dm24s1

Topic 05: Exploratory Data Analysis2

Part 01: EDA Pass2 3

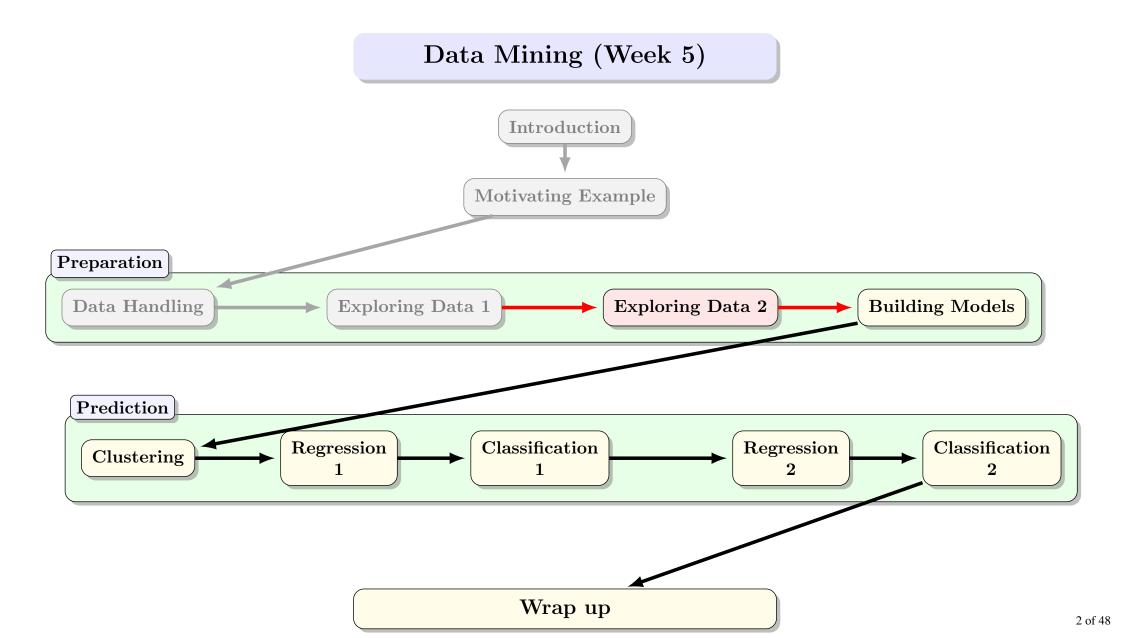
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Autumn Semester, 2024

Outline

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



EDA Pass2 3 — Summary

- 1. Review of previous week
- 2. Second Pass Individual Features and Target
- 2.1 Target
- 2.2 Individual Features
- 3. Third Pass Relationships Between Features and Target
- 3.1 Correlations
- 3.2 Multi-relation Plots
- 4. Visualisation selection of seaborn plots
- 5. Resources

Acknowledgment

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

First Pass—Load Dataset and Initial Clean

Load dataset

- Typically either csv or more general "table" format
- Can be local file or url (read over network)

Check variables names

- Should be meaningful and distinct
- Avoid clashes with reserved words (python or statistical)

Verify variable types

- Convert strings to categories, possibly grouping, where possible
- Ensure numeric data is stored as number (watch out for "Unknown" etc.)

• Identify (and possibly address) missing values

- Missing values by row or column
- Leave blank, impute value, drop row/column?

Categorical vs Numerical Variables

Recall statistical *Levels of Measurement*

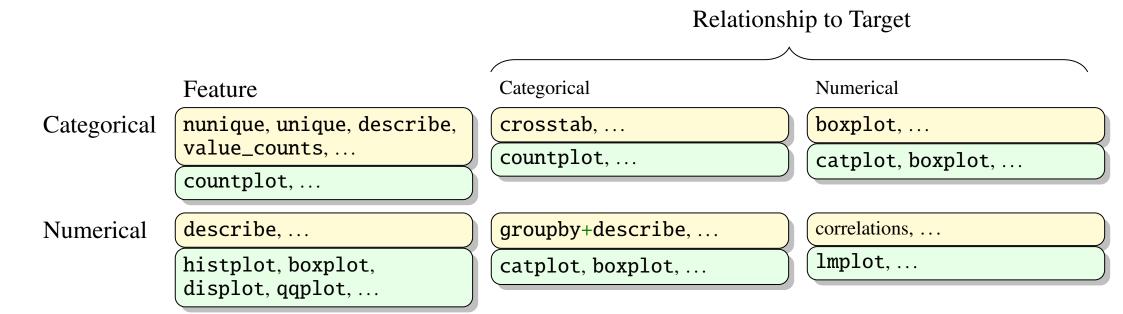
Туре	Drawn from	Examples	Used to		
Nominal	Finite Set, Unrelated	Manufacturers, Countries, Gender	Categorise with descriptive label		
Ordinal	Finite Set, Ordered	Size (S,M,L), Army Ranks, Satisfaction	Categorise with descriptive label		
Interval	Ordered, Differences matter	Exam Scores, Temperatures (Celsius)	Assign numeric score to		
Ratio	Ordered, Differences and ratios matter	Distance (m), Cost (\$), Temperatures (Kelvin)	Assign numeric score to		

Generally, *Nominal* and *Ordinal* are considered categorical, *Interval* and *Ratio* are considered Numerical

But what about a variable which contains *Months of the year*?

Categorical and Numerical variables

A Selection of Statistical Visualisations and Metrics



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?

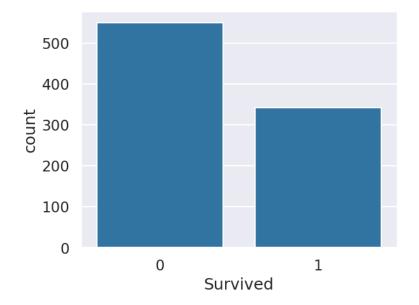
df.Survived.value_counts(normalize=True, dropna=False)

df.Survived.describe()

Survived 0 0.616162 1 0.383838

Name: proportion, dtype: float64

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



count 891
unique 2
top 0
freq 549

Name: Survived, dtype: int64

df.Survived.unique()

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

- 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 on the majority class.

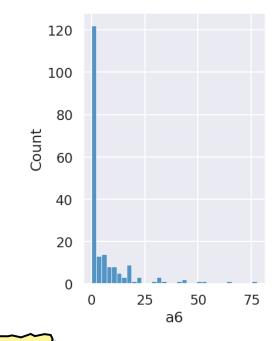
Dataset: Algae Blooms, Target: a1,..., a7

```
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()

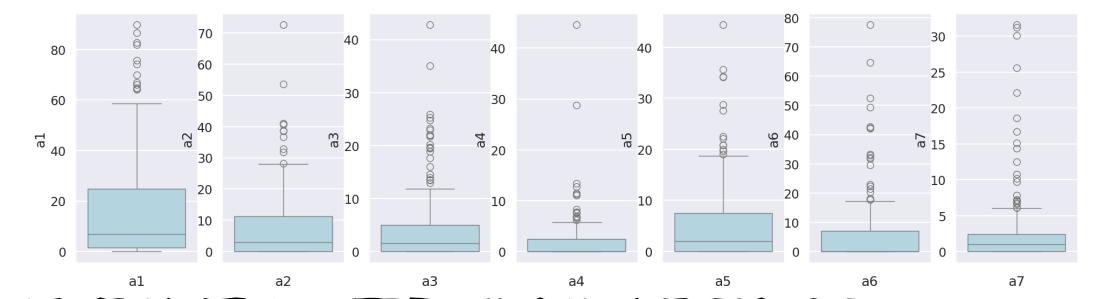
	a1	a 2	a 3	a4	a 5	a 6	a 7
count	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000	198.000000
mean	16.996465	7.470707	4.334343	1.997475	5.115657	6.004545	2.487374
std	21.421713	11.065461	6.976788	4.439205	7.511846	11.711053	5.181536
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	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

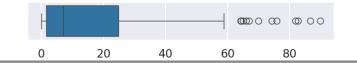
To keep this more manageable we will focus more on the Algae Blooms data set ...

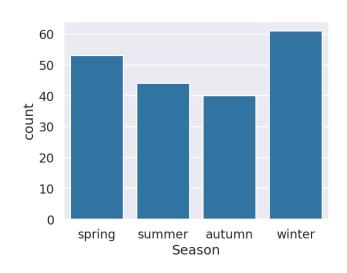
	Season	Size	Speed 1	max_pH	min_C)2 mean_(Cl mean_	_NO3 mean_N	NH4 mean_	_oPO4_mean_P	O4 mean_	Chlor	a1	a2	a 3	a4	a 5
0	winter	small n	nedium 8	8.00	9.8	60.800	6.238	578.000	00 105.00	000 170.000	00 50.000	0).0 (0.0	0.0	0.0	34.2 {
1	spring	small n	nedium 8	8.35	8.0	57.750	1.288	370.000	00 428.75	000 558.750	00 1.300	1	1.4	7.6	4.8	1.9	6.7 (
2	autumn	small n	nedium 8	8.10	11.4	40.020	5.330	346.666	99 125.66	700 187.0570	01 15.600	3	3.3	53.6	1.9	0.0	0.0
3	spring	small n	nedium 8	8.07	4.8	77.364	2.302	98.1820	0 61.182	00 138.700	00 1.400	3	3.1	41.0	18.9	0.0	1.4 (

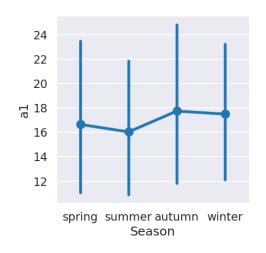
Sneak perview

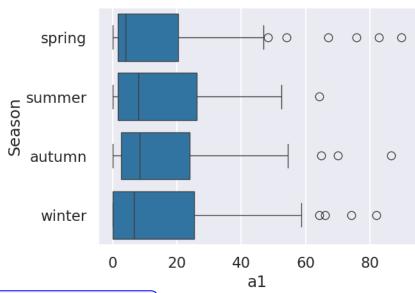
- Three categorical variables Season, Size, and Speed.
 - No missing values
 - No high cardinality, and reasonable balanced.
- Eight numerical variables max_pH, ..., mean_Chlor
- Missing values present
- Some variables heavily skewed might need to transform.
- Possibility of features being interrelated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

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







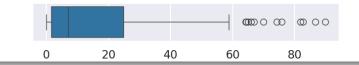


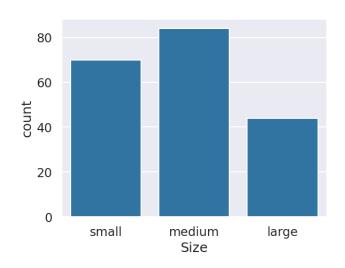
df.groupby("Season")["a1"].agg(["min","max","mean","count","std"])

	min	max		mean	count	std
Season			$\bar{\mathcal{X}}$	n		σ
spring	0.0	89.8	16.6	649057	53	23.093786
summer	0.0	64.2	16.0	038636	44	17.920798
autumn	0.0	86.6	17.	745000	40	21.611203
winter	0.0	81.9	17.4	498361	61	22.568256

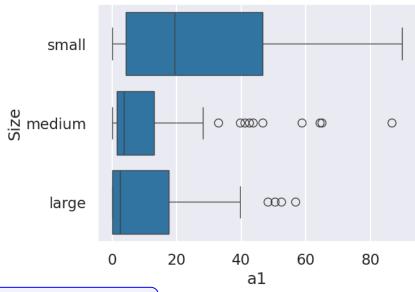
- Countplot shows no issues with feature Season all levels approximately equally represented.
- Countplots show slightly less spread in a1 for Season="summer" observations.
- No/weak relationship between Season feature and a1 target.

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







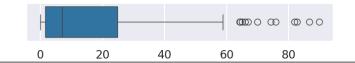


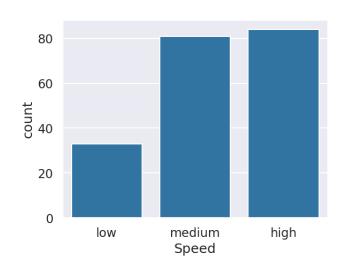
df.groupby("Size")["a1"].agg(["min","max","mean","count","std"])

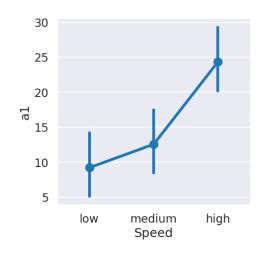
	min	max	mean	count	std
Size					
small	0.0	89.8	27.255714	70	24.895426
medium	0.0	86.6	11.267857	84	17.163124
large	0.0	56.8	11.611364	44	16.556123

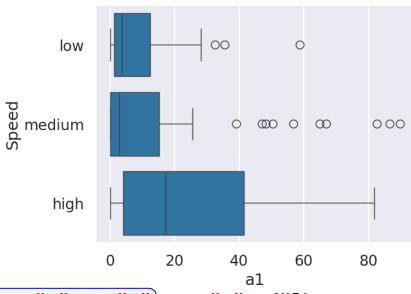
- Countplot shows no issues with feature Size.
- Size="small" rivers have higher frequencies of a1 alga ((point) catplot), and observed frequencies for small rivers is much more widespread across the domain of frequencies than for other types of rivers (boxplot).

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







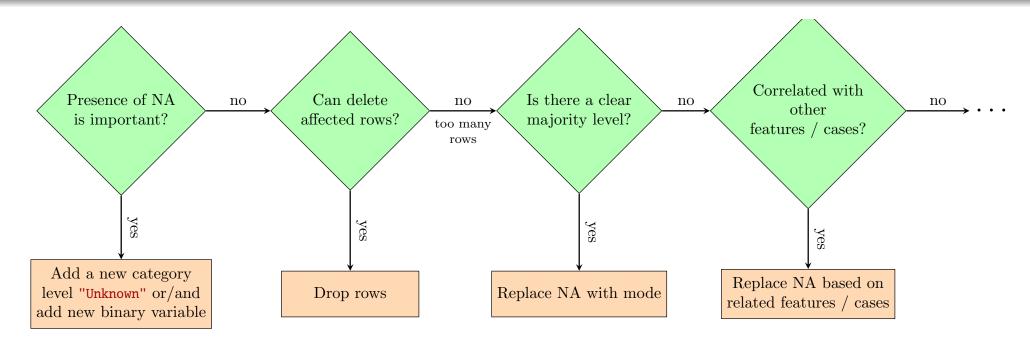


df.groupby("Speed", observed=False)["a1"].agg(["min","max","mean","count","std"])

	min	max	mean	count	std
Speed					
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 average population of a1 alga ((point) catplot), and observed frequencies is much more widespread across the domain of frequencies than for other types of rivers (boxplot).

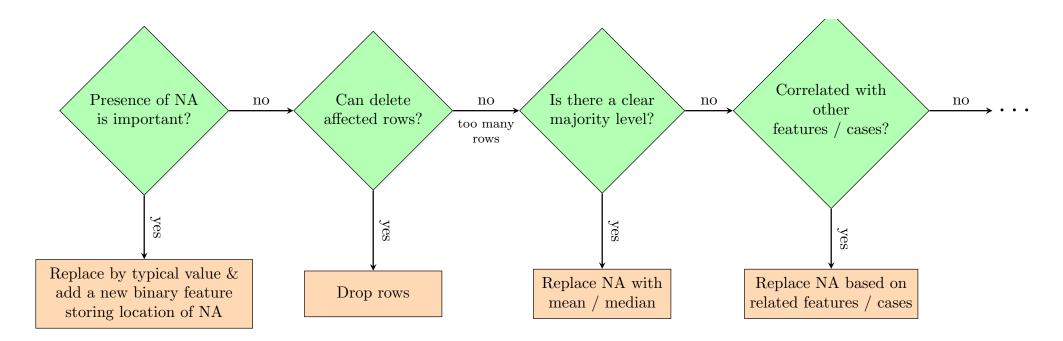
Categorical Variables — Dealing with Missing Values



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.

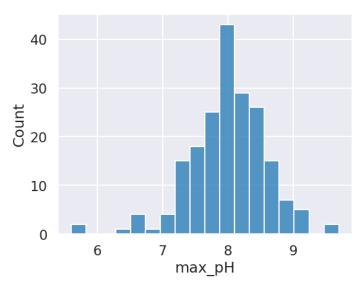
Numerical Variables — Dealing with Missing Values

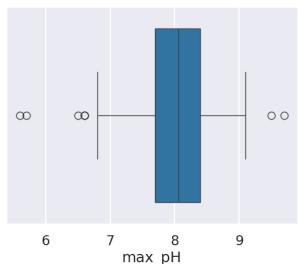


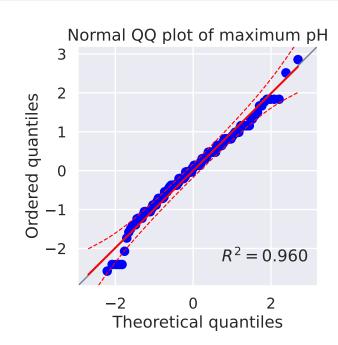
In terms of our three datasets:

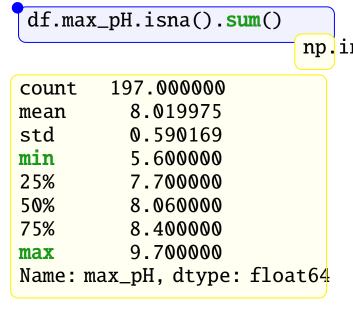
- In Titanic, feature Fare appears to have no missing values, but has 15 zero entries. Are these missing values? or free tickets due to age? ...
- In Algae Blooms, some of the 8 numeric features have NAs ... next few slides.

Dataset: Algae Blooms, Feature: max_ph









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

df.max_pH = df.max_pH.fillna(df.max_pH.mean())

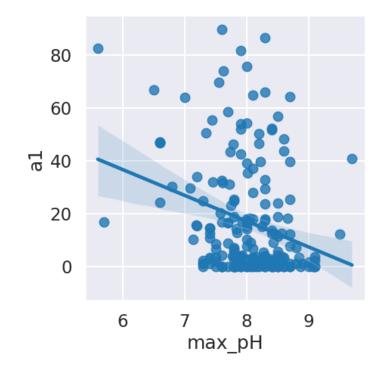
Dataset: Algae Blooms, Feature: max_ph, Target: a1

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.

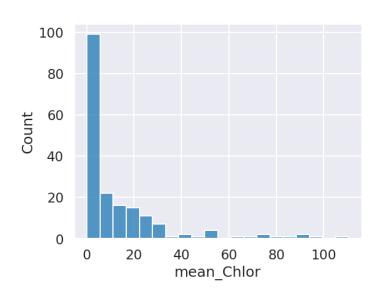
- near zero means no/weak linear relationship.
- near ± 1 zero means strong linear relationship.
- sign indicates direction of relationship

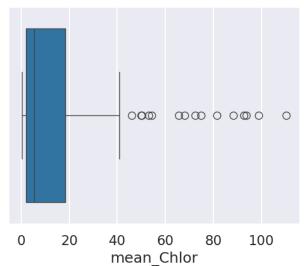
sns.lmplot(x="max_pH", y="a1", data=df);

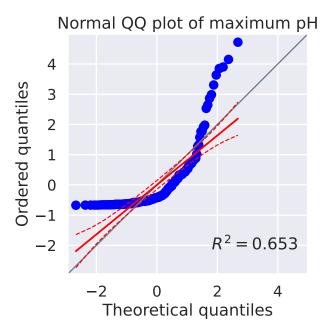


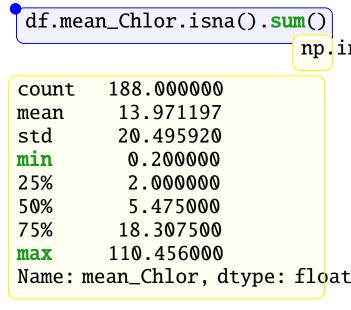
- Correlation coefficient, r = -0.27, shows (at most) a weak negative linear relationship.
- No obvious relationship visible in scatter plot.

Dataset: Algae Blooms, Feature: mean_Chlor









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

df.mean_Chlor = df.mean_Chlor.fillna(df.mean_Chlor.median()

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.

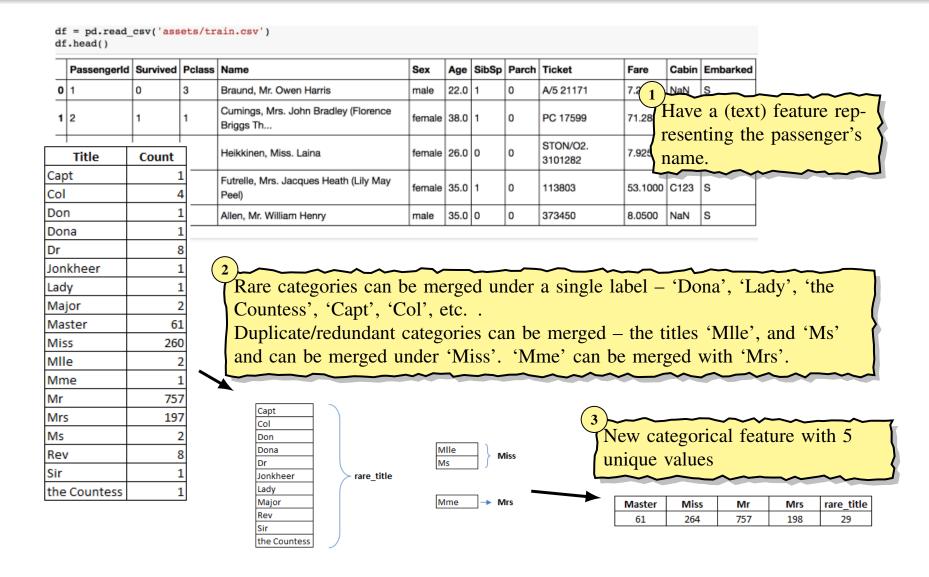
Titanic >

- Reviewed each feature location, spread, shape, issues.
- Generated ToDo list for 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

We distinguish later between feature-feature and feature-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, au

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

$$\overline{>}$$
 Phi-k, ϕk

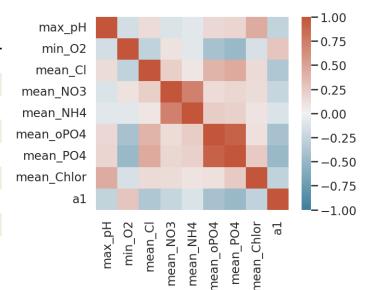
is a new and practical correlation coefficient that works consistently between categorical, ordinal and interval variables, captures non-linear dependency and reverts to the Pearson correlation coefficient in case of a bivariate normal input distribution. Its value also lies between 0 and +1, with values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

Pearson's Correlation Coefficient — Dataset: Algae Blooms

columns = df.columns[:12] corr

cmap = sns.diverging_palette(230, 20, as_cmap=True) corr = df[columns].corr(numeric_or sns.heatmap(corr, square=True, vmin=-1, vmax=1, cmap=cmap);

	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



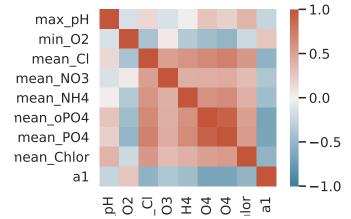
- Categorical variables are not included.
- Suggests best predictors for a1 are mean_P04, mean_oP04, and meanC1.
- mean_P04 and mean_oP04 are highly correlated (0.91) could use values of one to estimate missing values of the other.

Spearman's Rank Correlation Coefficient — Dataset: Algae Blooms

columns = df.columns[:12] corr

cmap = sns.diverging_palette(230, 20, as_cmap=T) corr = df[columns].corr(method='spearman', nume sns.heatmap(corr, square=True, vmin=-1, vmax=1,

	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



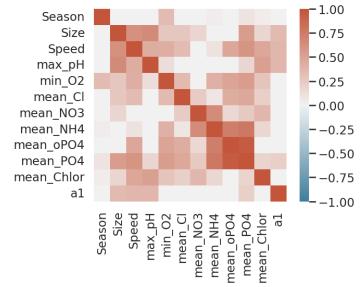
• Now best predictors for a1 also include mean_Chlor and mean_NH4.

Phik Correlation Coefficient — Dataset: Algae Blooms

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

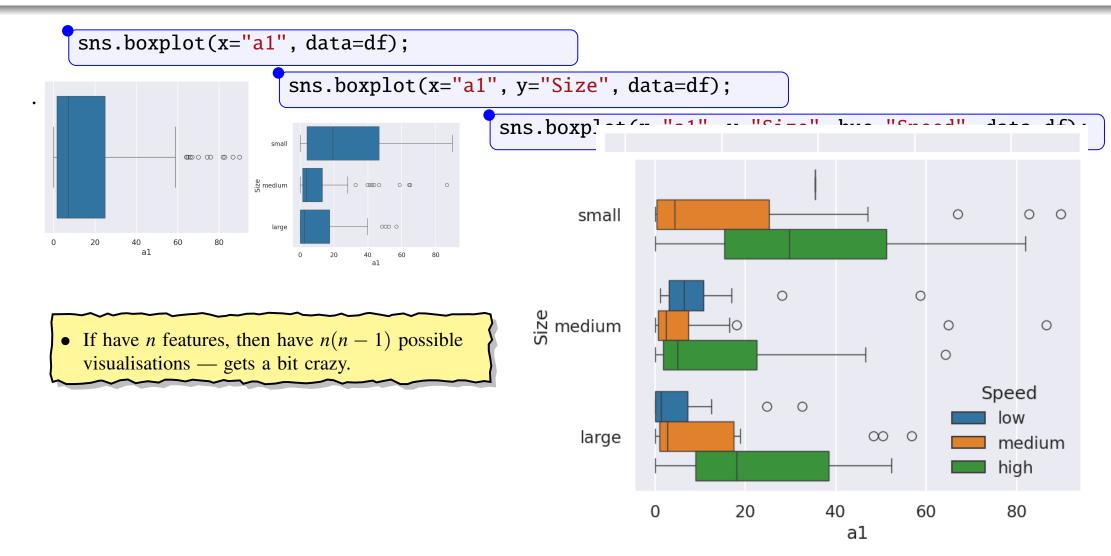
cmap = sns.diverging_palette(230, 20, as_cmap=Tr sns.heatmap(corr, square=True, vmin=-1, vmax=1,

	Season	Size	Speed	max_pH	min_O2	mean_Cl	mean_NO	3 mean_NH4	mean_oPO	4 mean_PO	l mean_Chlo	r 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



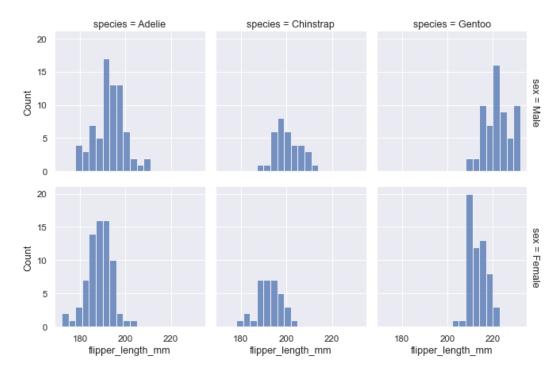
After Third Pass — Where are we?

- 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.

Selected seaborn-based visualisations

- We could easily spend several weeks on EDA visualisation
- There is a long history of visualisation, from infographics to bubble plots
- Seaborn provides a gallery of data science-related visualisation examples
- We consider a selection today that are useful in practice

Histograms with facets



Source: https://seaborn.pydata.org/ examples/faceted_histogram.html

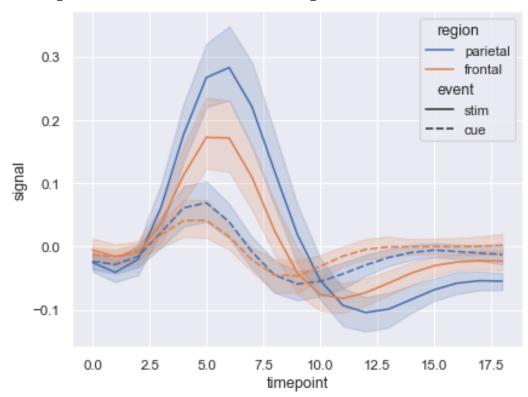
What it does

- Facets: show a grid of related plots
- Conditioned by 1 or 2 categorical variables
- Here: flipper length of penguins, by sex × species.

- Have a key variable, represented by a suitable plot
- Wish to view dependence on 1 or 2 categorical variables in same plot group

Line plots with error bands

Source: https://seaborn.pydata.org/ examples/errorband_lineplots.html



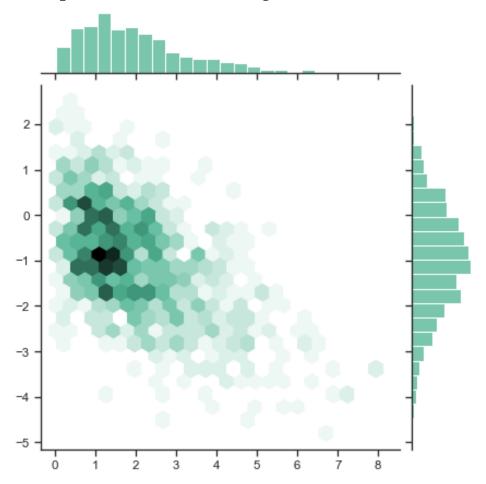
What it does

- Multiple numeric variables as lineplots
- Use of colour and linetype
- Overlaid on error bands

- Multiple numeric variables on same scale
- Highlight uncertainties

Binning with distribution plots

Source: https://seaborn.pydata.org/ examples/hexbin_marginals.html



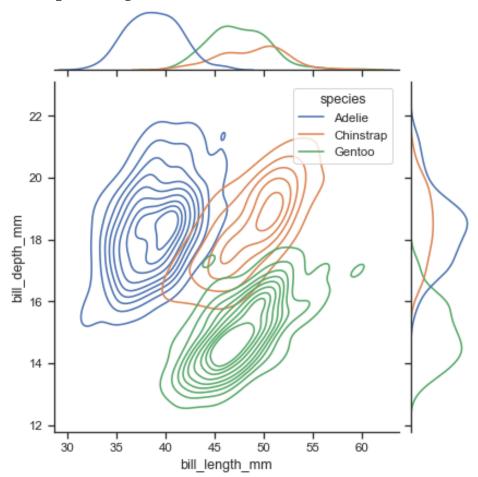
What it does

- Compare histograms of 2 numeric columns
- Binning provides a heatmap

- Interested in the co-occurrence of 2 numeric columns
- Columns are correlated, wish to understand this

Contour plots of distributions

Source: https://seaborn.pydata.org/examples/joint_kde.html



What it does

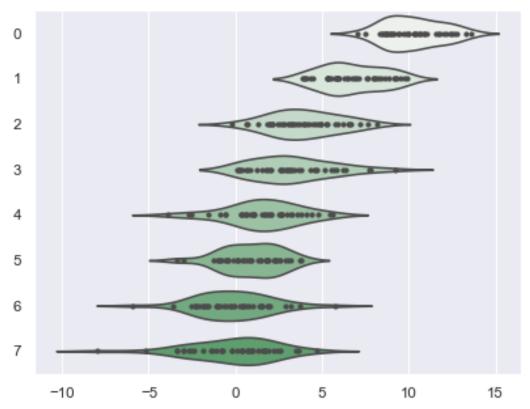
- Penguin bill length \times bill width per species
- Two ways of showing distributions

When to use it

• 2 numeric features, split by 1 categorical feature

Violin plots

Source: https://seaborn.pydata.org/ examples/simple_violinplots.html



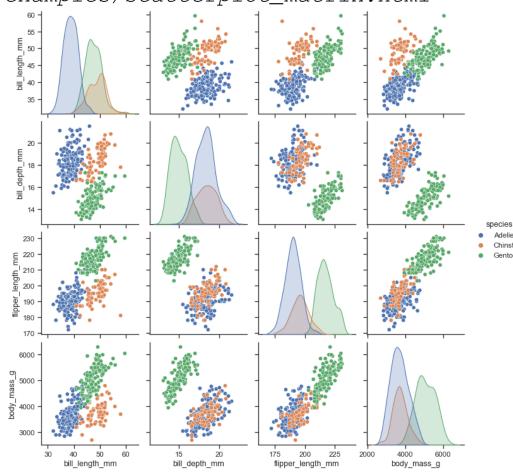
What it does

- Numeric variable, split by category
- Alternative to boxplot
- data points shown here

- Numeric attibute by categorical feature
- Interested in the shape of the distribution

Scatterplot matrix

Source: https://seaborn.pydata.org/ examples/scatterplot_matrix.html



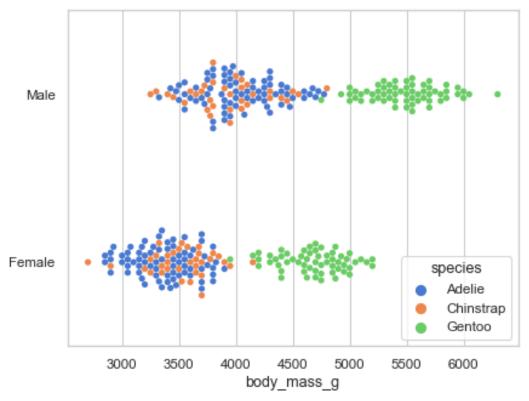
What it does

- Penguin data 4 numeric features (bill length, bill depth, flipper length, body mass), 1 categorical feature (species) with 3 levels
- All combinations shown

- Look at many numeric variables together
- Can use colour or other indicator to show categorical variable

Scatterplot with categorical variables

Source: https://seaborn.pydata.org/ examples/scatterplot_categorical.html



What it does

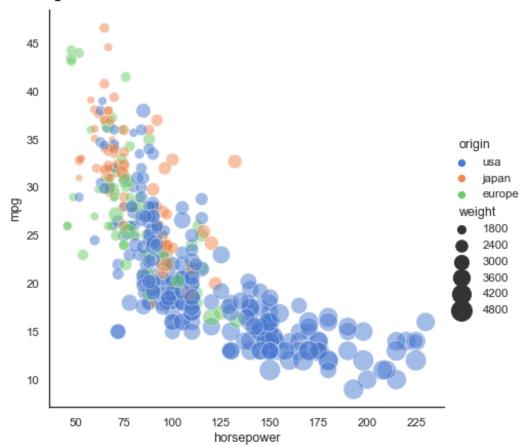
• Show numerical variable in terms of 1 or more categorical variables

When to use it

• More detailed alternative to violinplot

Scatterplot with bubbles

Source: https://seaborn.pydata.org/ examples/scatter_bubbles.html



What it does

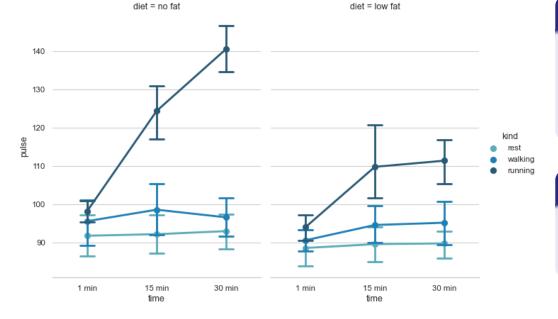
- Auto mpg data, mpg \times horsepower
- Plot features represent categorical features
- Note grouping of numeric variable to create categories

When to use it

• Represent multiple categorical variables in terms of 2 numerical variables

Pointplot for Analysis of Variance

Source: https://seaborn.pydata.org/ examples/pointplot_anova.html



What it does

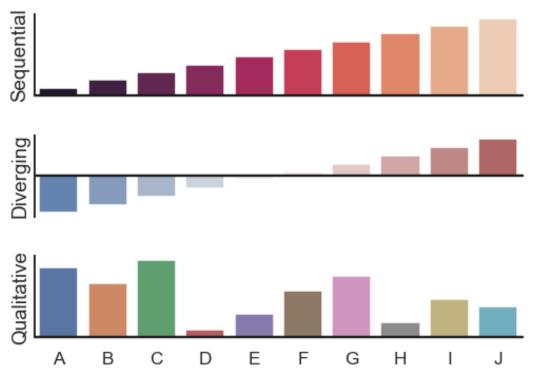
- Trend in pulse rates, by time × activity (ordered categories)
- Rich plot, with drill down capability

When to use it

 Numeric target as function of multiple categorical features

Colour palettes

Source: https://seaborn.pydata.org/ examples/palette_choices.html



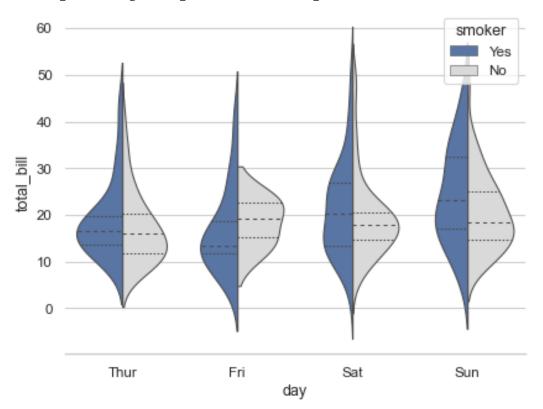
What it does

- Options for choosing palettes
- Qualitative, Sequential, Diverging

- Qualitative: unordered categorical variable
- Sequential: ordered categorical variable
- Diverging: ordered sequential variable

Grouped Violinplots

Source: https://seaborn.pydata.org/ examples/grouped_violinplots.html



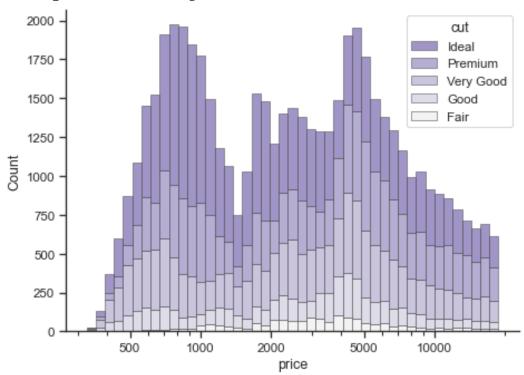
What it does

- Tips data: total_bill by day × smoker
- Note splits in "violins" to accommodate a category

- Adding a second categorical variable to violinplot
- Alternative to faceting

Stacked histograms

Source: https://seaborn.pydata.org/ examples/histogram_stacked.html



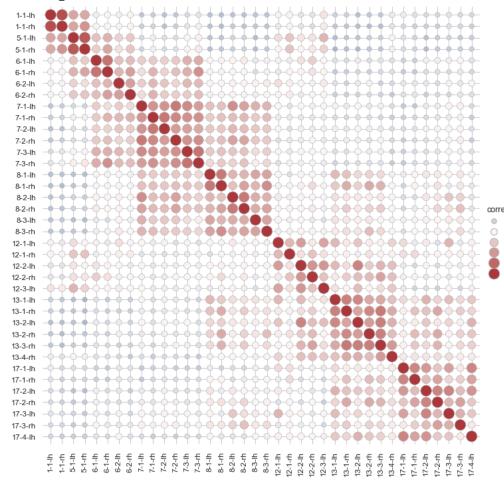
What it does

- Diamond valuation data
- Show distribution of price by cut
- Be careful: stacked not overlaid!

- Can compare histograms by category variable
- Alternative to faceting

Heatmap with scatterplot

Source: https://seaborn.pydata.org/ examples/heat_scatter.html



What it does

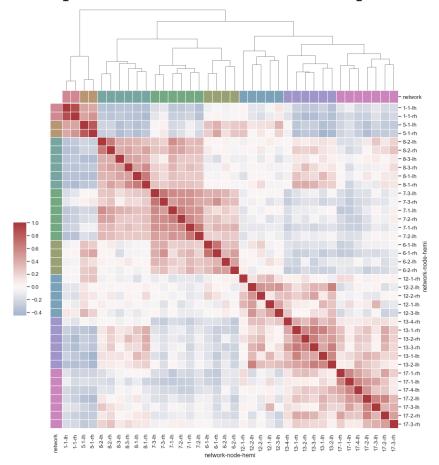
- Network data
- Highlighting correlated flows
- Use of colour and size of bubbles

When to use it

• Emphasise sign and magnitude of correlations

Heatmap with dendrogram

Source: https://seaborn.pydata.org/ examples/structured_heatmap.html



What it does

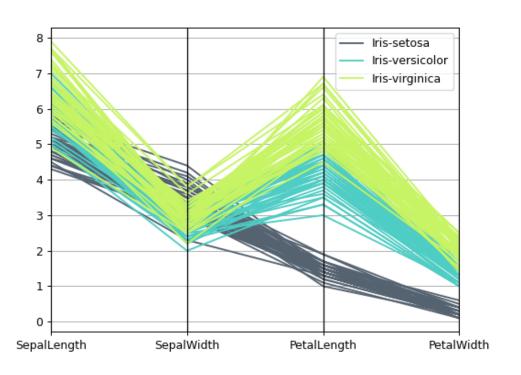
- Heatmap of correlations
- Dendrogram clusters them to highlight similar values

When to use it

Need to identify groups of correlated numerical variables

Parallel coordinate plots

Source: https://pandas.pydata.org/docs/ reference/api/pandas.plotting.parallel_ coordinates.html



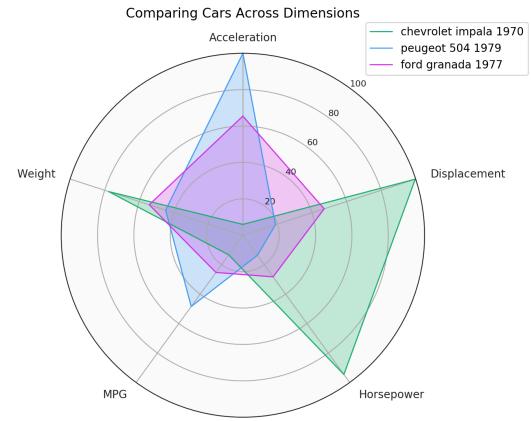
What it does

- Each piecewise linear "line" represesents an instance
- Each vertical split (context) line represents a numerical variable (feature or target)
- Instance lines pass through values they take on the context variables

- Need to compare subsets of instances (note use of colour to distinguish)
- Compare instances based on a (subset) of their numerical values

Radar charts

Source: https://www.pythoncharts.com/matplotlib/radar-charts/



What it does

- Each polygon represents an instance, colour legend identifies the instance
- Each radial line represents a numerical variable
- Vertices of the polygon indicate the value an instance takes on that variable

- Have a small number of instances to compare over selected numerical variables
- Visualise correlations between numerical variables, for selected instances

Resources

Resources

Guides

• 1 hour, Youtube on generating seaborn plots — excellent (but wrong on interpretation of box plot)
www.youtube.com/watch?v=6GUZXDef2U0&t=1363s

Articles on Exploratory Data Analysis

- Exploratory Data Analysis (EDA) and Data Visualization with Python www.kite.com/blog/python/data-analysis-visualization-python/
- When Should You Delete Outliers from a Data Set?

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

Visualisation

• (Seaborn) Example Gallery

https://seaborn.pydata.org/examples/index.html