Exploratory data analysis

How to start making data talk

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Today's objectives

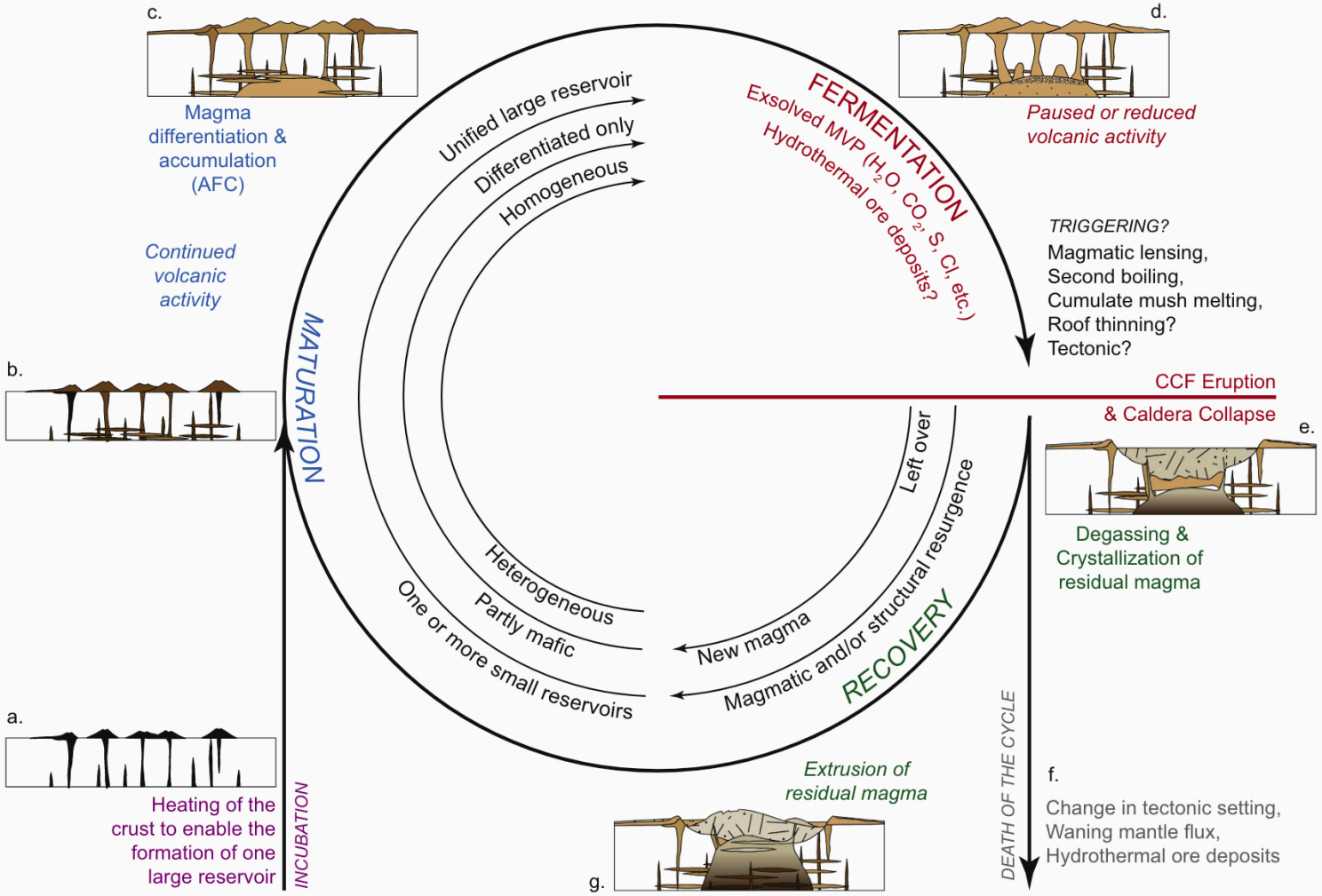
- **Last week**: We learned how to handle data using `Pandas`
  - → Load, access, query, filter, sort and operate on data

The dataset

Case study

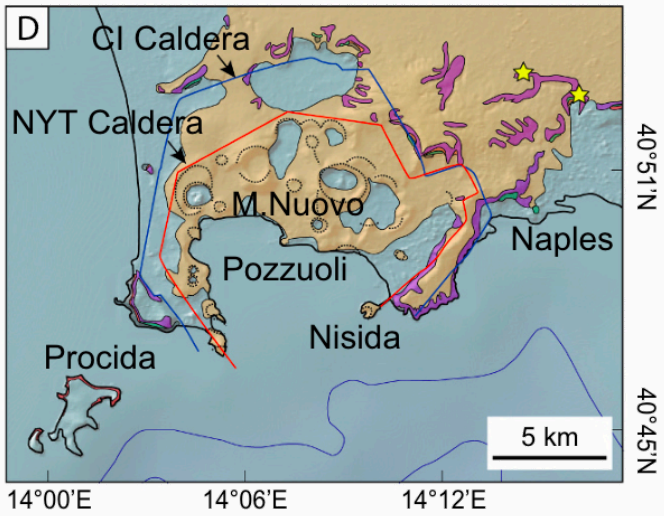
- **Campi Flegrei**: Home to 1.5 million people
- **Caldera-forming** eruptions
  - → Campanian Ignimbrite (CI), ~39 ka ago
  - → Neapolitan Yellow Tuff (NYT), ~15 ka ago 

Caldera-forming eruptions cycles



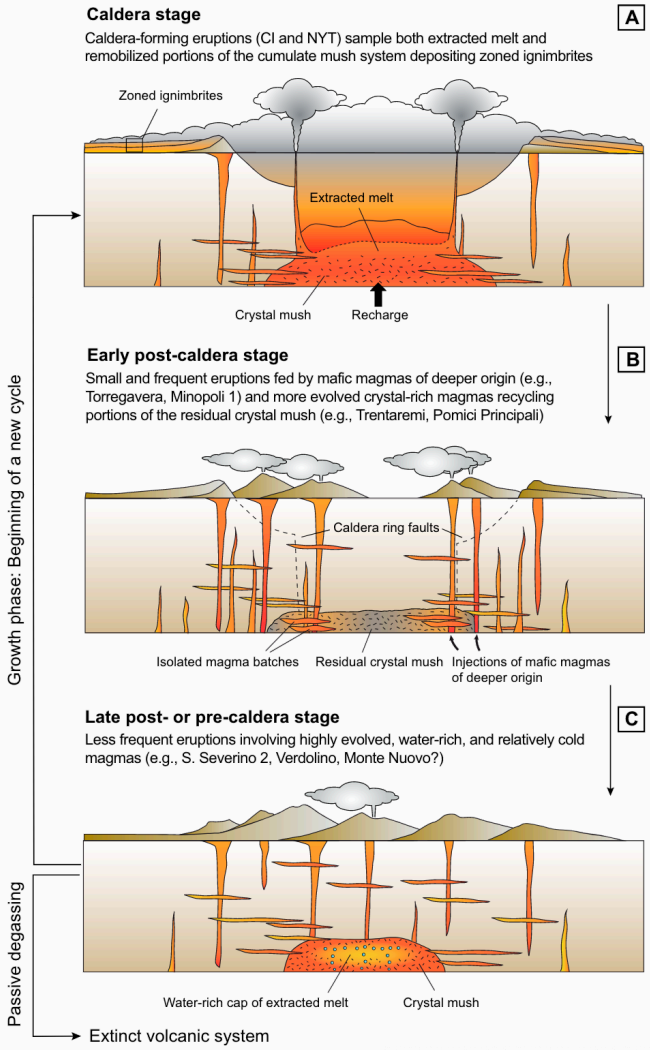
Bouvet de Maisoneuve et al. (2021)

Caldera cycles at Campi Flegrei



D) CAMPI FLEGREI CALDERA

- Post-NYT
- **Neapolitan Yellow Tuff (NYT)**
- Post-CI/Pre-NYT
- **Campanian Ignimbrite (CI)**
- Pre-CI
- Masseria del Monte Tuff (sampling locations)

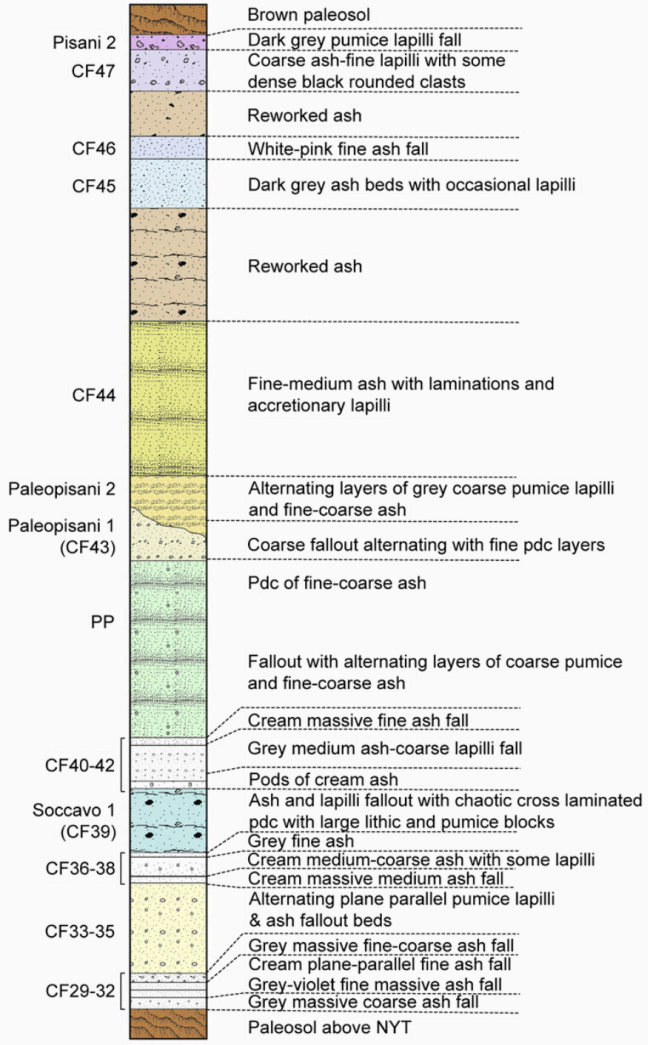


Bouvet de Maisoneuve et al. (2021), Forni et al. (2018) →

Dataset

Tephrostratigraphy and glass compositions of post-15 kyr Campi Flegrei eruptions

- Smith et al. (2011)
- Major and trace elements



Loading the dataset

- Import `pandas`
- Load an **excel** file using `pandas`
- Specify **which sheet** to read from using the `sheet_name` argument
  - → *Supp_majors* → `df_majors`
  - → *Supp_traces* → `df_traces`

```
1 # Load Pandas
2 import pandas as pd # Import pandas
3
4 # Import the dataset specifying which Excel sheet name to load the data from
5 df_majors = pd.read_csv('https://raw.githubusercontent.com/ELSTE-Master/Data-Science/main/Data/
6 df_traces = pd.read_csv('https://raw.githubusercontent.com/ELSTE-Master/Data-Science/main/Data/
```

Inspecting the dataset

```
1 df_traces.head(5)
```

	Analysis no.	Strat. Pos.	Eruption	controlcode	Sa
0	1915	63	Astroni 7	1	79
1	1916	63	Astroni 7	1	79
2	1917	63	Astroni 7	1	79
3	1918	63	Astroni 7	1	79
4	1919	63	Astroni 7	1	79

5 rows × 37 columns

```
1 df_traces.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 370 entries, 0 to 369
Data columns (total 37 columns):
 #   Column            Non-Null Count  Dtype
---  ------            --------------  -----
 0   Analysis no.      370 non-null    int64
 1   Strat. Pos.       370 non-null    int64
 2   Eruption          370 non-null    object
 3   controlcode       370 non-null    int64
 4   Sample            370 non-null    object
 5   Epoch             370 non-null    object
 6   Crater size       370 non-null    int64
 7   Date of analysis  370 non-null    object
 8   Si/bulk cps       370 non-null    float64
 9   SiO2* (EMP)       370 non-null    float64
 10  Sc                370 non-null    float64
 11  Rb                370 non-null    int64
 12  Sr                369 non-null    float64
```

Types of data

Basic types of data

- `int`: **Integer** numbers → 0, 1, 2, ...
- `float`: **Decimal** numbers → 1.1, 1.2, 1.3, ...
- `object`: **Strings** → “Campi Flegrei”

Families of data

Numerical data

- Represent quantities or measurable values
- **Quantitative**
  - → *Discrete*: Earthquake counts
  - → *Continuous*: Temperature
- Stored as **numerical** values
- **Operations** → arithmetic

Families of data - cheat sheet

Feature	Categorical Data	Numerical Data
Definition	**Categories or groups** of data	**Quantities or measurable values**
Nature	Qualitative (describes qualities)	Quantitative (describes amounts or measurements)
Data Type	Non-numeric (often text or labels)	Numeric (numbers only)
Examples	Eruption type	Element concentration
Possible Operations	Counting, grouping, mode	Arithmetic operations
Measurement Scale	Nominal or Ordinal	Interval or Ratio
Visualization Tools	Bar chart, Pie chart	Histogram, Box plot, Scatter plot
Subtypes	**Nominal:** Categories with no order (e.g., color); **Ordinal:** Categories with order (e.g., rank)	**Discrete:** Countable numbers (e.g., number of earthquakes); **Continuous:** Measurable values (e.g., temperature)
Examples of Statistical Summary	Frequency, mode	Mean, median, standard deviation
Storage Format	Strings or labels	Integers or floats

Plotting data

Plotting libraries

There are two main plotting libraries:

- `matplotlib` (and its module `pyplot`): core of plotting in Python

  → Matplotlib gallery

- `seaborn`: based on `matplotlib`, designed for statistical exploration, integration with `pandas`

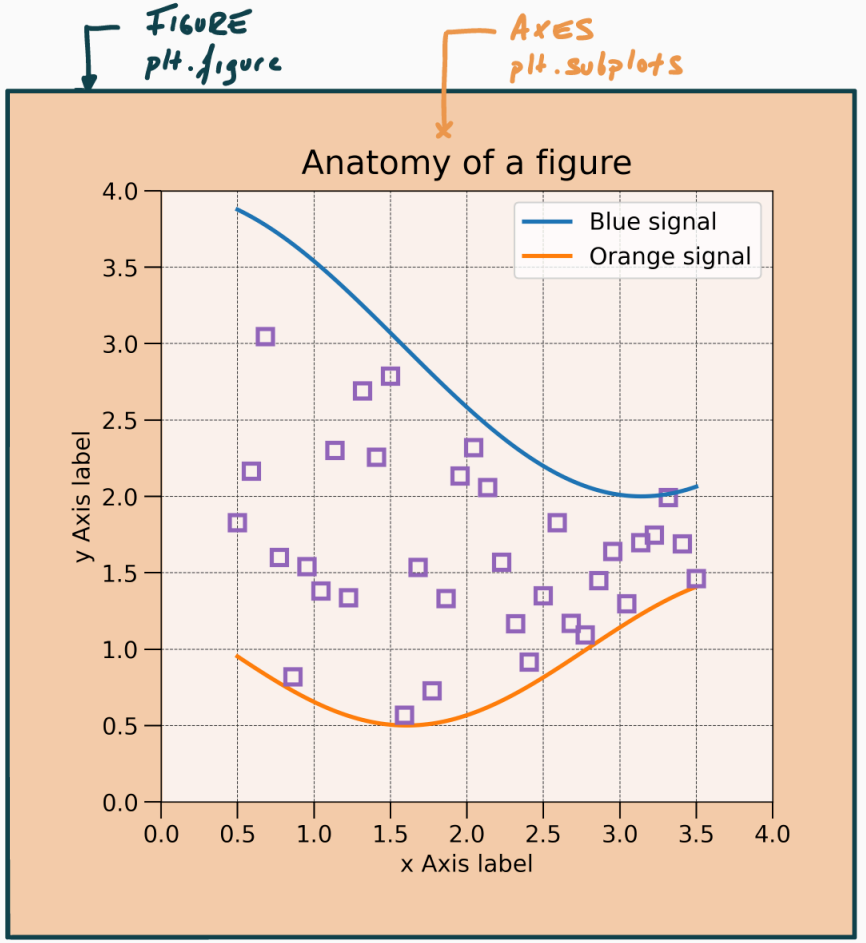
  → Seaborn gallery

```
1 import matplotlib.pyplot as plt # Import the pyplot module from matplotlib
2 import seaborn as sns # Import seaborn
```

Anatomy of a figure

- Setup figure:
  `plt.subplots()`
- Returns:
  - → `fig` → figure
  - → `ax` → axes

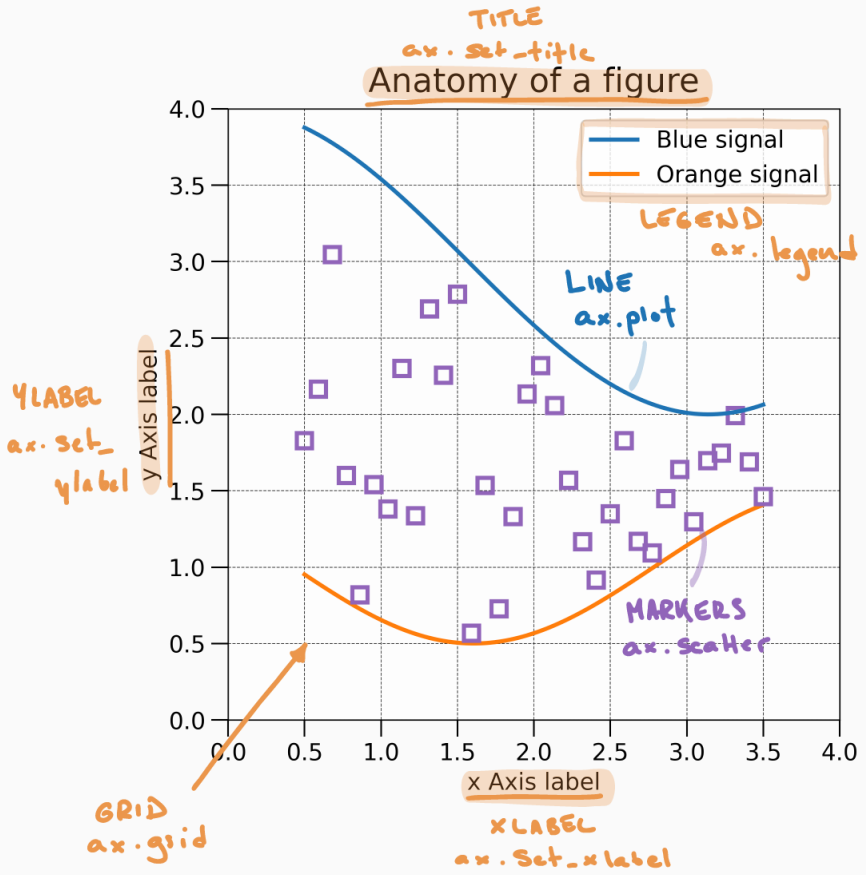
```
1  fig, ax = plt.subplots()
```



Anatomy of a axes

Axes: Where most of the magic occurs

Function	Description
`ax.set_title`	Sets the title of the axes
`ax.set_xlabel`	Sets the label for the x-axis
`ax.set_ylabel`	Sets the label for the y-axis
`ax.legend`	Displays the legend
`ax.grid`	Shows grid lines



Plotting example

```
# Define some data
data1 = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
data2 = [7, 3, 9, 1, 5, 10, 8, 2, 6, 4]

# Set the figure and the axes
fig, ax = plt.subplots()

# Plot the data
ax.plot(data1, data1, color='aqua', label='L
ax.scatter(data1, data2, color='purple', lab
```

Plotting example

```
# Define some data
data1 = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
data2 = [7, 3, 9, 1, 5, 10, 8, 2, 6, 4]

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# Plot the data
ax.plot(data1, data1, color='aqua', label='L
ax.scatter(data1, data2, color='purple', lab

# Set labels
ax.set_xlabel('x Label')
ax.set_ylabel('y Label')

# Only to make it look pretty on the present
plt.show()
```

Seaborn

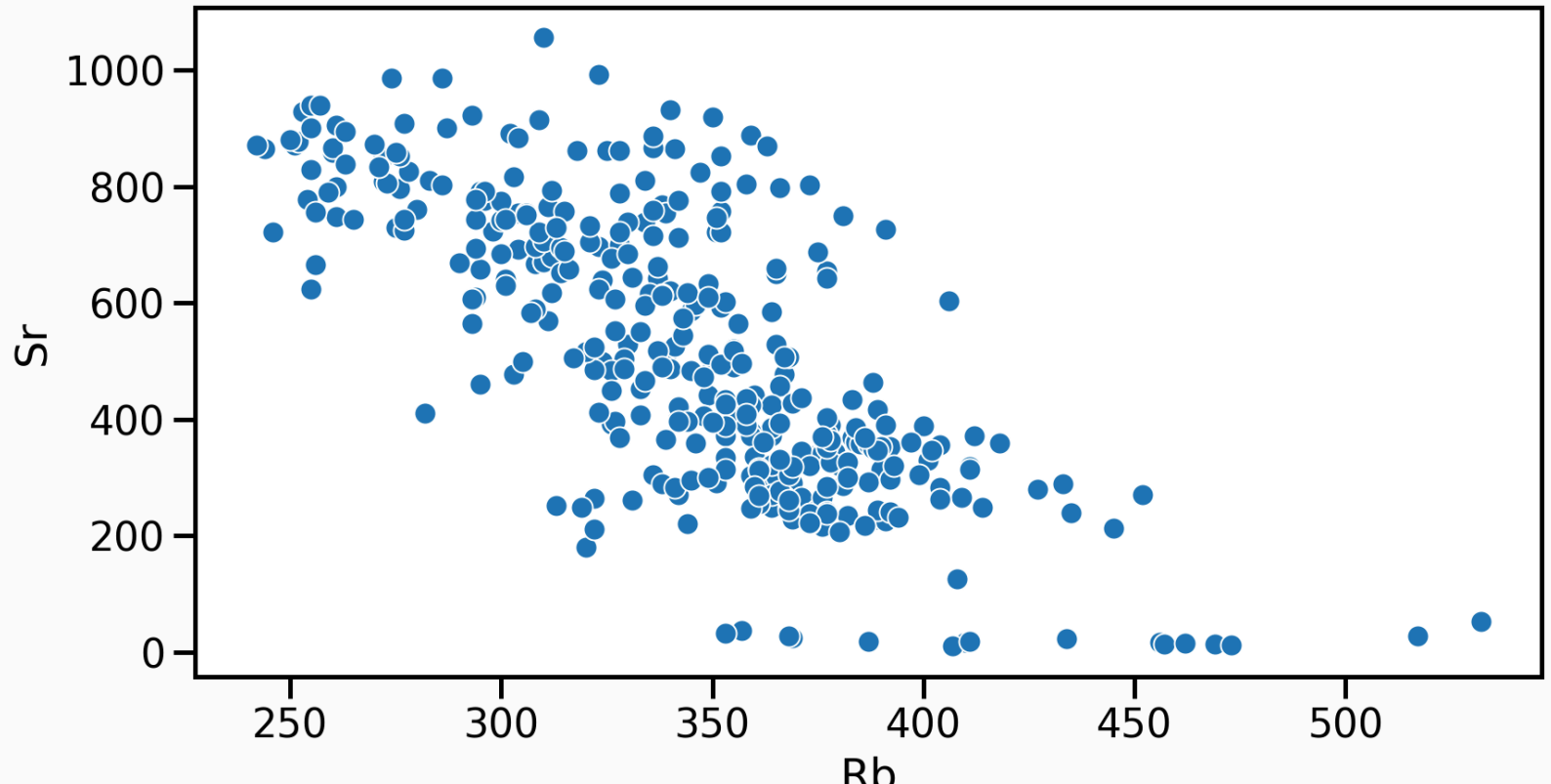
Why Seaborn?

> Seaborn provides a high-level interface for drawing attractive and informative statistical graphics.

- Makes plotting `pandas` DataFrames **easy**
- Produces **clean** graphics
- Drawback: difficult customisation

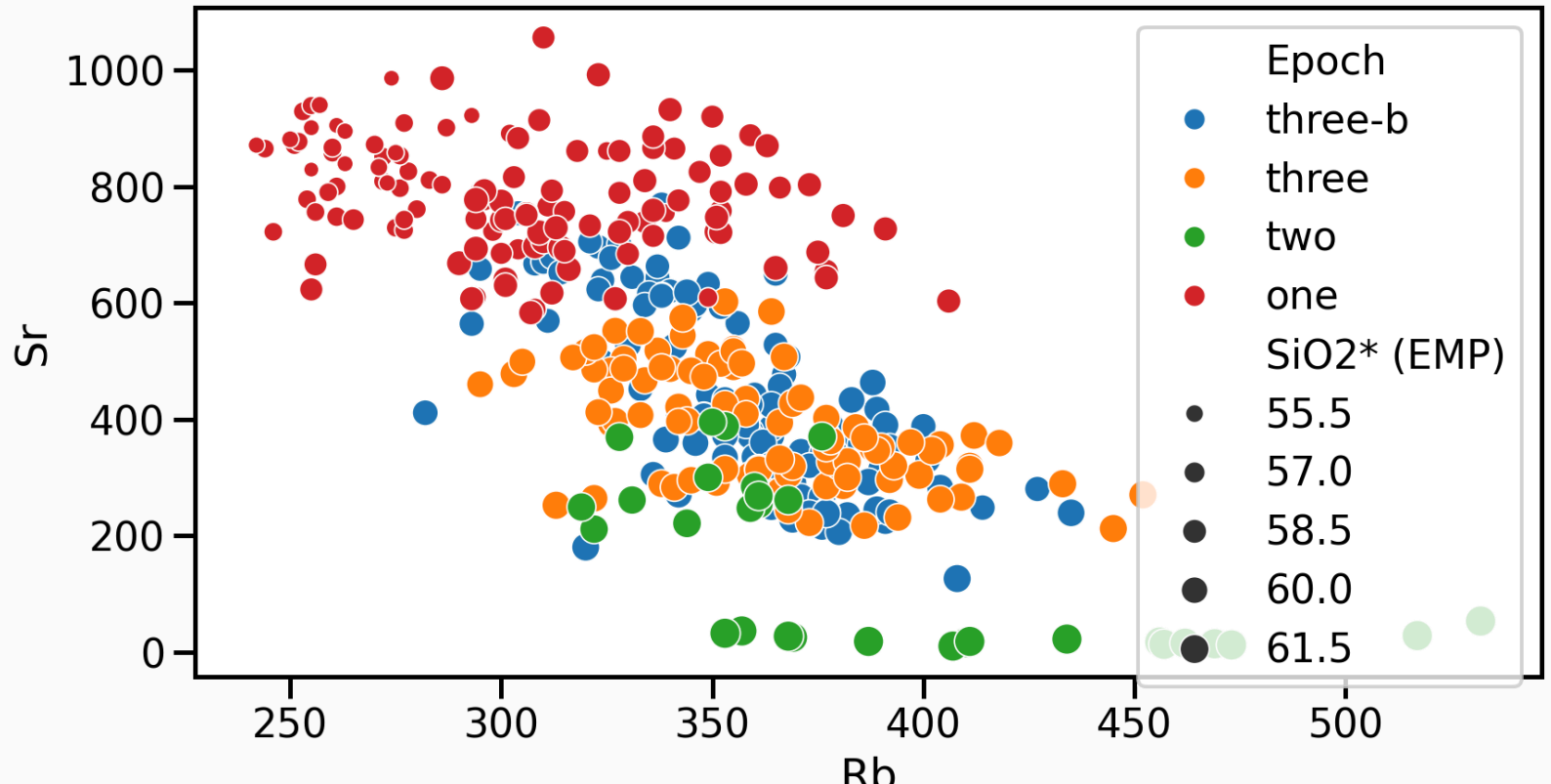
Seaborn example

```
# Define figure + axes
fig, ax = plt.subplots()
# Plot with seaborn (remember, we imported it as sns)
# df_traces is the geochemical dataset imported previously
sns.scatterplot(ax=ax, data=df_traces, x='Rb', y='Sr')
```



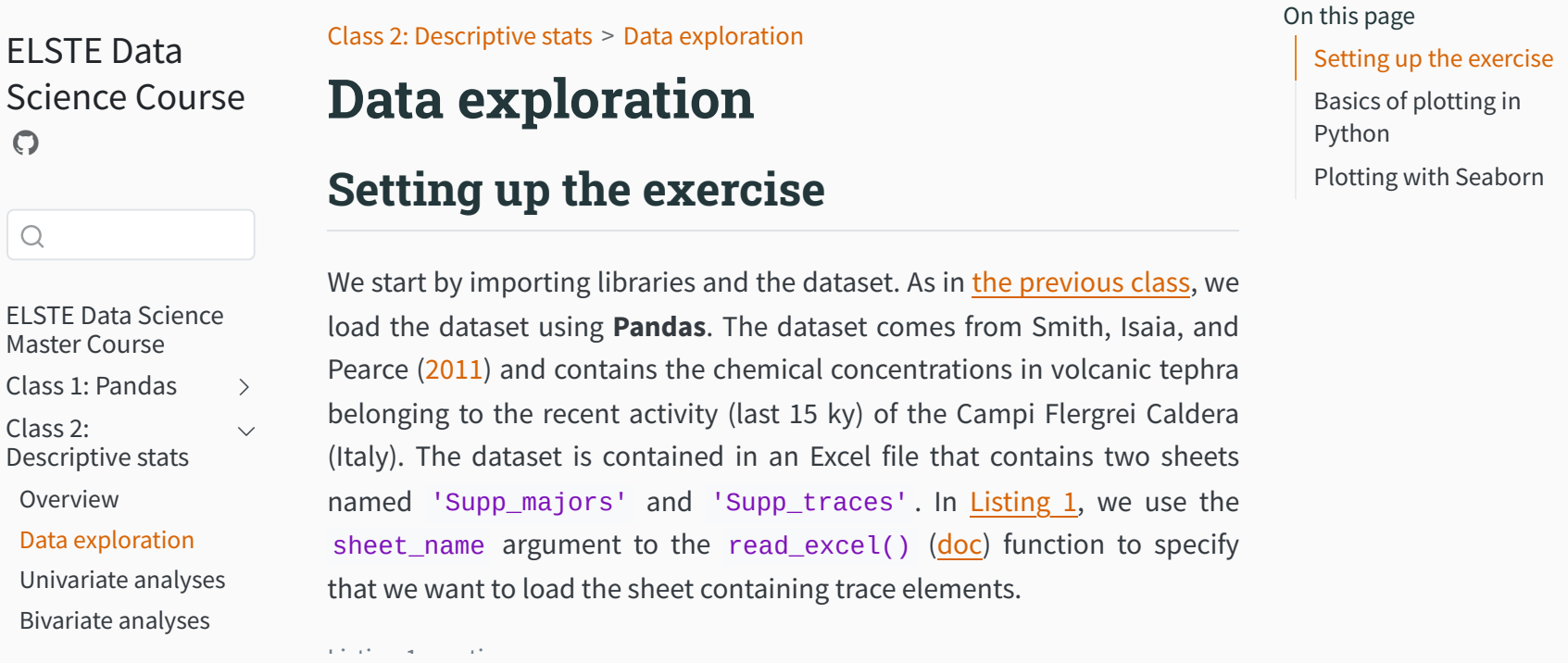
Seaborn example

```
# Define figure + axes
fig, ax = plt.subplots()
# Plot with seaborn (remember, we imported it as sns)
# df_traces is the geochemical dataset imported previously
sns.scatterplot(ax=ax, data=df_traces, x='Rb', y='Sr', hue='Epoch', size="SiO2* (EMP)")
```



Your turn!

- Go to https://elste-master.github.io/Data-Science/
  - → Class 2 > Data exploration
  - → Explore the structure of the glass geochemistry or your dataset
  - → Get used to plotting functions



Descriptive statistics

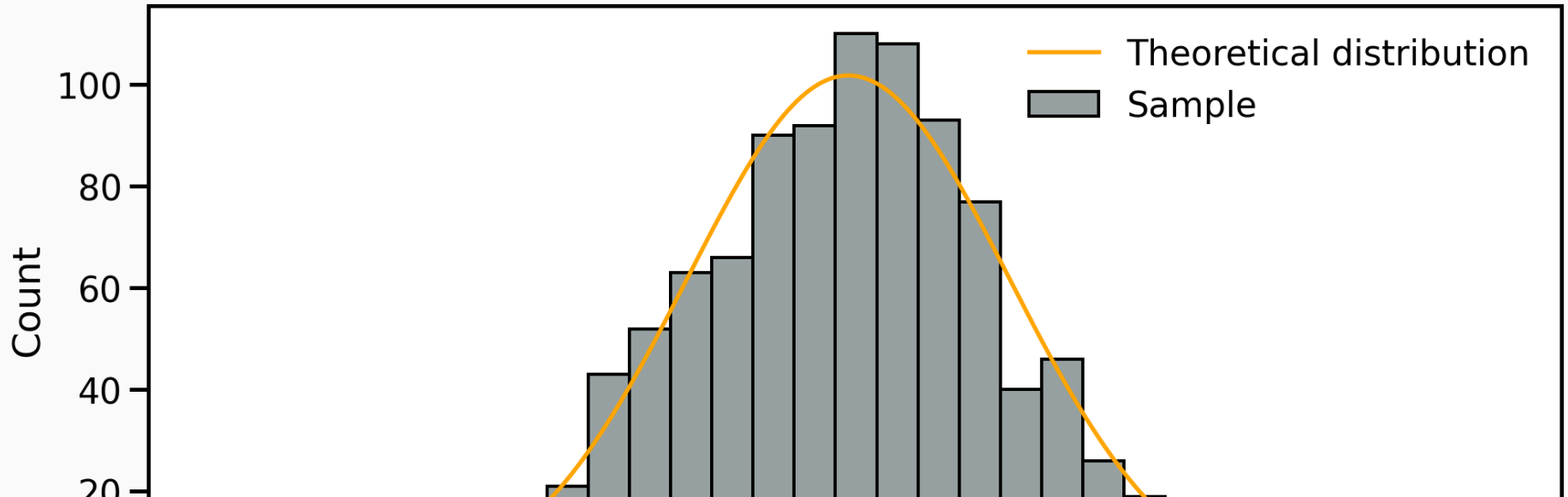
Descriptive statistics

- **Descriptive statistics** → provide ways of capturing the properties of a given data set or sample.
- `Pandas` and `Seaborn` → review metrics, tools, and strategies to summarize a dataset
- Providing us with a quantitative basis to describe it and compare it to other datasets

Univariate analyses

Univariate analyses

- **Objective** capturing the properties of **single** variables at the time
- Fist step: review the samples distribution using **histograms**
  - → Divides dataset into **equal intervals** → bins
  - → **Counts the value** in each bin
  - → Represents the distribution of data



Univariate analyses

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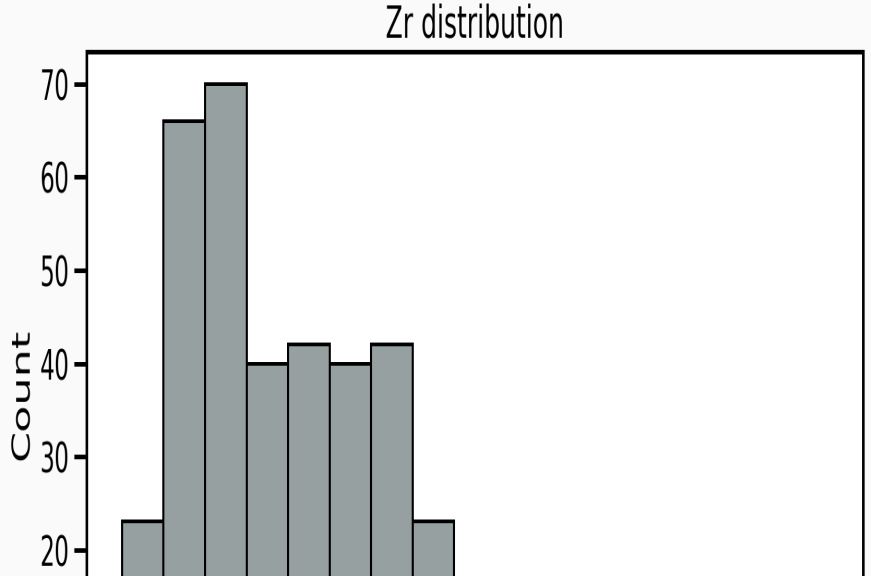
Automatic number of bins:

```
1  fig, ax = plt.subplots()
2  # Plot histogram
3  sns.histplot(data=df_traces, x='Zr', color
4  ax.set_xlabel('Zr (ppm)');
5  ax.set_title('Zr distribution');
```



Univariate analyses

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- Fist step: review the samples distribution using **histograms**
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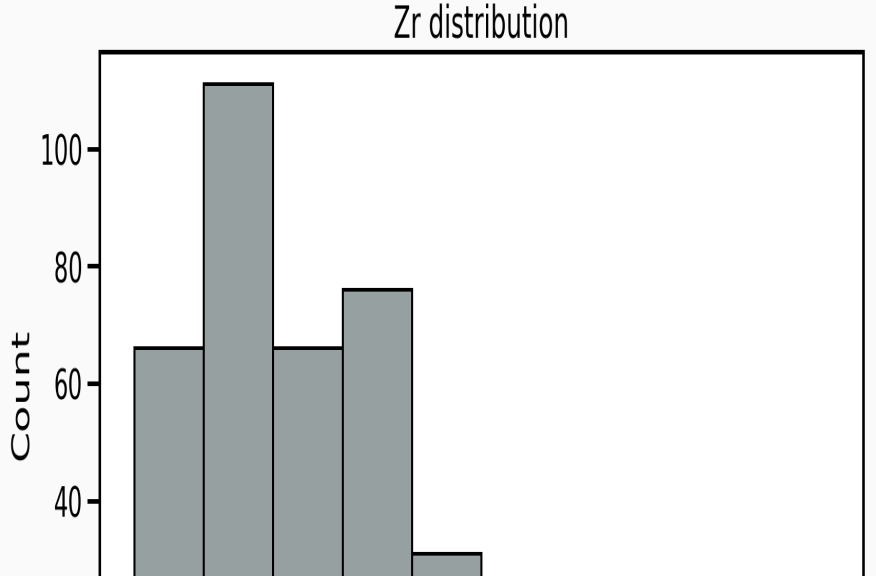
10 bins:

```
1  fig, ax = plt.subplots()
2  # Plot histogram
3  sns.histplot(data=df_traces, x='Zr', bins=
4  ax.set_xlabel('Zr (ppm)');
5  ax.set_title('Zr distribution');
```

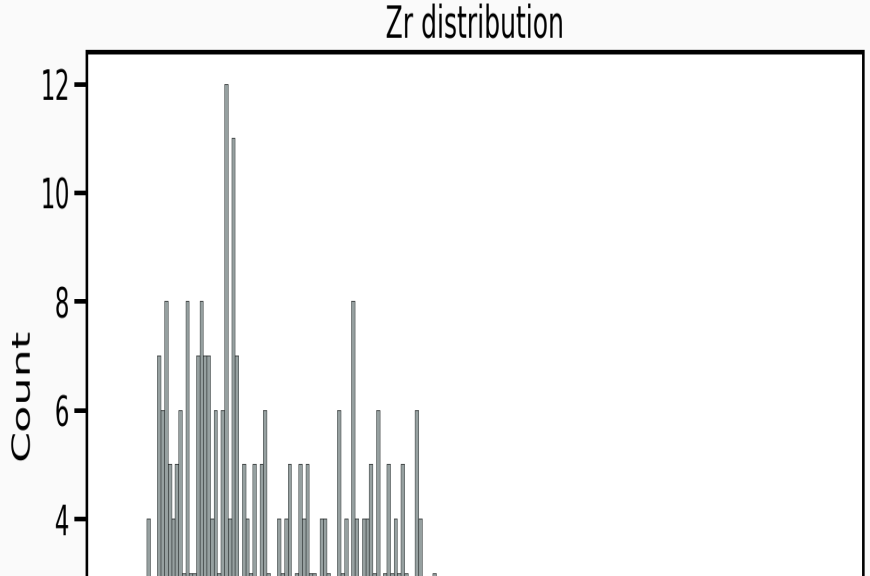


Univariate analyses

- **Objective** capturing the properties of **single** variables at the time
- Fist step: review the samples distribution using **histograms**
  - → Divides dataset into **equal intervals** → bins
  - → **Counts the value** in each bin
  - → Represents the distribution of data

200 bins:

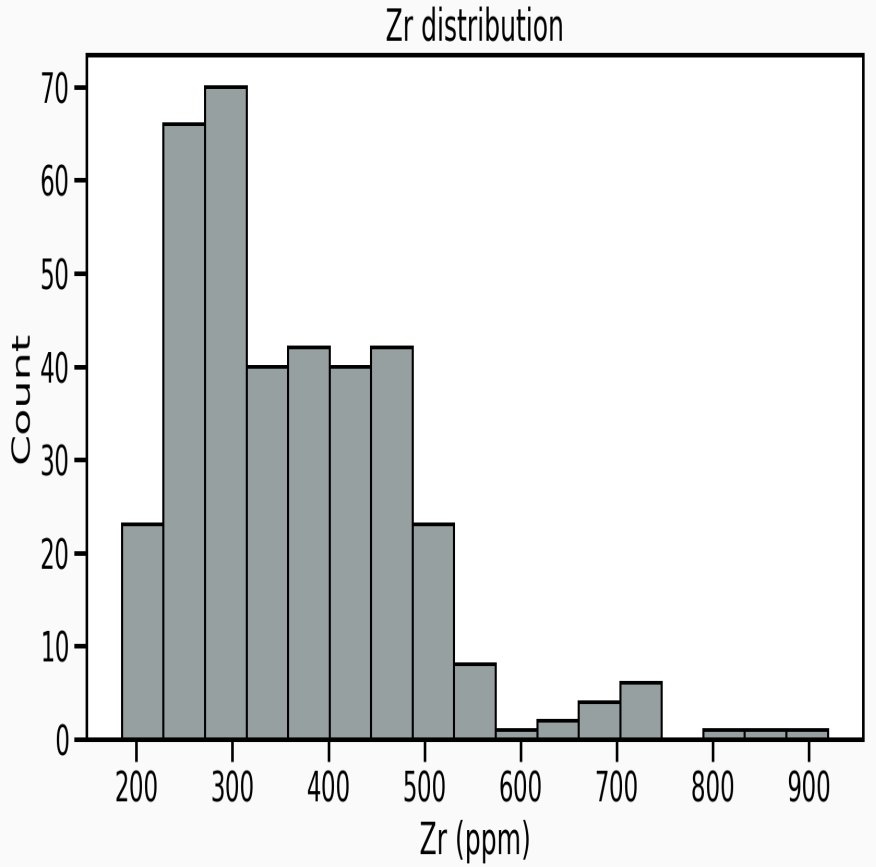
```
1  fig, ax = plt.subplots()
2  # Plot histogram
3  sns.histplot(data=df_traces, x='Zr', bins=
4  ax.set_xlabel('Zr (ppm)');
5  ax.set_title('Zr distribution');
```



Descriptive parameters

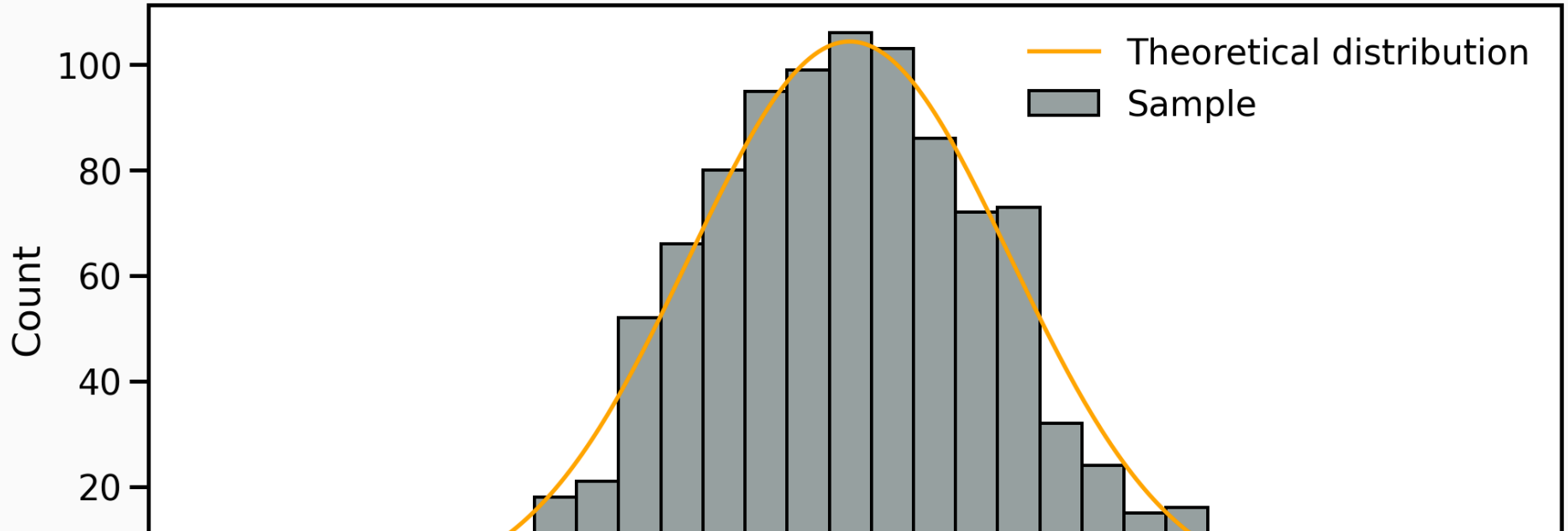
Intuitive importance of describing **three different characteristics** of the distribution:

- The **location** - or where is the central value(s) of the dataset;
- The **dispersion** - or how spread out is the distribution of data compared to the central values;
- The **skewness** - or how symmetrical is the distribution of data compared to the central values;



Descriptive parameters

- **Ideally** → able to constrain full distributions of X
  - → **theoretical moments**
- **In practice** → only observe a finite sample of X
  - → **estimators**



Location I: Mean

The **mean** is the sum of the values divided by the number of values:

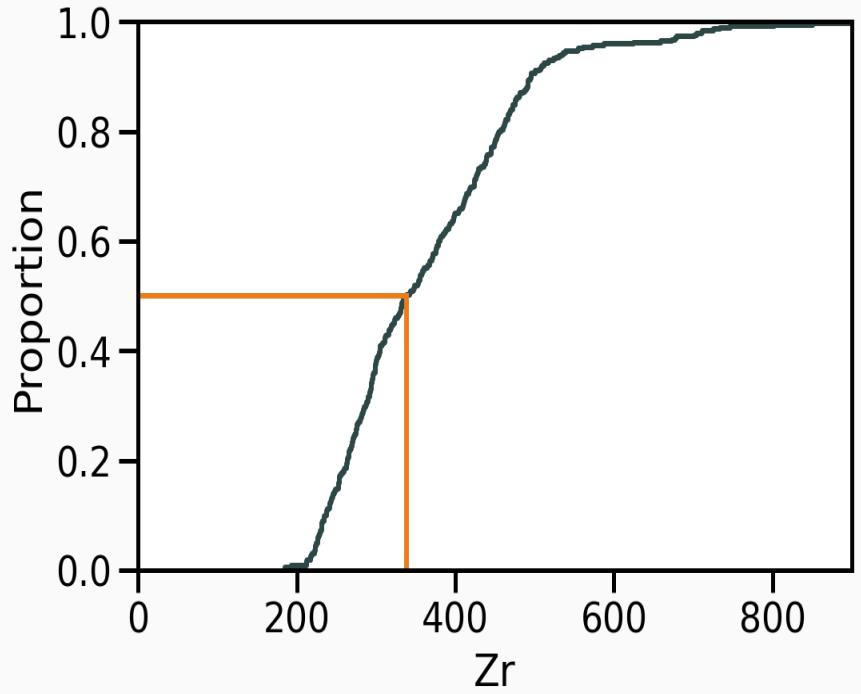
$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

- Meaningful to describe symmetrical distributions
- Very **sensitive** to outliers
- `df.mean()`

Location II: Median

The **median** is the value at the exact middle of the dataset.

- No equation, use of ECDF
- `df.median()`




```
1  # One column
2  df_traces[['Zr']].median().round(2)
3  # Multiple columns
4  df_traces[['Zr','Rb','Sr']].median().round
```

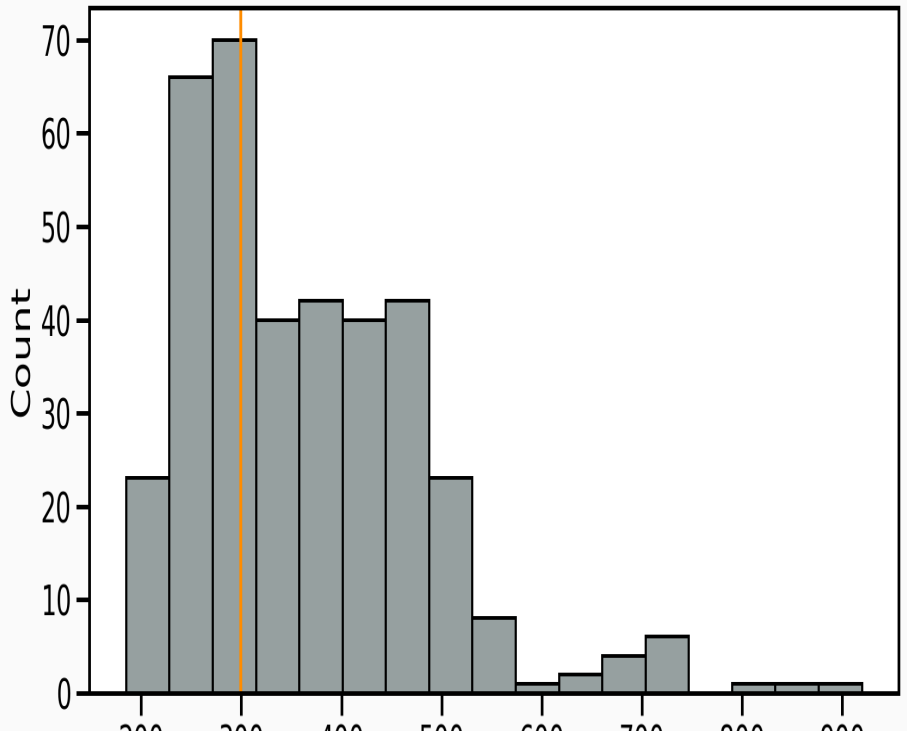
```
Zr     339.0
Rb     347.5
Sr     490.0
dtype: float64
```

Location III: Mode

The **mode** is the value that occur most frequently in a dataset.

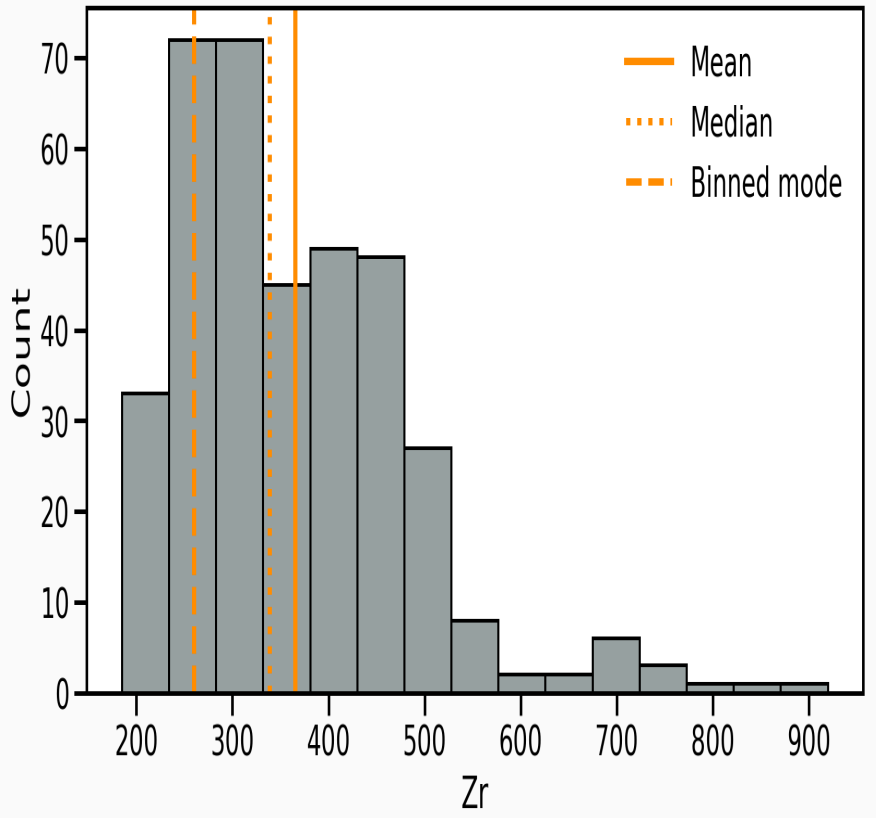
- **Categorical** or **discrete numerical data**: value(s) that appear most often.
- For **continuous data**, exact duplicates may be rare

```
# Calculate the modes
modes = df_traces['Zr'].mode().round(2)

# Plot the histogram
fig, ax = plt.subplots()
sns.histplot(data=df_traces, x='Zr', ax=ax,

# Plot the modes
[ax.axvline(m, color='darkorange', lw=2) for

ax.set_xlabel('Zr (ppm)')
plt.show()
```



Location: Summary

- **Mean**: Best for symmetric distributions
  - → Sensitive to outliers
- **Median**: Best for skewed or outlier-prone data
  - → Only based on rank, not magnitude
- **Mode**: Best for describing the most frequent range in grouped or categorical-like data.
  - → Otherwise requires binning



Dispersion 1: Range

The **range** is the range of value covered in the dataset

- Min → `df.min()`
- Max → `df.max()`
- Range:

$$\text{Range} = \max(x) - \min(x)$$

```
1  df_min = df_traces['Zr'].min()
2  df_max = df_traces['Zr'].max()
3  df_range = df_max - df_min
4  print(f"The range of Zircon concentrations
```

```
The range of Zircon concentrations is 735.00
```

Dispersion 2: Standard deviation

The **sample standard deviation** (s) is the sum of squares differences between data points x_i and the mean $\bar{x}$ over n observations:

$$s = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}}$$

- s is in the same unit as the data
  - → Easy to interpret
- `df.std()`

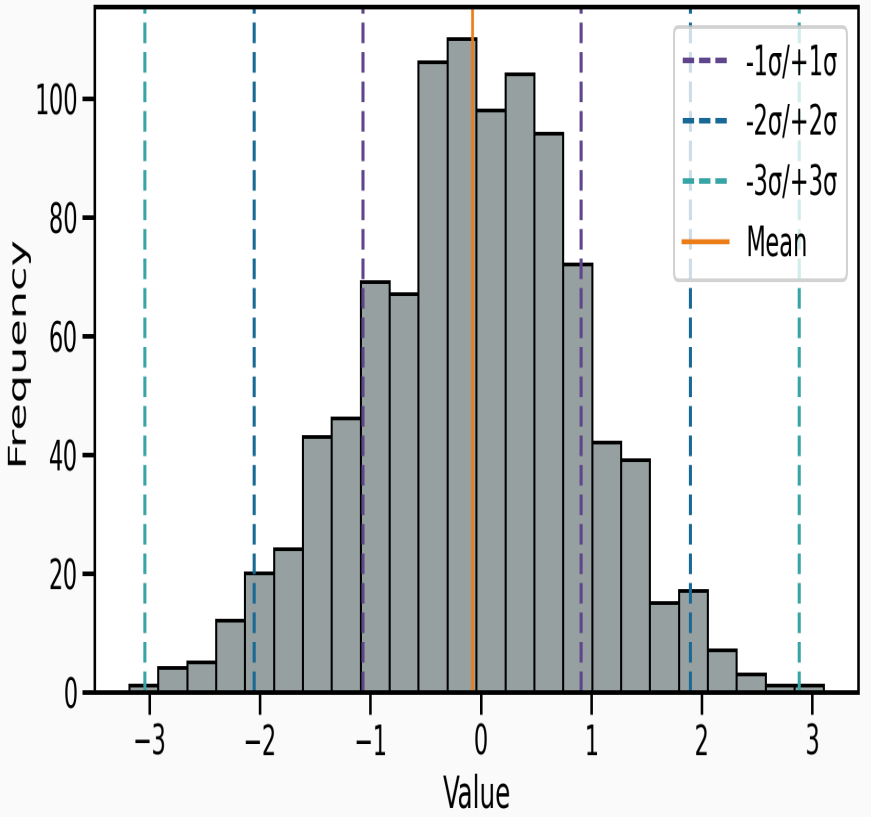
```
1 df_traces['Zr'].std()
```

```
np.float64(118.39358315895393)
```

Dispersion 2: Standard deviation

The **theoretical standard deviation** (σ) is closely related to the **normal distribution** as:

- $1\sigma \rightarrow$ ~68% of the data
- $2\sigma \rightarrow$ ~95% of the data
- $3\sigma \rightarrow$ ~99.7% of the data



Dispersion 2.1: Variance

The **variance** (s^2) is the average of squared deviations from the mean (→ the square of the standard deviation):

$$s^2 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}$$

- s^2 is in **not** the same unit as the data
- Used in modelling (e.g., ANOVA)
- `df.var()`

```
1 df_traces['Zr'].var()
```

```
np.float64(14017.04053321614)
```

Rule of thumb

- Comparing data spread → standard deviation
- Statistical modelling → variance

Dispersion 3: Interquartile range

The **interquartile range** (IQR) indicates how spread out the middle 50% of the data is.

- Difference between the third quartile (Q3) and the first quartile (Q1):

$$\text{IQR} = Q_3 - Q_1 \qquad (1)$$

- Q1: The value below which **25% of the data fall**
- Q3: The value below which **75% of the data fall**

Dispersion 3: Interquartile range

Table 1: Relationship between quartiles, deciles and percentiles.

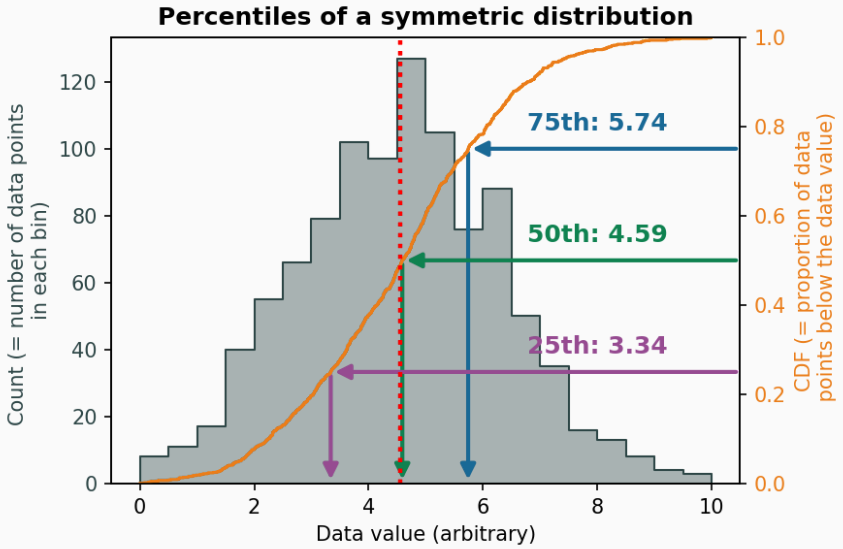
Measure	Number of Divisions	Position(s) in Data / Percentile Equivalent
Quartiles (Q1, Q2, Q3)	4 equal parts	Q1 = 25th percentile, Q2 = 50th percentile (median), Q3 = 75th percentile
Deciles (D1 … D9)	10 equal parts	D1 = 10th percentile, D2 = 20th percentile, …, D9 = 90th percentile
Percentiles (P1 … P99)	100 equal parts	P1 = 1st percentile, P2 = 2nd percentile, …, P99 = 99th percentile

- median =
  - → 2nd quartile = Q2
  - → 5th decile = D5
  - → 50th percentile = P50

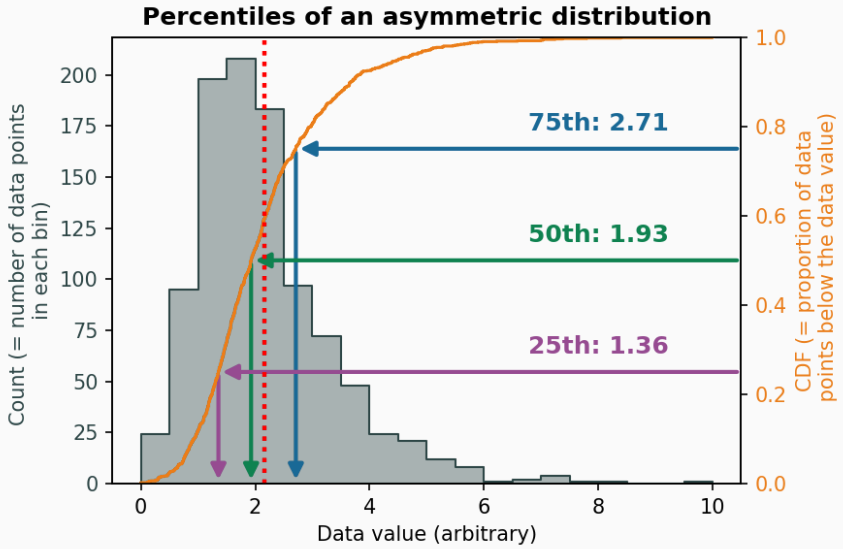
Dispersion 3: Interquartile range

The **interquartile range** (IQR) indicates how spread out the middle 50% of the data is.

Q_1 and Q_3 for a **symmetrical** distribution:



Q_1 and Q_3 for an **asymmetrical** distribution:



Shape: Skewness

The **skewness** measures the asymmetry of a distribution and is computed as:

$$\text{Skewness} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{x_i - \bar{x}}{s}\right)^3$$

In *Pandas*, the skewness can be computed using `.skew()`

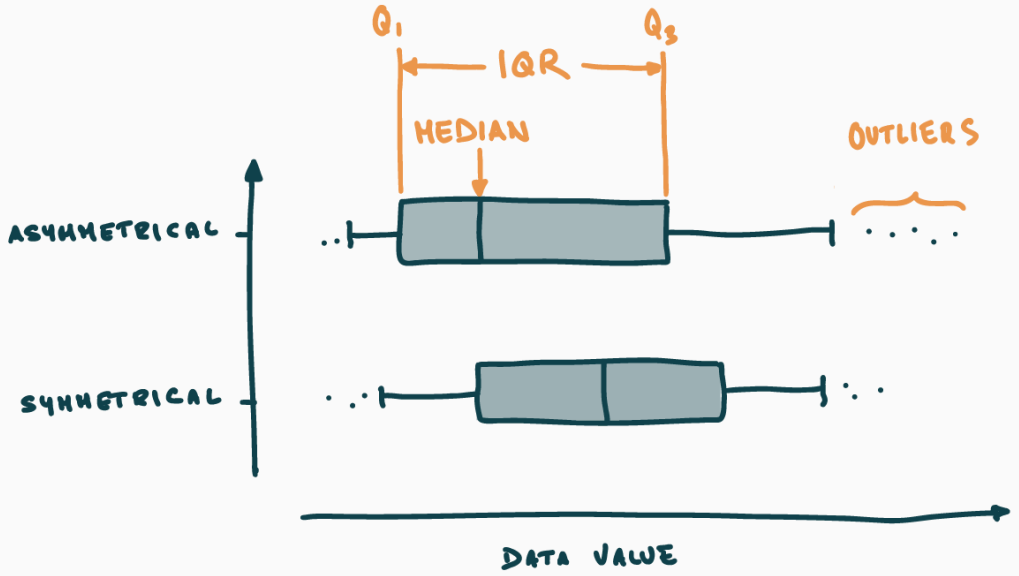
- **0**: Symmetric → e.g., normal distribution
- **>0**: Righ-skewed → a tail extends to the right
- **<0**: Left-skewed → a tail extends to the left

Distribution visualisation

Beyond **histograms** → some plot types report empirical indications of **location**, **dispersion** and **skewness**.

Box and whisker plots

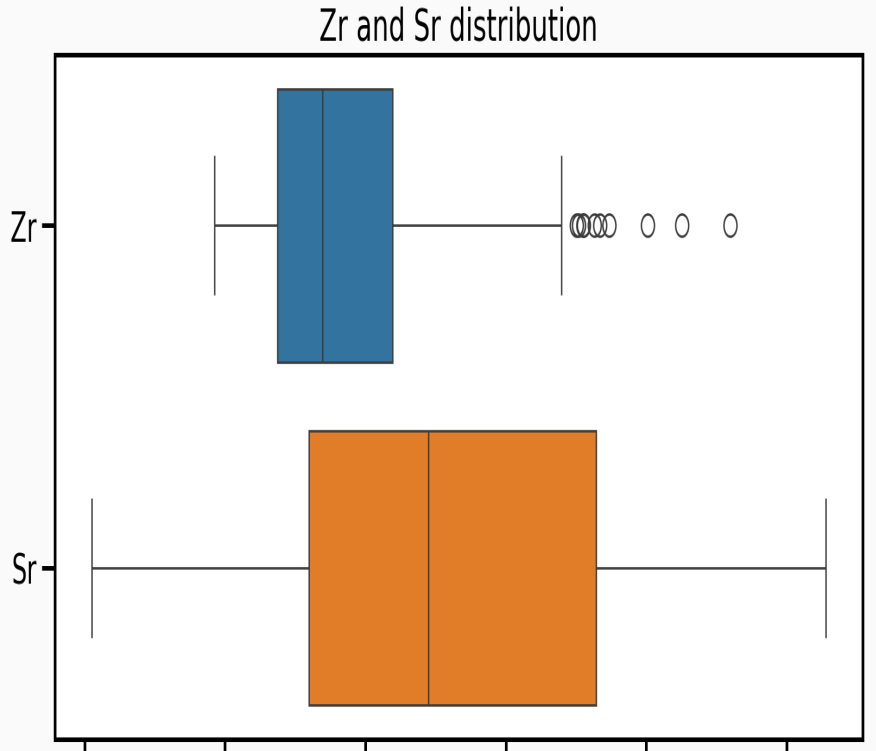
- **Box** → IQR + median
- **Whiskers** 1.5 times the IQR from Q1/Q3
- **Outlier** → differs from the majority of observations



Distribution visualisation: Box plots

- `sns.boxplot()`
- No density
- No tail resolution

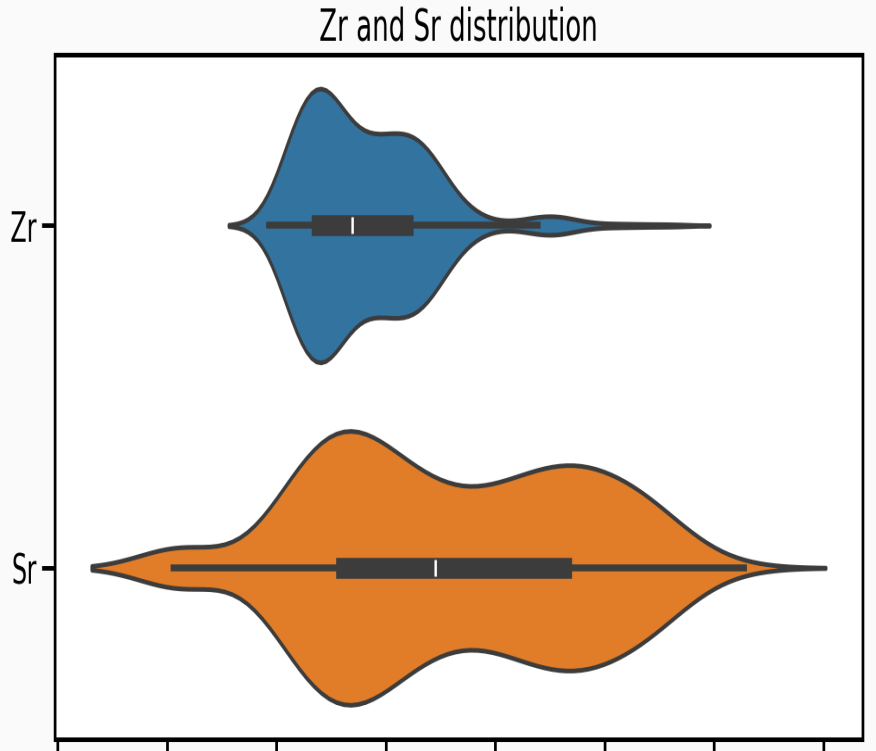
```
1  fig, ax = plt.subplots()
2  sns.boxplot(data=df_traces[['Zr', 'Sr']],
3  ax.set_xlabel('Concentration (ppm)');
4  ax.set_title('Zr and Sr distribution');
```



Distribution visualisation: Violin plots

- `sns.violinplot()`
- Density estimate through Kernel Density Estimator → artefacts
- Some tail resolution, not always realistic

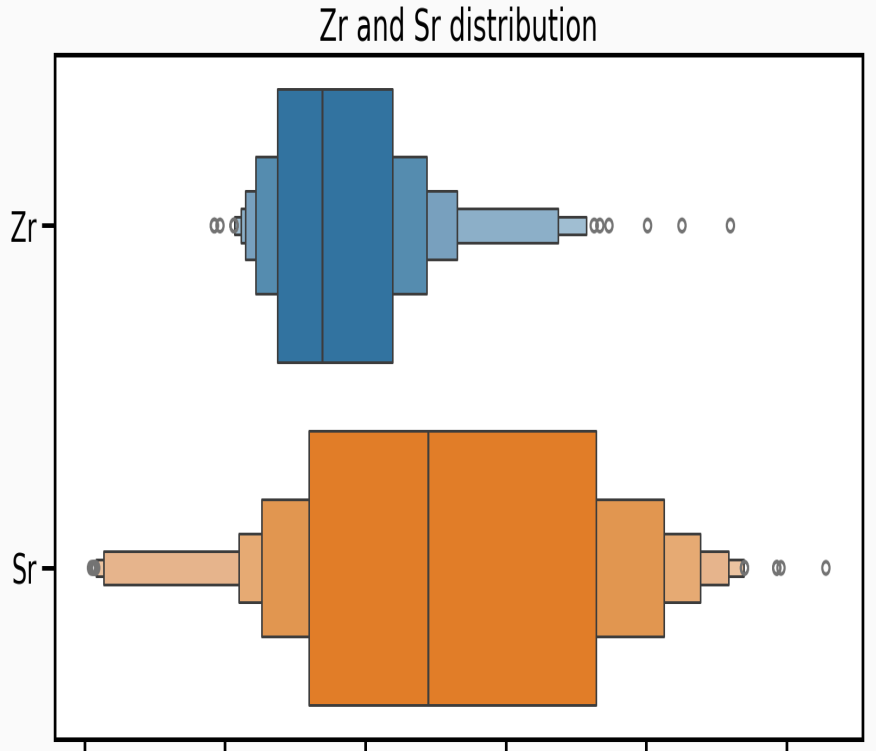
```
1  fig, ax = plt.subplots()
2  sns.violinplot(data=df_traces[['Zr', 'Sr']]
3  ax.set_xlabel('Concentration (ppm)');
4  ax.set_title('Zr and Sr distribution');
```



Distribution visualisation: Boxen plots

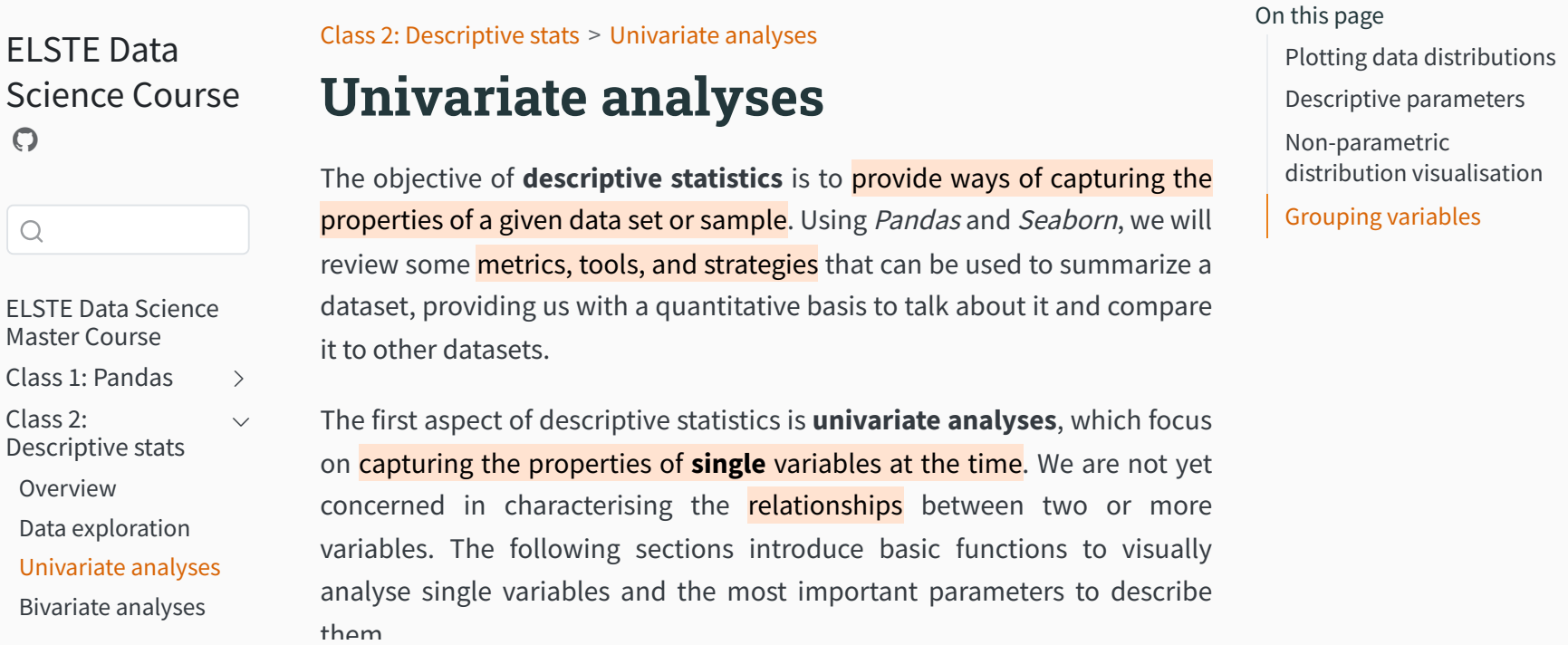
- `sns.boxenplot()`
- Plots deciles → some density estimate
- Good tail resolution

```
1  fig, ax = plt.subplots()
2  sns.boxenplot(data=df_traces[['Zr', 'Sr']]
3  ax.set_xlabel('Concentration (ppm)');
4  ax.set_title('Zr and Sr distribution');
```



Your turn!

- Go to https://elste-master.github.io/Data-Science/
  - → Class 2 > Univariate analyses
  - → Explore the structure of the glass geochemistry or your dataset
  - → Get used to the various functions



Bivariate analyses

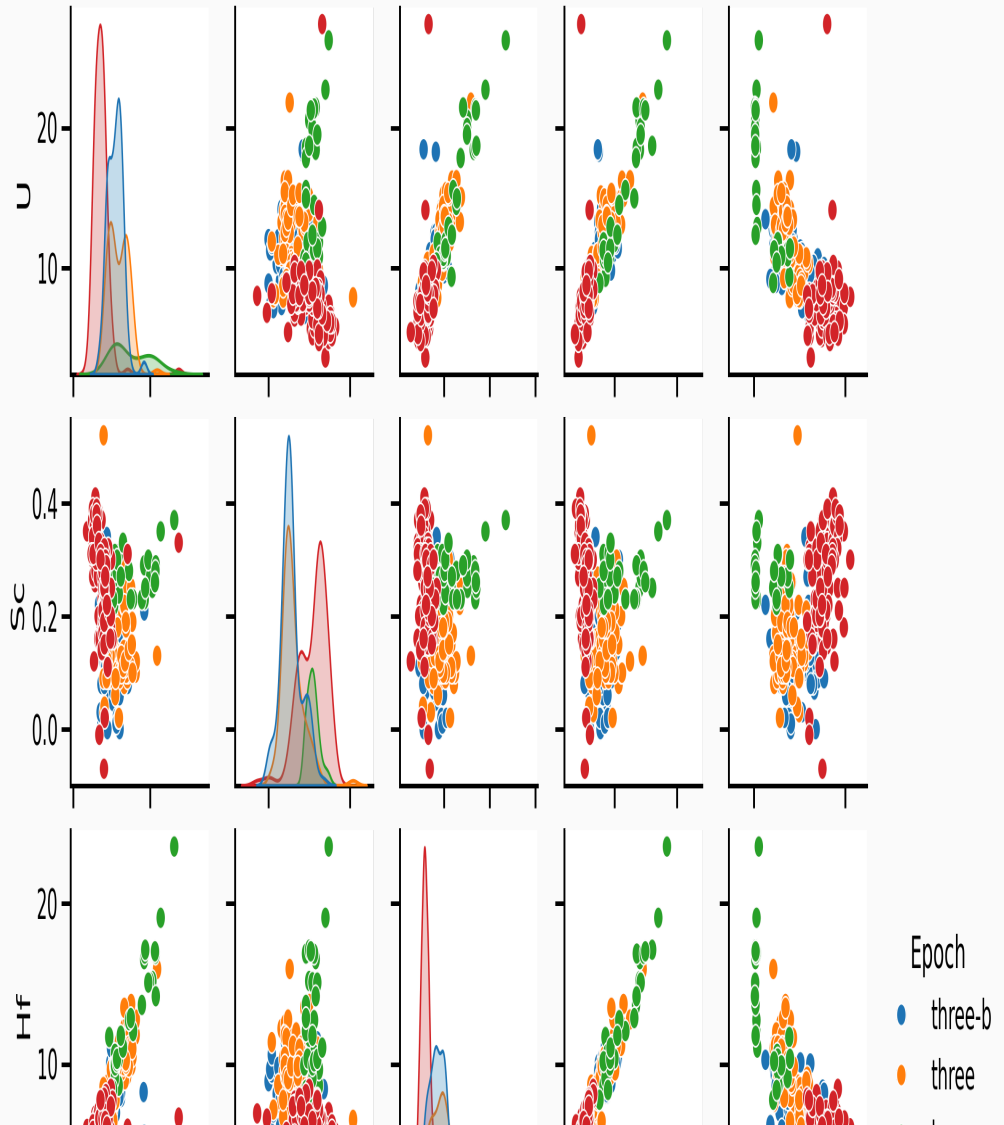
Bivariate analyses

- **Univariate analyses**: properties of one variable at the time
- **Bivariate analyses**: investigate the **relationship** between two variables

Pairwise comparison

A first visual inspection using `sns.pairplot()`

- Numerical values
- One categorical value



Covariance

- The covariance captures **the direction and magnitude of the linear relationship between the two variables**
- The sample covariance is an **estimator** of the theoretical covariance:

$$\mathrm{Cov}(X, Y)_{\mathrm{emp}} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}),$$

- **Positive**: Increase in $X \rightarrow$ increase in Y
- **Negative**: Increase in $X \rightarrow$ decrease in Y

Problem: depends on the magnitudes of the variables, so it does not directly reflect the strength of the relationship

Correlation

- The correlation coefficient provides **a normalized version** of the covariance
  - → Ranges from -1 to 1
  - → Indicates both the direction and the strength of the linear relationship
- The sample correlation is computed as:

$$r(X,Y)_{\text{emp}} = \frac{\text{Cov}(X,Y)_{\text{emp}}}{s_X s_Y} = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2}},$$

- $r(X,Y) = -1/1 \rightarrow$ "perfect" **relationship** between X and Y
- $r(X,Y) = 0 \rightarrow$ **independence** between X and Y.

Correlation matrix

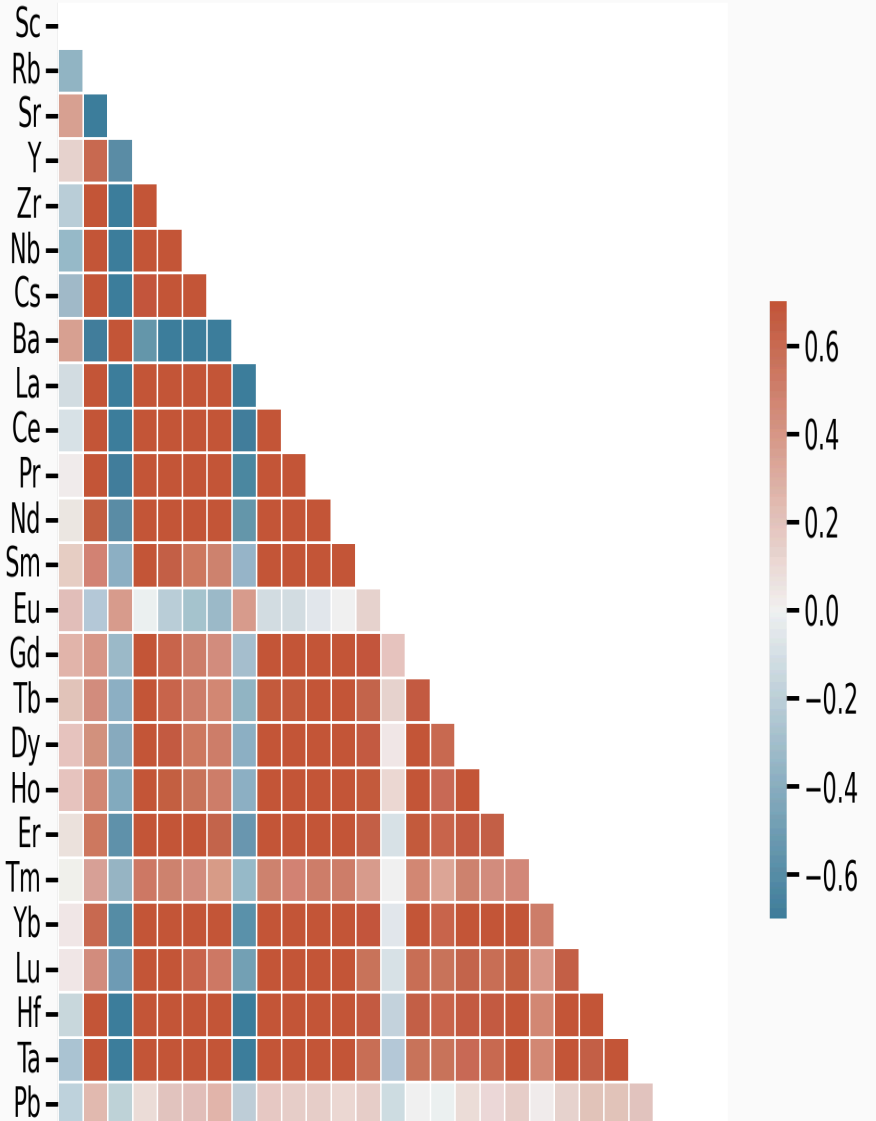
- Correlation matrix → square table showing the pairwise correlations between all variables in a dataset
- Suppose we have p variables $(X_1, X_2, \dots, X_p)$ → the correlation matrix $\mathbf{C}$ is:

$$\mathbf{C} = \begin{pmatrix} 1 & r(X_1, X_2) & \dots & r(X_1, X_p) \\ r(X_2, X_1) & 1 & \dots & r(X_2, X_p) \\ \vdots & \vdots & \ddots & \vdots \\ r(X_p, X_1) & r(X_p, X_2) & \dots & 1 \end{pmatrix}.$$

Correlation matrix

Correlation matrix for trace elements

- Use **sample** correlation coefficient r
  - → **Red:** positive relationship
  - → **Blue:** negative relationship
  - → **White:** no relationship



Linear regression

- Correlation coefficients → measure of coupling between two continuous variables
- linear regressions attempt modelling this relationship

$$y = a + bx + \varepsilon$$

where:

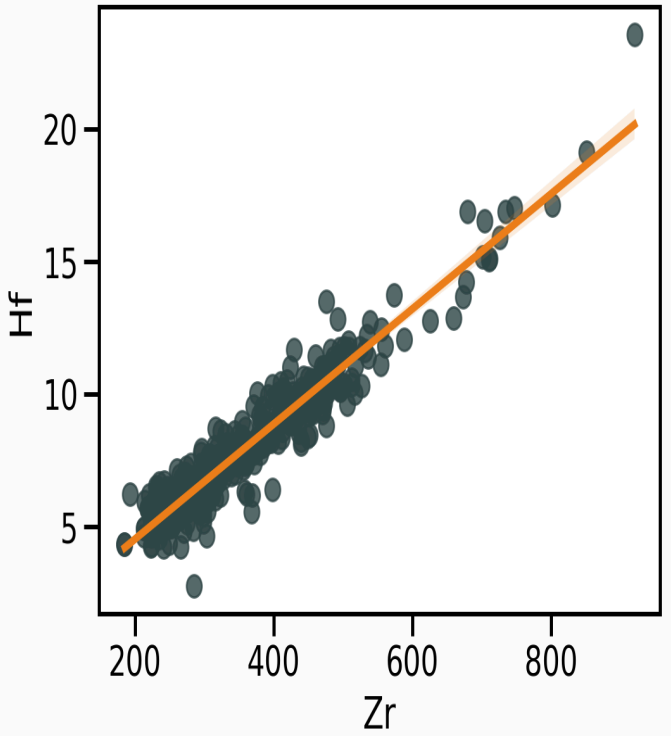
- y: dependent (response) variable
- x: independent (predictor) variable
- a: intercept → value of y when $x = 0$
- b: slope → how much y changes by unit of x
- ε: error term

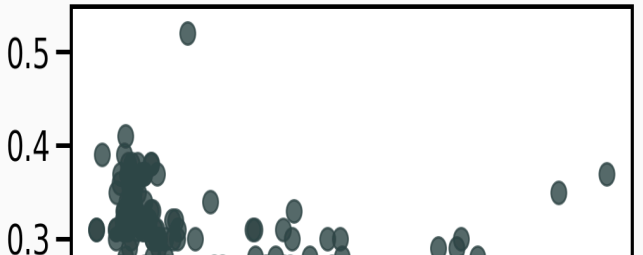
→ **Objective:** Estimate the values of a and b that best fit the observed data

Linear regression with Seaborn

Seaborn has high level functions to **visualise** regressions → `sns.regplot()` that produce:

1. A scatter plot;
2. A linear regression model fit;
3. A confidence interval



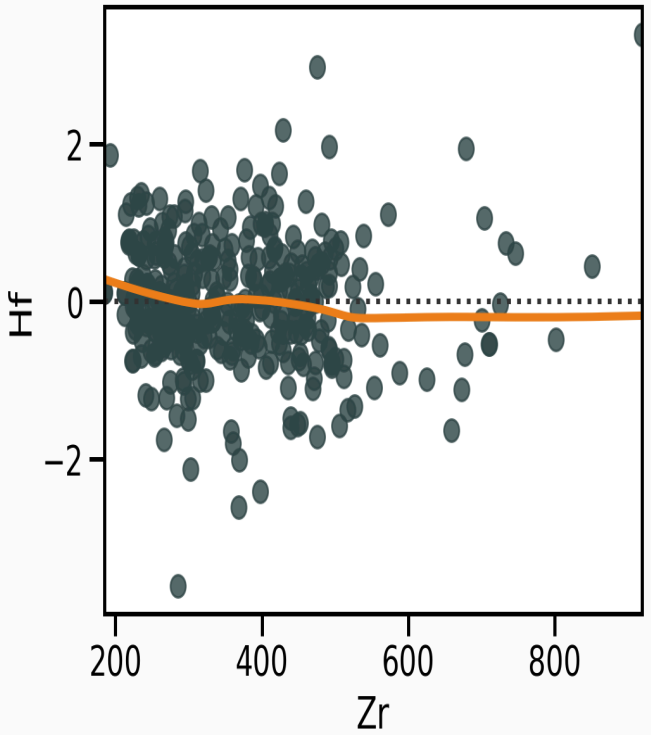


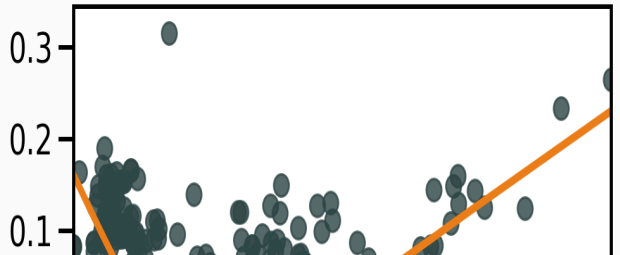
Residual analysis with Seaborn

Linear regression → do residuals show any structure?? → `sns.residplot()`

Residuals are necessary to:

1. **Diagnose model fit** (→ how much **unexplained variation** remains);
2. **Detect patterns** that indicate problems (non-linearity, heteroscedasticity, outliers).





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