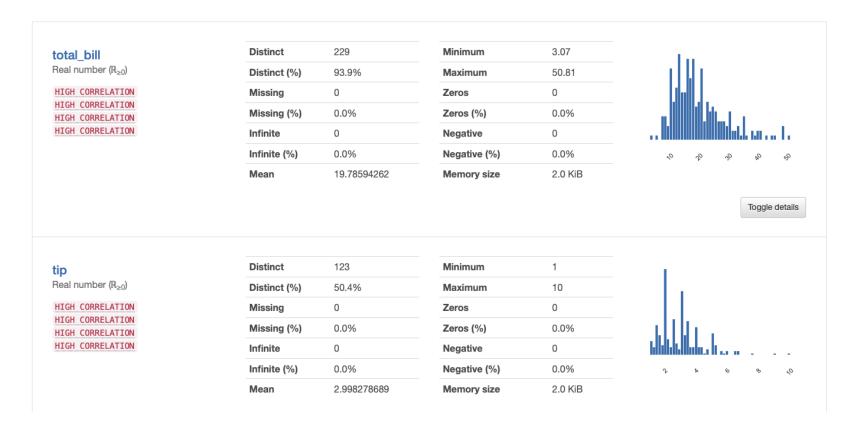
Finally we set options ...

```
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

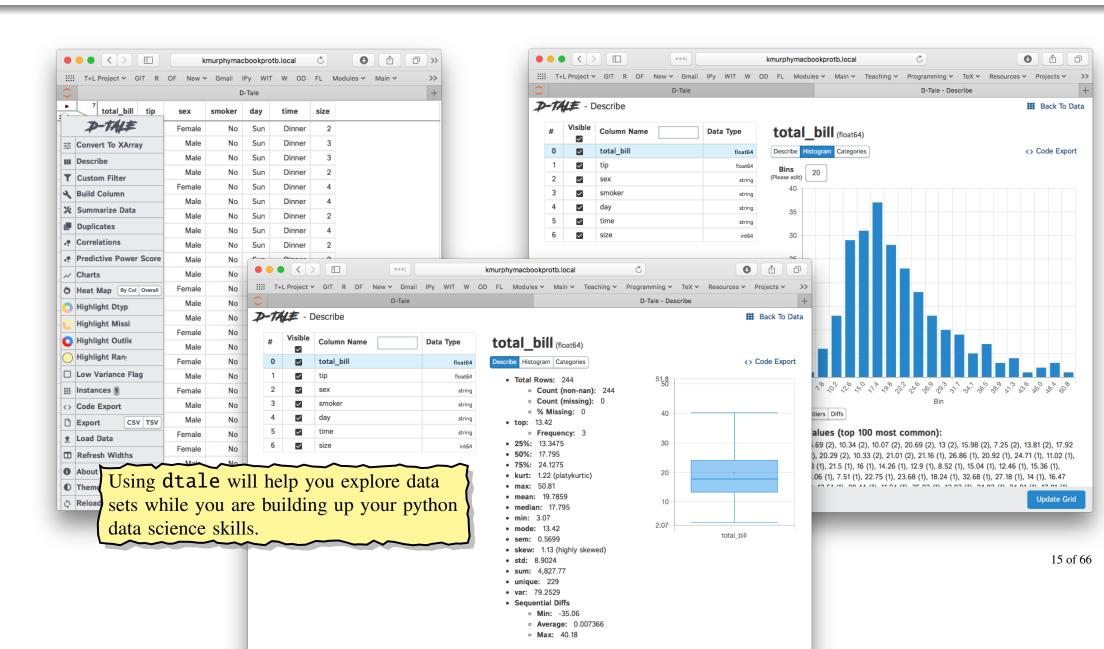


Variables



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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

	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
              244 non-null
                           float64
    tip
              244 non-null
                           object
    sex
    smoker
              244 non-null
                           object
          244 non-null
                           object
    day
              244 non-null
                           object
    time
    size
              244 non-null
                           int64
dtypes: float64(2), int64(1), object(4)
memory usage: 13.5+ KB
```

Issue: categorical data treated as object (string).

Tips — Fix Data Types

```
df.smoker.unique()
df.sex.unique()
array(['Female', 'Male'], dtype=object)
                                                      array(['No', 'Yes'], dtype=object)
df.sex = pd.Categorical(df.sex)
                                                      df.smoker = pd.Categorical(df.smoker)
df.sex.unique()
                                                      df.smoker.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.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']</pre>
```

Tips — Fix Data Types

```
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:

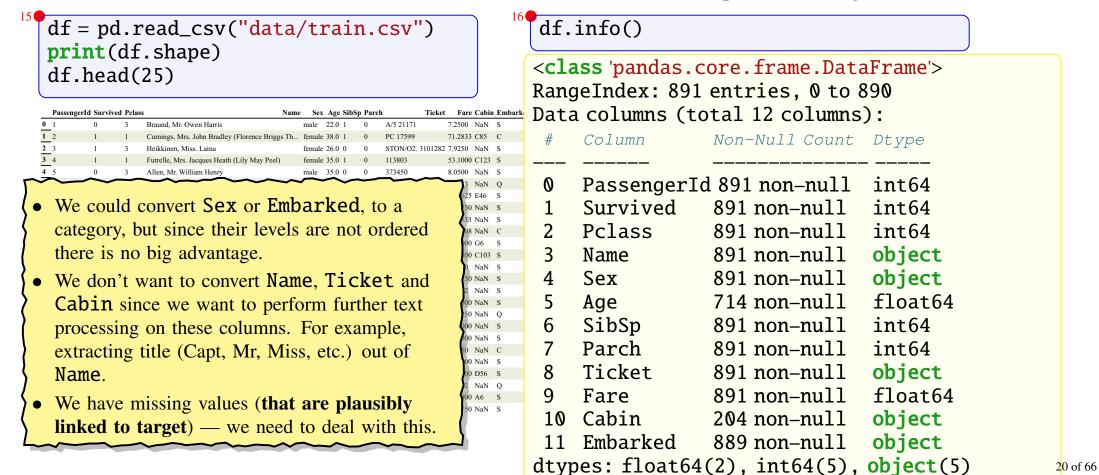
- Simplify visualisation (order can be preserved).
- Reduce memory usage (not that big a deal for us).
- Speed up I/O (depending on file format).
- ⇒ Converting to category is a bigger deal for features where the levels have an order.

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
```

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

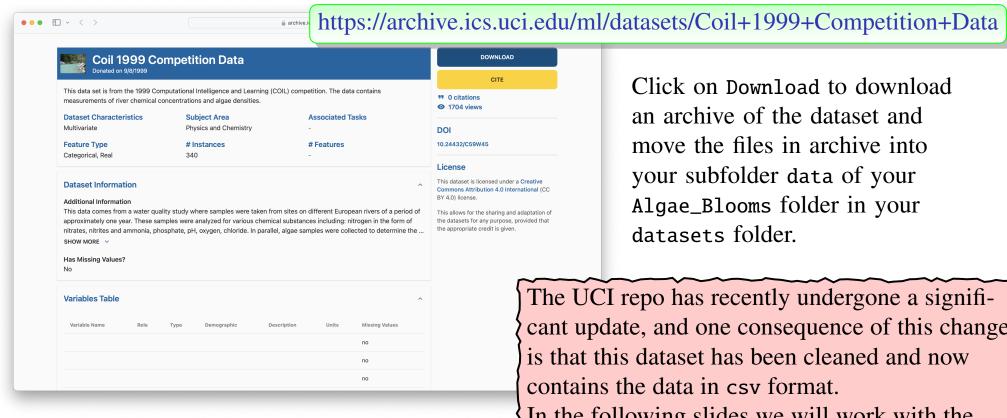
Titanic — Load

- 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.



memory usage: 83.7+ KB

$Algae_Blooms - Load$



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.

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

```
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)

```
df = pd.read_table('data/analysis.txt', sep='\s+', header=None)

print(df.shape)
df.head()

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

ouinter 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 "\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 a4 **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 <class 'pandas.core.frame.DataFrame'> 370.0000 1 spring small medium 8.35000 8.00000 57.75000 1.28800 RangeIndex: 200 entries, 0 to 199 2 autumn small medium 8.10000 11.40000 40.02000 5.33000 346.6669 Data columns (total 18 columns): spring small medium 8.07000 4.80000 77.36400 2.30200 98.18200 Column Non-Null Count Dtype **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.

```
object
              200 non-null
0
   Season
   Size
              200 non-null
                             object
                             object
   Speed
              200 non-null
3
   max_pH
                             object
              200 non-null
4
                             object
   min_02
              200 non-null
                             object
5
   mean Cl
              200 non-null
6
              200 non-null
                             object
   mean_NO3
7
   mean NH4
              200 non-null
                             object
              200 non-null
                             object
   mean_oPO4
                                            24 of 66
9
   mean PO4
                             object
              200 non-null
   mean_Chlor 200 non-null
                             object
11
   a1
               200 non-null
                             float64
12
   a2
               200 non-null
                              float64
```

Algae_Blooms — Load (4th attempt)

Season	Size	Speed max	_pH min	_O2 mean_	_Cl mean_	_NO3_mean_N	NH4 mean	_oPO4 m	ean_PO4	mean	_Chlor	a1	a2	a3	a4	a5	a6	a7
0 winter	small	medium 8.00	9.8	60.800	6.238	578.000	000 105.00	00 17	70.00000	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	370.000	clas	s 'pand	as.co	re.fı	rame.	Dat	aFr	ame	!'>			1
2 autumn	small	medium 8.10	11.4	40.020	5.330	346.666	Range Data o	ınaex:	200 e. s (tot	ntri al 18	es, w	TO imns	:). 199					7
3 spring	small	medium 8.07	4.8	77.364	2.302	98.1820	W1	olumn										4
4 autumn	small	medium 8.06	9.0	55.350	10.416	5 233.700								<u></u>)

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
   Season
   Size
                             object
              200 non-null
   Speed
                             object
              200 non-null
3
              199 non-null
                             float64
   max_pH
   min_02
              198 non-null
                             float64
              190 non-null
                             float64
   mean_Cl
   mean_NO3
              198 non–null
                             float64
   mean NH4
              198 non-null
                             float64
   mean_oPO4 198 non-null
                             float64
                                           25 of 66
9
   mean PO4
              198 non-null
                             float64
   mean Chlor 188 non-null
                             float64
11
   a1
              200 non-null
                             float64
12
   a2
              200 non-null
                             float64
```

Algae_Blooms — Fix Data Types

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=Ti
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>
```

Algae_Blooms — Identification of Missing Values (NA)

Which columns have missing values?

df.isna().sum()

Season 0 Size Speed max_pH min_02 mean Cl mean_NO3 mean_NH4 mean_oP04 mean_P04 mean Chlor a 1 a2 **a**3 a4 a5 a6 a7 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 ⇒ remove.
- Removing other rows with a NA will result in a loss 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()

0 184 1 7 2 7 6 2

Name: count, dtype: int64

Rows / Cols to drop?

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

	Season	Size	Speed	max_pH	min_O	z mean_	_CI_mean_	NO3 mean_	NH4 mean_	_oPO4_mean_	_PO4_mean_	Chior al	l az	a3	a 4
61	summer	small	medium	6.4	NaN	NaN	NaN	NaN	NaN	14.0	NaN	19.4	1 0.0	0.0	2.0
19	winter	large	medium	8.0	7.6	NaN	NaN	NaN	NaN	NaN	NaN	0.0	12.5	3.7	1.0

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

After Loading and Initial Clean — Where are we?

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? \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('output/analysis.csv', index=False)
```

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

```
df.to_pickle('output/analysis.pkl')
```

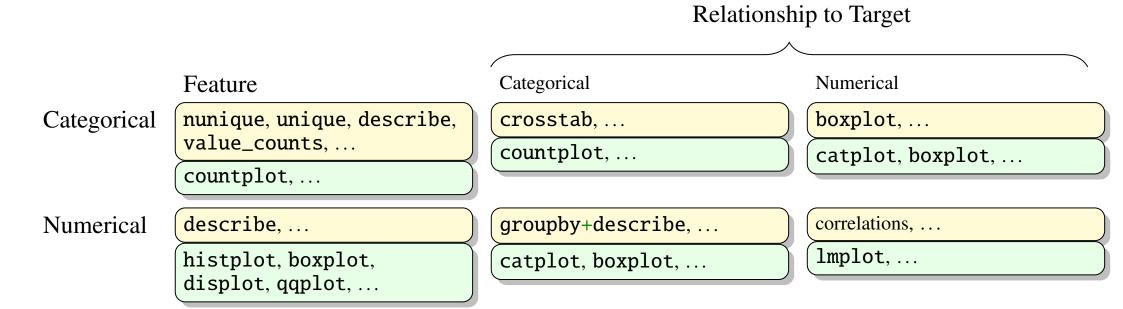
Later can read dataframe back in using

```
df = pd.read_pickle('output/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('output/analysis_sample.pkl)
```

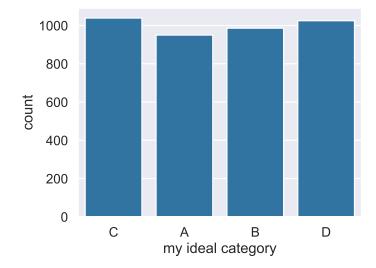
A Selection of Statistical Visualisations and Metrics



Categorical Variable

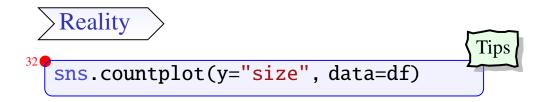
The Ideal

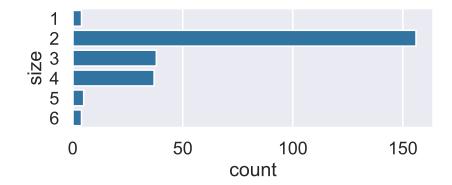
- Each level equally likely.
- Not too many levels: 2–12(ish).



Tools

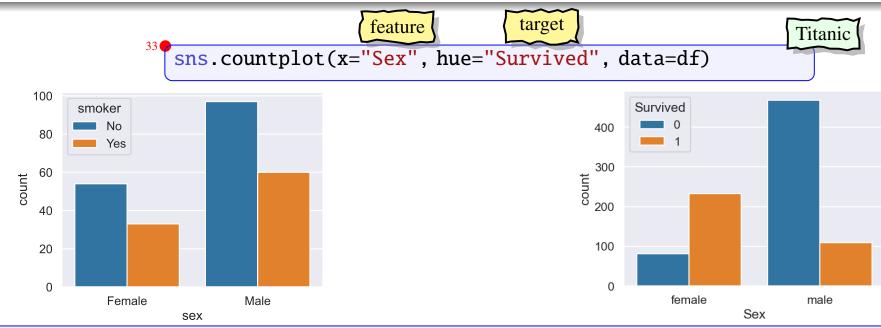
• nunique, unique, value_counts.





- 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



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

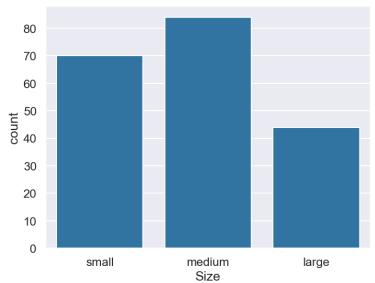
No relationship between sex and smoker

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

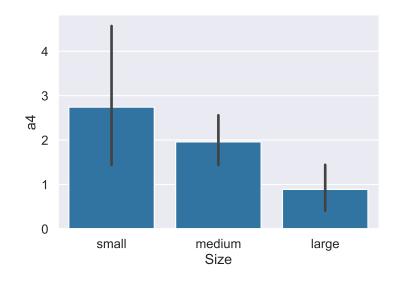
sns.countplot(x="Size", data=df)



• Shows the counts of observations in each categorical level using bar (height/width).

Is it usable?

sns.catplot(x="Size", y="a4", data=df, kind='bar')

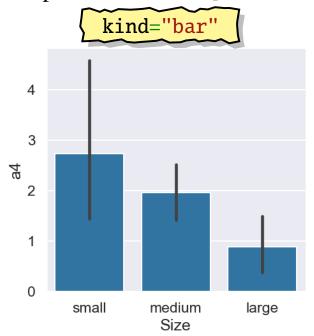


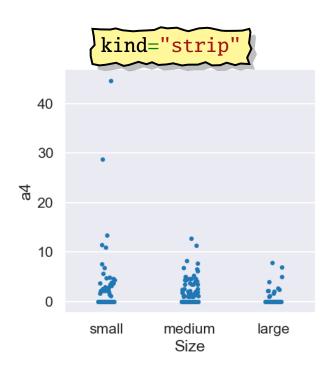
- Shows the average level (mean) and uncertainty (std) of the numerical target (a4) in each categorical level of the categorical variable.
- Vertical bar shows 95% confidence interval.

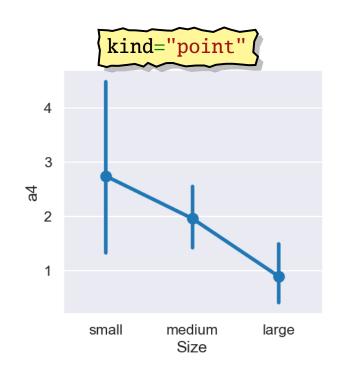
Is it useful?

Categorical Variable — Relationship with (Numerical) Target

The option kind in catplot can be:

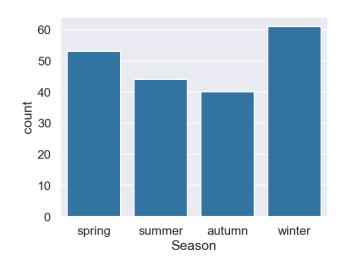


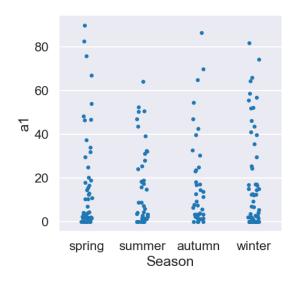


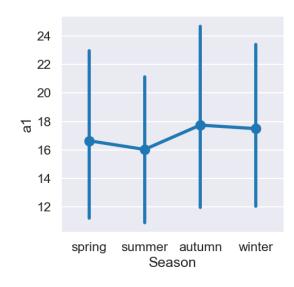


- bar and point show essentially the same information, but point is more compact when comparing multiple categorical features to a continuous target on the same plot.
- strip shows individual observations useful (as in this case) to show that the larger uncertainty in Size="small" observations is mainly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

Example — Dataset: Algae Blooms, Feature: Season, Target: a1





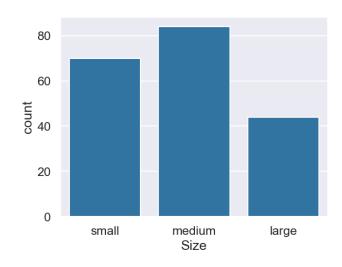


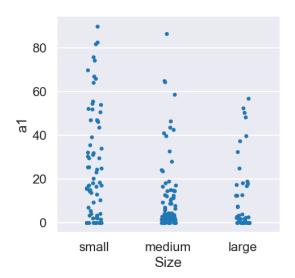
df.groupby("Season",observed=False)["a1"].agg(["mean","count","std"])

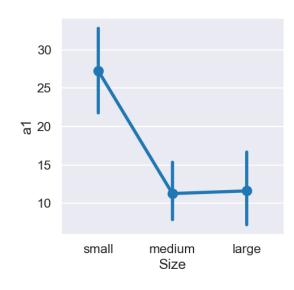
	mean	count	std
Season	\bar{x}	n	σ
spring	16.649057	53	23.093786
summer	16.038636	44	17.920798
autumn	17.745000	40	21.611203
winter	17.498361	61	22.568256

- 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).
- \Rightarrow 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







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

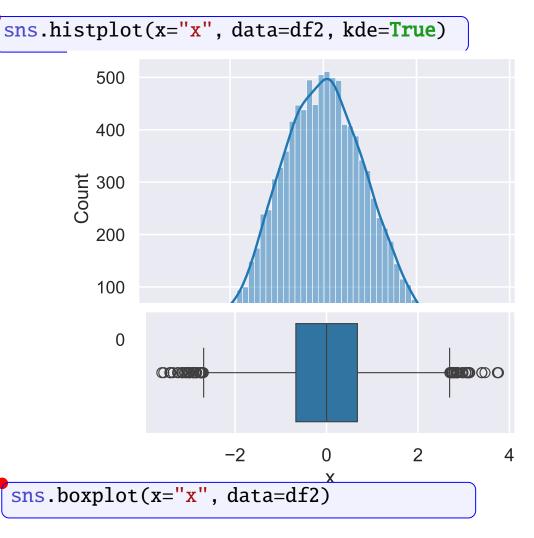
- Countplot shows no issues with feature Size.
- Catplot (point) shows that levels of a1 are higher for Size="small" observations.
- ⇒ Confidence interval for Size="small" observations do not overlap with CI for other levels, so significant relationship between categorical feature and numerical target.

Numerical Variable

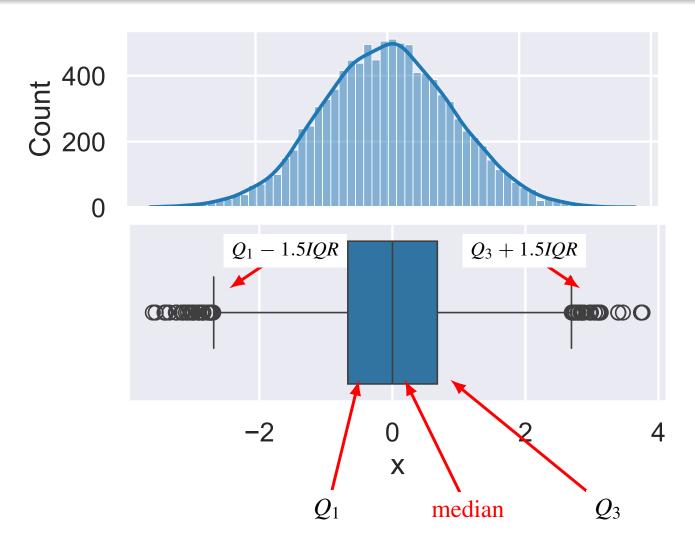
Things here are more complicated as a numerical variable could follow many different distributions. Here we look at data following the
standard normal distribution. To start we generate 10,000 values and put in to new DataFrame,
df2.

```
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
```



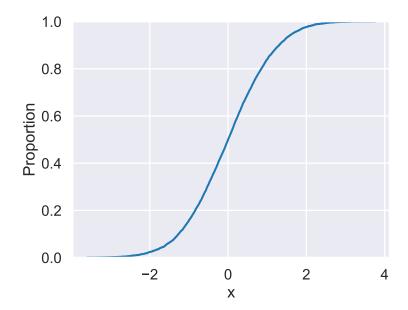
Histplot (Histogram) and Boxplot



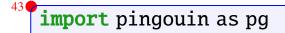
- Histogram is useful in depicting location, spread and shape.
- Curve, is estimate of shape given infinite data and infinite number of bins.
- Boxplots also depicts location, spread and shape, but uses median for estimate of centre, and quartiles for spread.
- Half the data is within the box, data points outside the whiskers (lines) are possible outliers, denoted by circles.

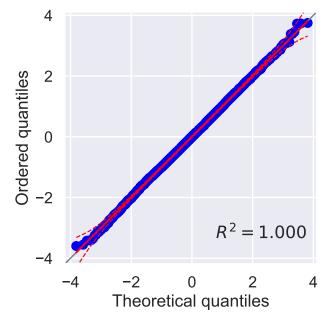
Cumulative Plot and QQ-Plot

sns.ecdfplot(data=df2, x="x")



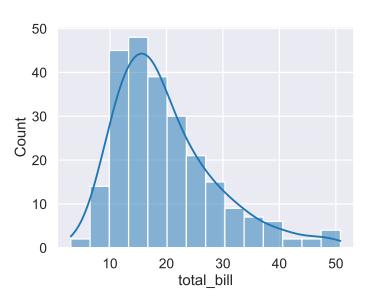
• Represents the proportion of observations less than or equal to given value.

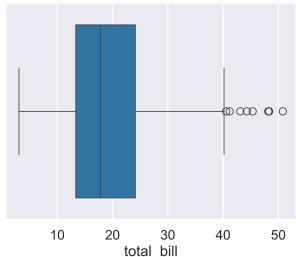


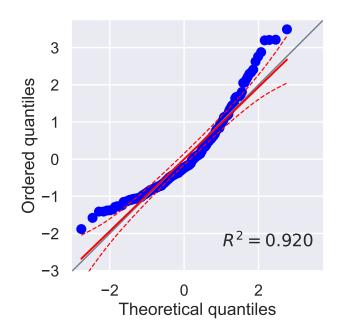


• Plot of observed quantiles against theoretical (assuming normal) quantiles. If both sets of quantiles came from the same distribution, we should see the points forming a line that's roughly straight.

Example — Dataset: Tips, Feature: total_bill





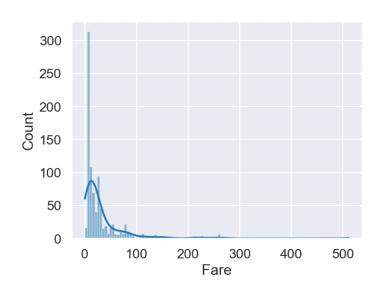


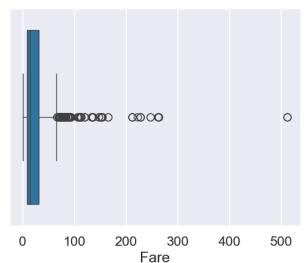
df.total_bill.describe()

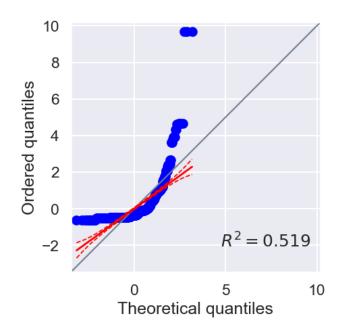
count	244.000000	
mean	19.785943	
std	8.902412	
min	3.070000	
25%	13.347500	
50 %	17.795000	
75%	24.127500	
max	50.810000	
Name:	<pre>total_bill, dtype:</pre>	flo

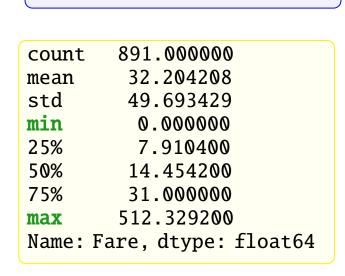
- Data is bell curve shaped, but right skewed (data is more spread out to the right).
- Outliners to the right.
- QQ-Plot indicate that data is not normal, but we could transform it to be more closer to normal.

Example — Dataset: Titanic, Feature: Fare









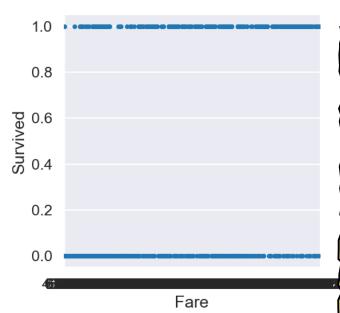
df.Fare.describe()

• This variable is more skewed and dominated by its outliers which need to be resolved.

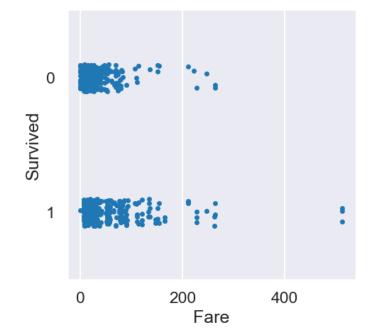
Warning — Plot Output Depends on Data Assumptions

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

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'



```
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
- Relationship to target.

Is it usable?

Is it useful?

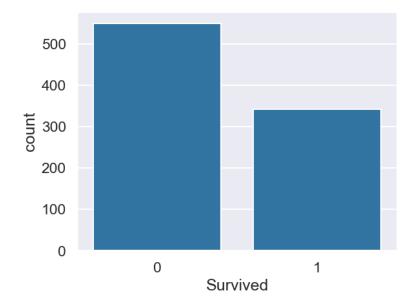
Dataset: Titanic, Target: Survived

df.Survived.value_counts(normalize=True, dropna=False)

df.Survived.unique()

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

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



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

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.

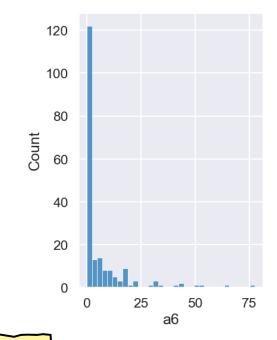
Dataset: Algae Blooms, Target: a1,..., a7

```
targets = [c for c in df.columns if c[0]=="a"]
targets ['a1', 'a2', 'a3', 'a4', 'a5', 'a6', 'a7']
```

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

df[targets].describe()

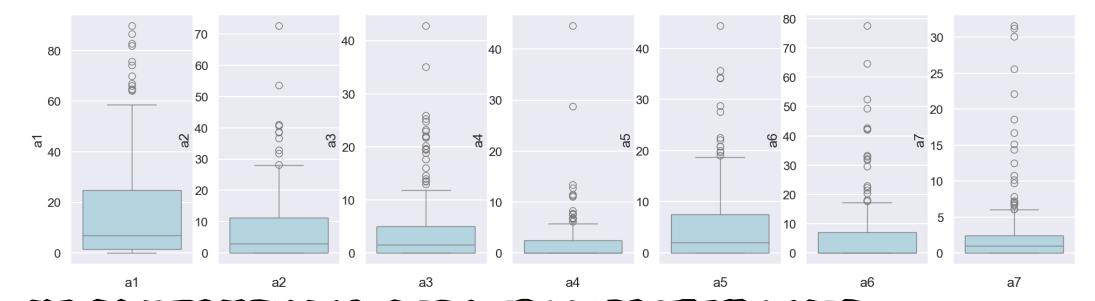
	a1	a2	a3	a4	a5	a 6	a7
count	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000
mean	16.996465	7.470707	4.334343	1.997475	5.115657	6.004545	2.487374
std	21.421713	11.065461	6.976788	4.439205	7.511846	11.711053	5.181536
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	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

```
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

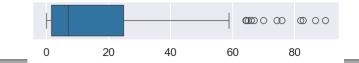
To keep this EDA overview more manageable we will focus on the Algae Blooms data set ...

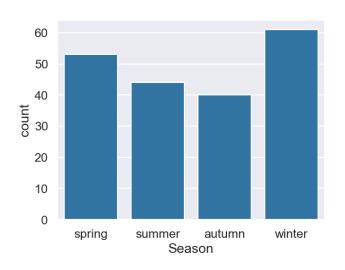
	Season	Size	Speed max_p	H min_	O2 mean_	Cl mean_	NO3 mean_N	NH4 mean_	_oPO4 mean_	_PO4 mean	_Chlor_a	1 a2	a3	a4	a5	a6	a7
0	winter	small 1	nedium 8.00	9.8	60.800	6.238	578.000	000 105.00	0000 170.00	0000 50.000	0.0	0.0	0.0	0.0	34.2	8.3	0.0
1	spring	small 1	nedium 8.35	8.0	57.750	1.288	370.000	000 428.75	5000 558.75	5000 1.300	1.4	7.6	4.8	1.9	6.7	0.0	2.1
2	autumn	small 1	medium 8.10	11.4	40.020	5.330	346.666	599 125.66	6700 187.05	5701 15.600	3.3	53.6	1.9	0.0	0.0	0.0	9.7
3	spring	small 1	medium 8.07	4.8	77.364	2.302	98.1820	00 61.182	200 138.70	0000 1.400	3.1	41.0	18.9	0.0	1.4	0.0	1.4

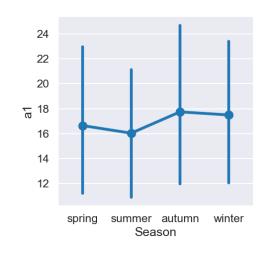
Sneak perview

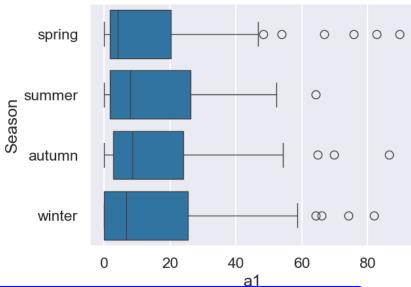
- Three categorical variables Season, Size, and Speed.
 - No missing values
 - No high cardinality, and reasonable balanced.
- Eight numerical variables max_pH, ..., mean_Chlor
- Missing values present
- Some variables heavily skewed might need to transform.
- Possibility of features being interrelated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

Dataset: Algae Blooms, Feature: Season, Target: a1







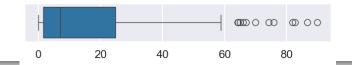


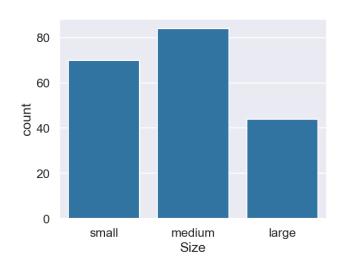
df.groupby("Season",observed=**True**)["a1"].agg(["min","max","mean","count","std"])

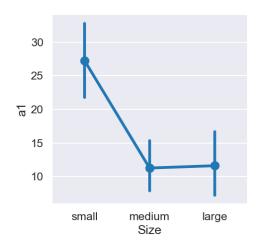
	min	max	mean	count	std
Season			\bar{x}	n	σ
spring	0.0	89.8	16.649057	53	23.093786
summer	0.0	64.2	16.038636	44	17.920798
autumn	0.0	86.6	17.745000	40	21.611203
winter	0.0	81.9	17.498361	61	22.568256

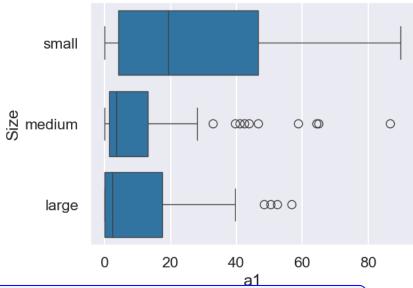
- Countplot shows no issues with feature Season all levels approximately equally represented.
- Catplots show slightly less spread in a1 for Season="summer" observations.
- No/weak relationship between Season feature and a1 target.

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







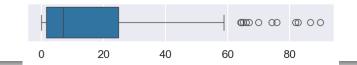


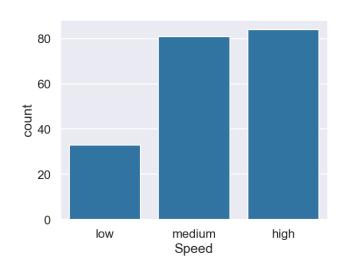
df.groupby("Size",observed=**True**)["a1"].agg(["min","max","mean","count","std"])

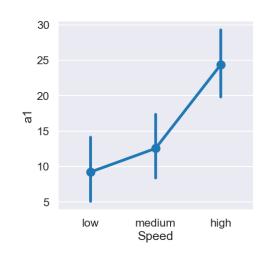
	min	max	mean	count	std
Size			\bar{x}	n	σ
small	0.0	89.8	27.255714	70	24.895426
medium	0.0	86.6	11.267857	84	17.163124
large	0.0	56.8	11.611364	44	16.556123

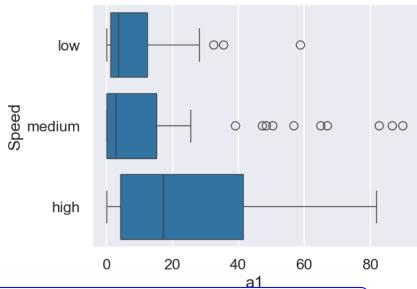
- Countplot shows no issues with feature Size.
- Size="small" rivers have higher frequencies of a1 alga ((point) catplot), and observed frequencies for small rivers is much more widespread across the domain of frequencies than for other types of rivers (boxplot).

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







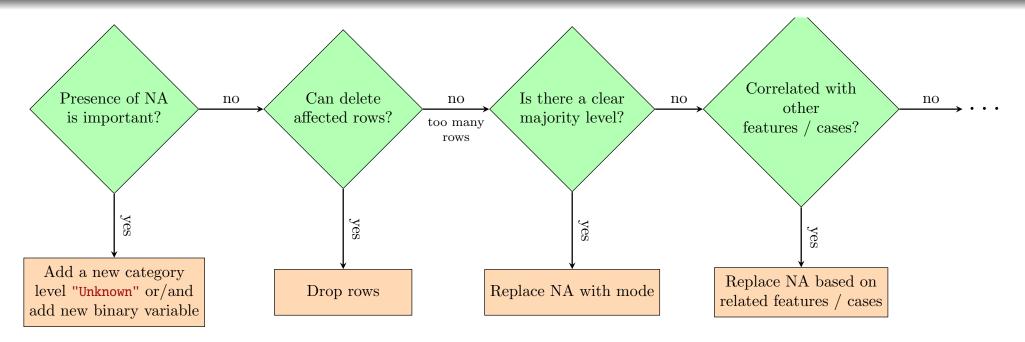


df.groupby("Speed",observed=**True**)["a1"].agg(["min","max","mean","count","std"])

	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

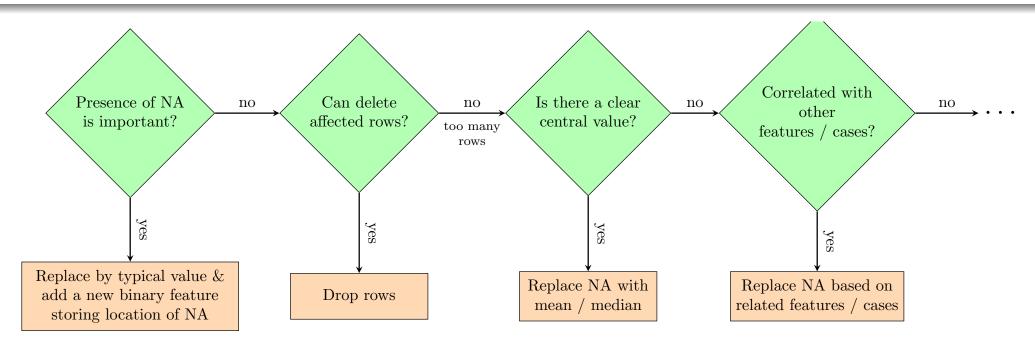


In terms of our three datasets, only Titanic has missing values in categorical features:

- 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.

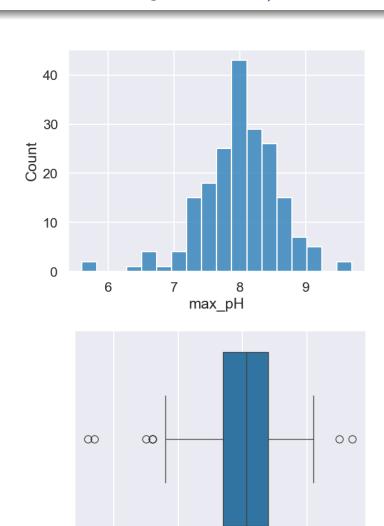
Numerical Variables — Dealing with Missing Values



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.

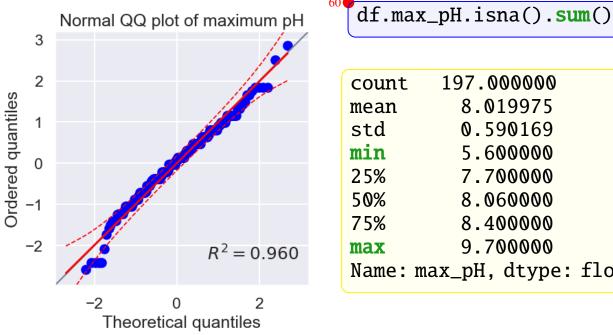
Dataset: Algae Blooms, Feature: max_ph

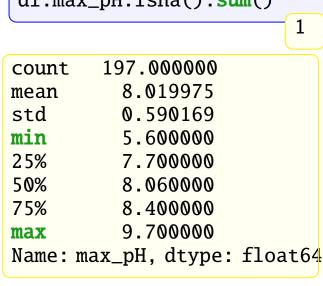


max pH

9

6





- Data is relatively normal minor issue with (left) outliers.
- Will replace (single) NA by mean
 - df.max_pH.fillna(df.max_pH.mean(), inplace=True)

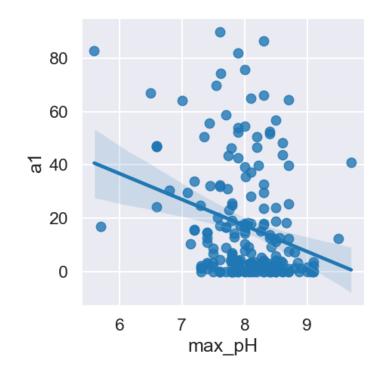
Dataset: Algae Blooms, Feature: max_ph, Target: a1

Is there a relationship between feature max_pH and target a1?

(Pearson's) Correlation coefficient, r, measures the strength of a **linear** relationship between two numerical variables.

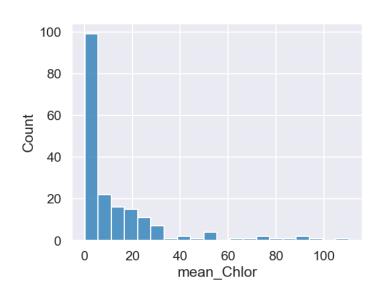
- near zero means no/weak linear relationship.
- near ± 1 zero means strong linear relationship.
- sign indicates direction.

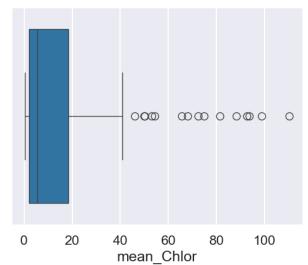
sns.lmplot(x="max_pH", y="a1", data=df)

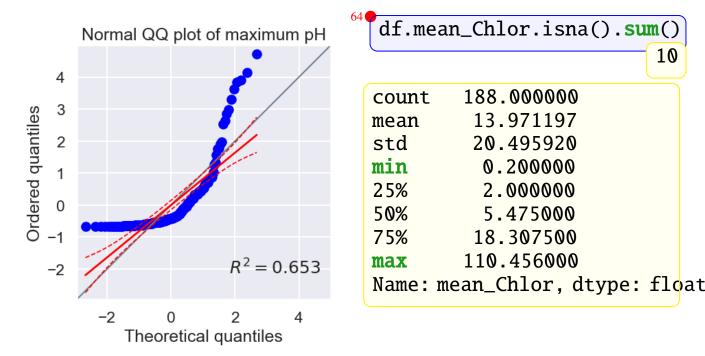


- Correlation coefficient, r = -0.27, shows (at most) a weak negative linear relationship.
- No obvious relationship visible in scatter plot.

Dataset: Algae Blooms, Feature: mean_Chlor







- Data is not normal, heavily skewed to the right \Rightarrow mean is a poor representative of the central location.
- ⇒ Will replace (single) NA by median

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

10

After Target and Individual Feature Pass — Where are we?

Tips `

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

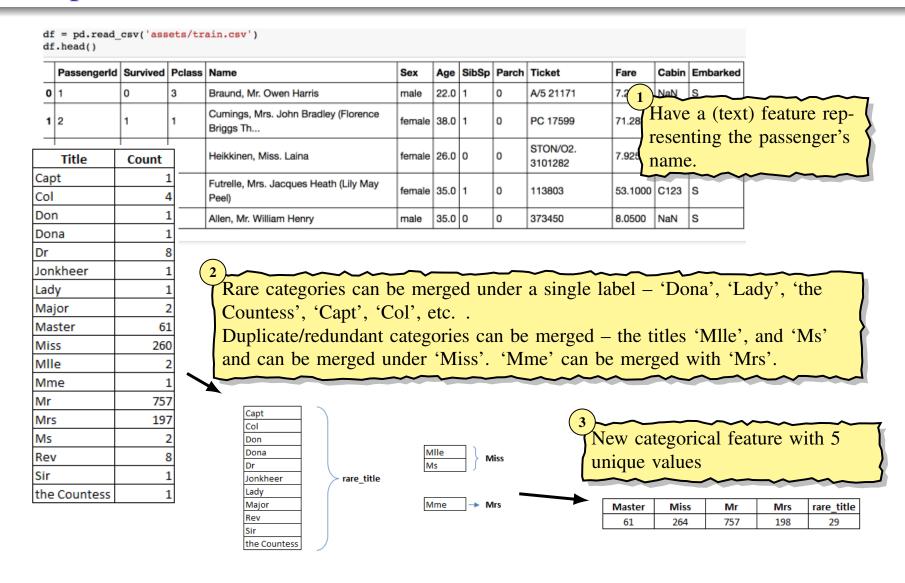
Titanic >

- 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



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, ho

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, au >

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

$$>$$
 Phi-k, ϕk

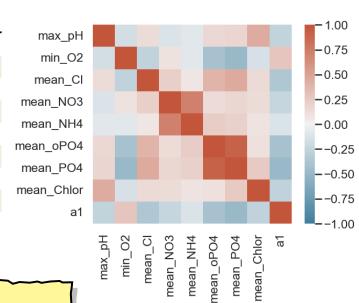
is a new and practical correlation coefficient that works consistently between categorical, ordinal and interval variables, captures non-linear dependency and reverts to the Pearson correlation coefficient in case of a bivariate normal input distribution. Its value also lies between 0 and +1, with values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

Pearson's Correlation Coefficient — Dataset: Algae Blooms

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

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
<u>a1</u>	-0.268539	0.285564	-0.371171	-0.241211	-0.132656	-0.417358	-0.487023	-0.277987	1.000000



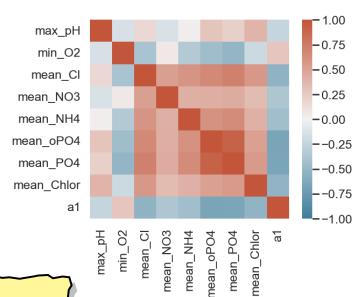
- Categorical variables are not included.
- Suggests best predictors for a1 are mean_PO4, mean_oPO4, and meanC1.
- mean_P04 and mean_oP04 are highly correlated (0.91) could use values of one to estimate missing values of the other.

Spearman's Rank Correlation Coefficient — Dataset: Algae Blooms

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

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



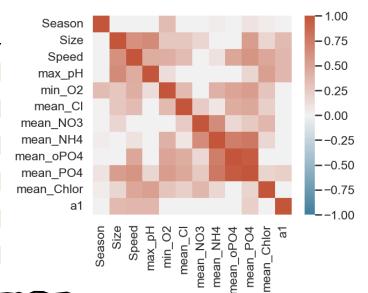
• Now best predictors for a1 also include mean_Chlor and mean_NH4.

Phik Correlation Coefficient — Dataset: Algae Blooms

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

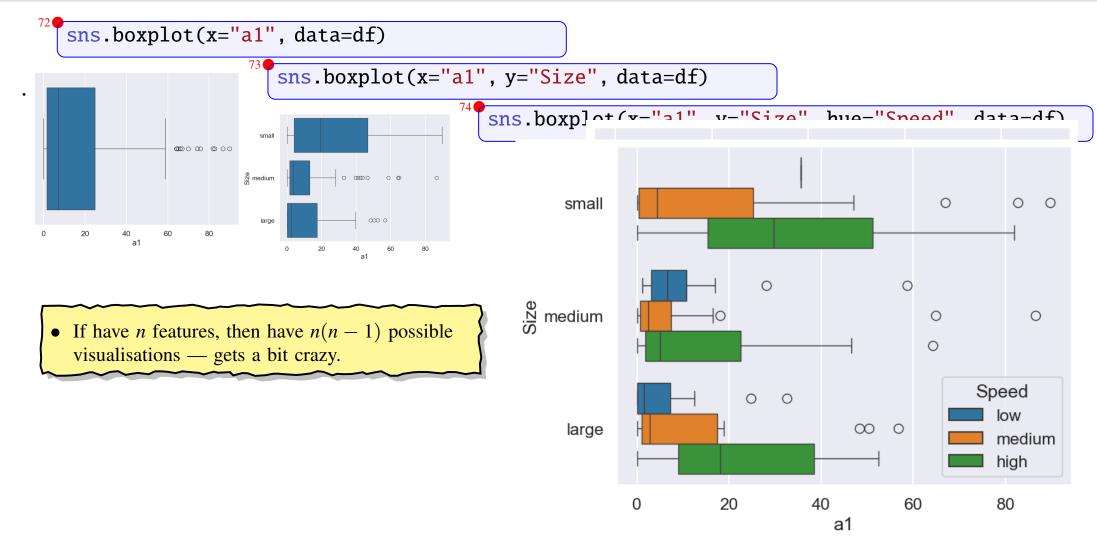
cmap = sns.diverging_palette(230, 20, as_cmap=Ti
sns.heatmap(corr, square=True, vmin=-1, vmax=1,
plt.show()

	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	6 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	5 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



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

Guides

• 1 hour, Youtube on generating seaborn plots — excellent (but has wrong on interpretation of box plot)
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)
 www.kaggle.com/mcromao/titanic-exploratory-data-analysis
- Titanic Exploratory Data Analysis

```
becominghuman.ai/
titanic-survival-dataset-part-1-2-exploratory-data-analysis-5b98f7917913
```

• When Should You Delete Outliers from a Data Set?

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