Lecture #4: Exploratory data analysis (EDA)

Slides by Artem Dembitskiy

Previously on

- Python for atomistic modeling
- ASE's Atoms and Pymatgen's Structure
  - Neighbor list
  - Voronoi partitioning
- Data in materials informatics
- Computational data
  - The Materials project API

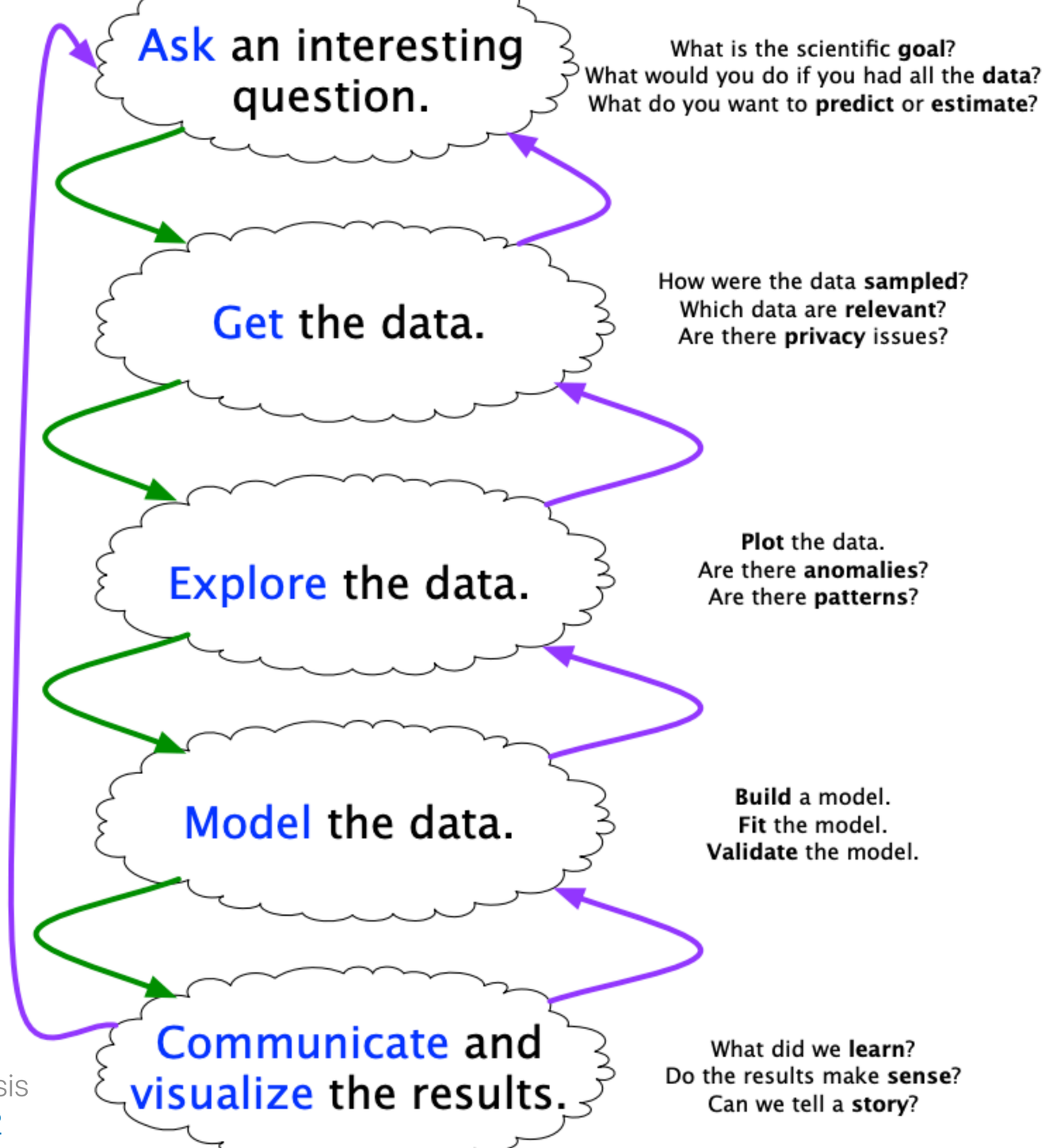
Goals/Agenda

- Explain why visualizing data is important when analyzing data
- Provide tips on how to use visualization to explore data

Attribution

- Parts of these slides are adapted from the excellent lecture on exploratory data analsysis from the course CS 109A: Introduction to Data Science by Pavlos Protopapas & Kevin Rader shared under MIT licence
  - https://harvard-iacs.github.io/2018-CS109A/lectures/lecture-3/presentation/lecture3.pdf
- Consider the following materials your reading homework

The data science workflow



From CS 109a: Data Science, Effective Exploratory Data Analysis and Visualization by Pavlos Protopapas & Kevin Rader, slide #2

Sample size

Number of observations in a dataset (study)

```
len(data)
```

Mean

```
np.mean(data)
```

$$\bar{x} = \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right) = \frac{x_1 + x_2 + \cdots + x_n}{n}$$

Median

"The median of a set of numbers is the value separating the higher half from the lower half of a data sample, a population, or a probability distribution."

```
np.median(data)
```

$$1, 3, 3, \mathbf{6}, 7, 8, 9$$

$$\text{Median} = \underline{\underline{6}}$$

$$1, 2, 3, \mathbf{4}, \mathbf{5}, 6, 8, 9$$

$$\text{Median} = (4 + 5) \div 2$$

$$= \underline{\underline{4.5}}$$

Standard deviation

"...is a measure of the amount of variation of the values of a variable about its mean."

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}, \text{ where } \mu = \frac{1}{N}\sum_{i=1}^{N} x_i.$$

```
np.std(data)
```

Correlation coefficient

"The Pearson correlation coefficient measures the linear relationship between two datasets. Like other correlation coefficients, this one varies between -1 and +1 with 0 implying no correlation."

scipy docs

The correlation coefficient is calculated as follows:

$$r = \frac{\sum(x - m_x)(y - m_y)}{\sqrt{\sum(x - m_x)^2 \sum(y - m_y)^2}}$$

where m_x is the mean of the vector x and m_y is the mean of the vector y.

Descriptive statistics of band gap (E_g) distribution in the Materials Project

Sample size

- 103,217

Mean of E_g

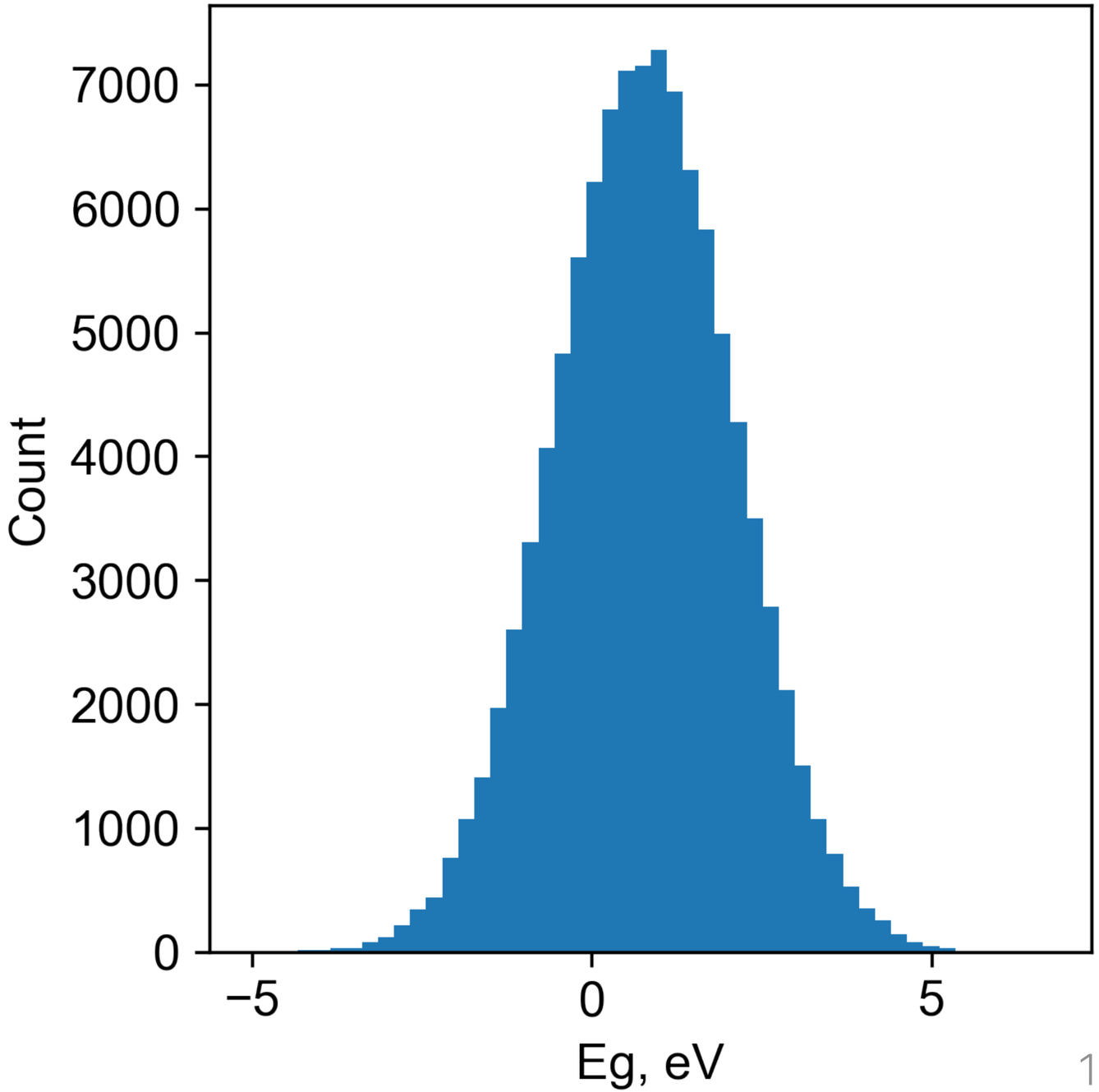
- 0.79 eV

Standard deviation of E_g:

- 1.37 eV

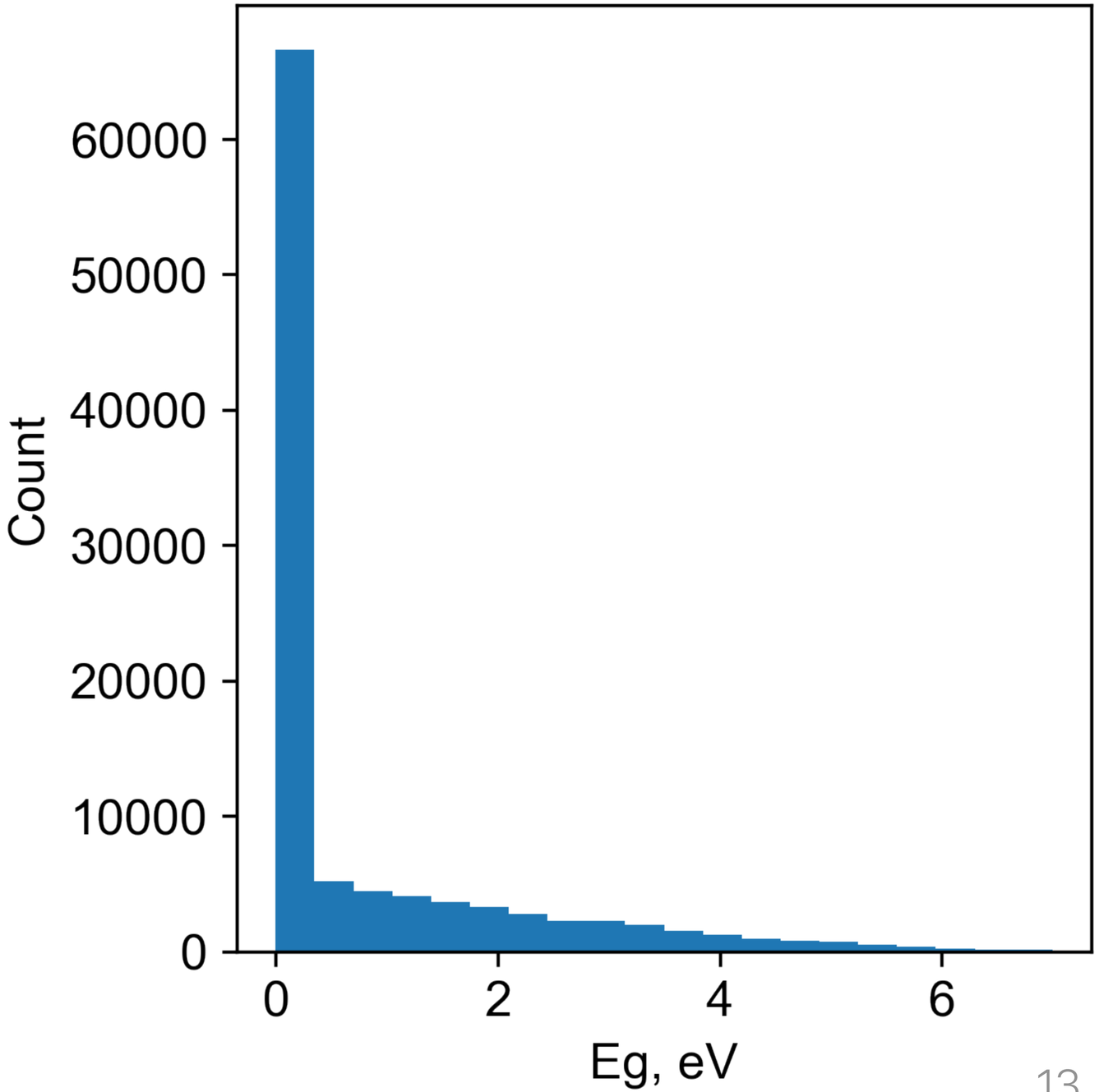
Is it what you expected?

- What wrong with this distribution?



This is the real distribution

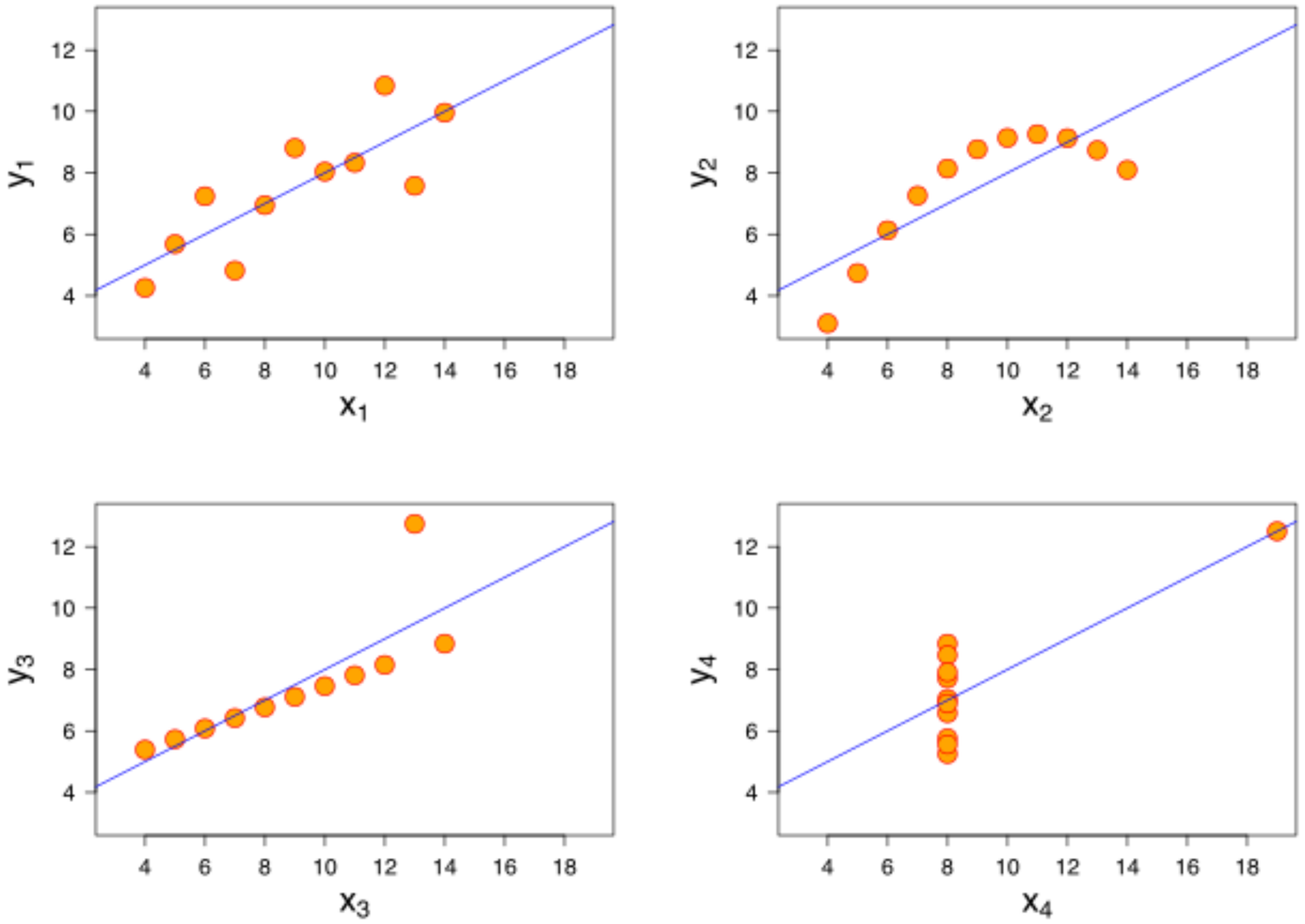
- Metals have a zero E_g
- Median(E_g) = 0.0 says that metals represent at least half of the sample



Why is visual inspection of data important?

- Same descriptive statistics
- Very different distributions

https://en.wikipedia.org/wiki/Anscombe%27s_quartet



Visulaization goals

- Communicate (Explanatory)
- Present data and ideas
- Explain and inform
- Provide evidence and support
- Influence and persuade
- Analyze (Exploratory)
- Explore the data
- Assess a situation
- Determine how to proceed
- Decide what to do

From CS 109a: Data Science, Effective Exploratory Data Analysis and Visualization by Pavlos Protopapas & Kevin Rader, slide #23

Communicate

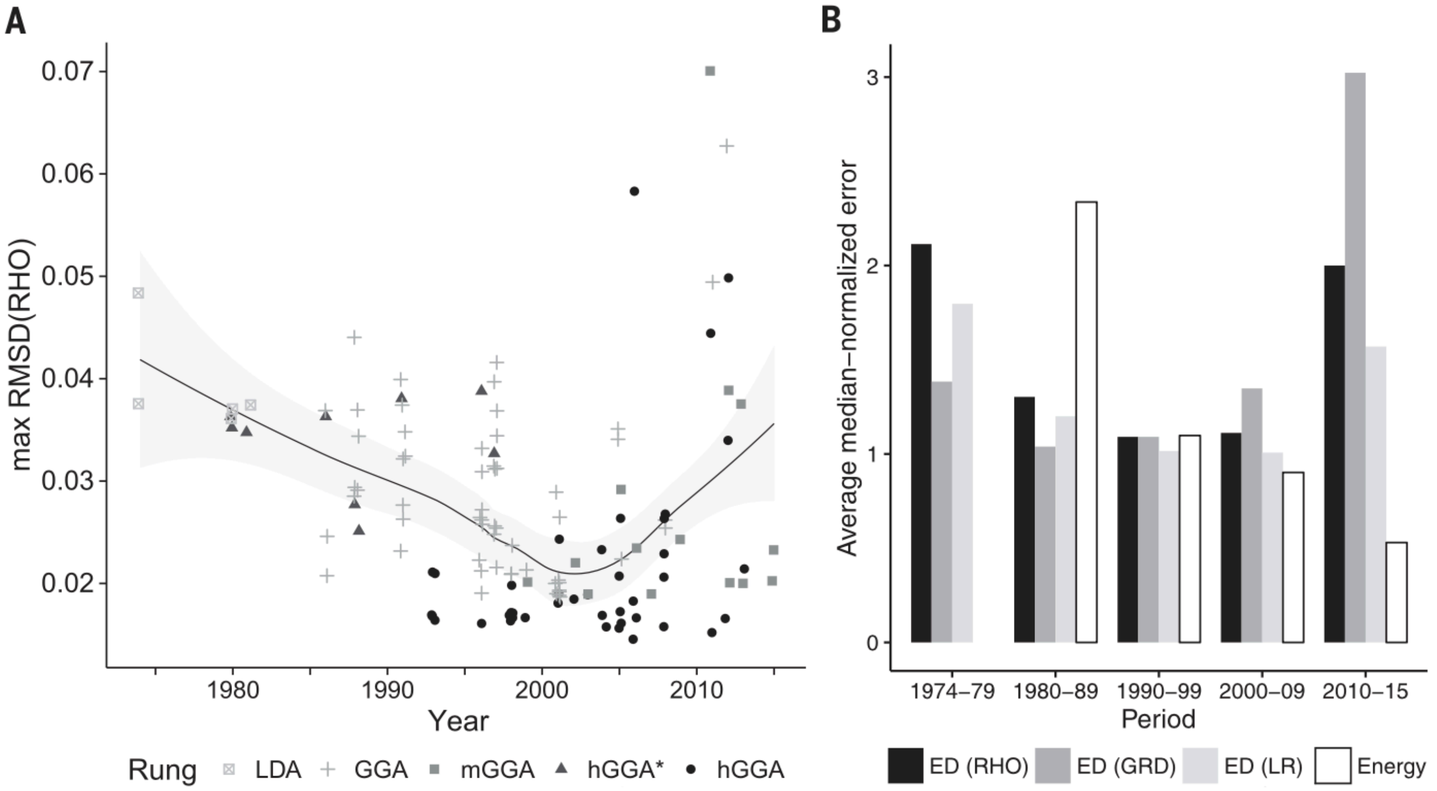
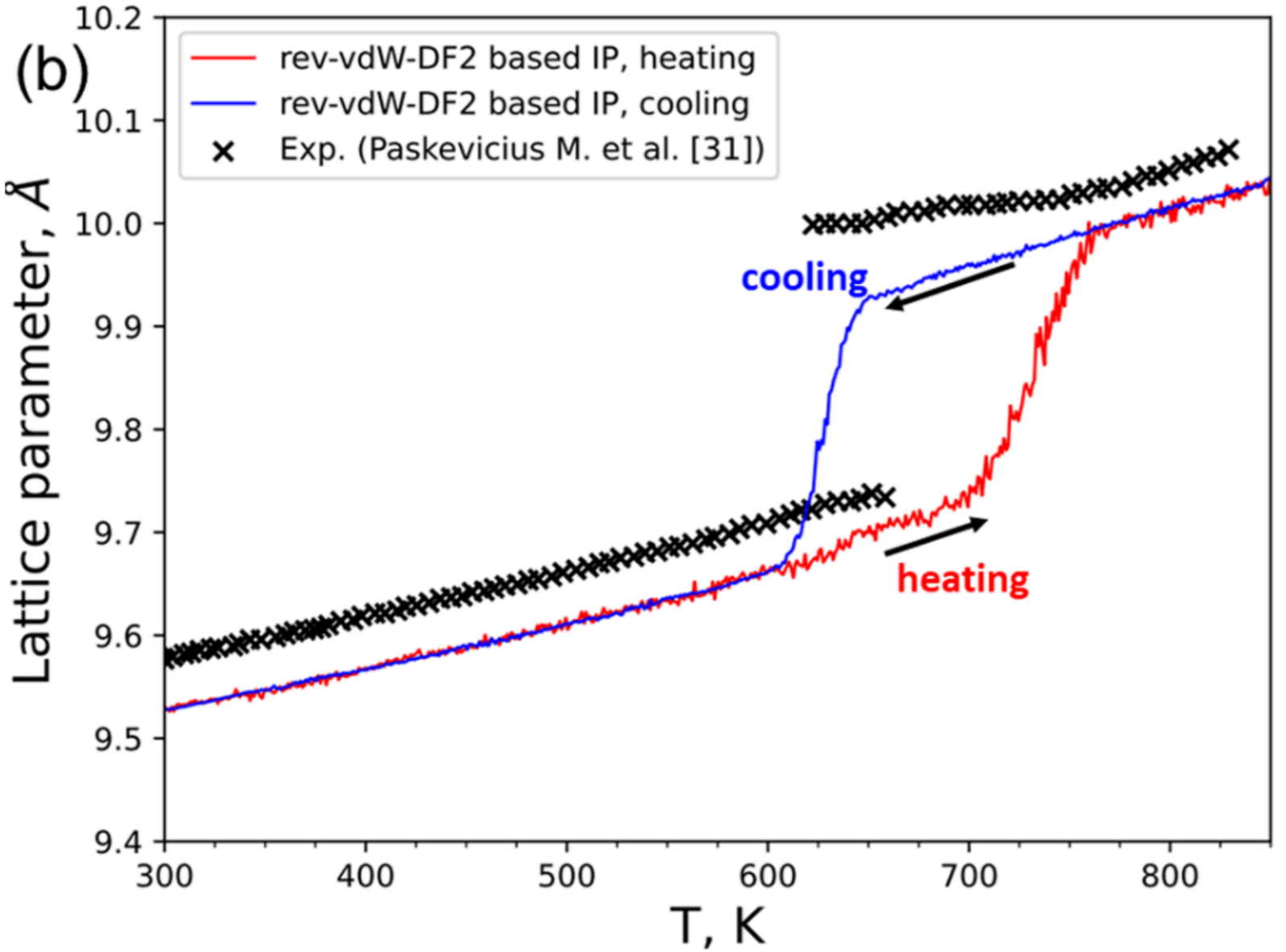


Fig. 1. The historical trends in maximal deviation of the density produced by various DFT methods from the exact one. (**A**) The line shows the average deviation, with the light gray area denoting its 95% confidence interval; hGGA* denotes 100% exact exchange-based methods. (**B**) The bars denote averages of DFT functionals' median-normalized absolute error for energy [open bars, Truhlar's data (*4*)] and electron density with its derivatives (solid bars, this work) per publication decade.

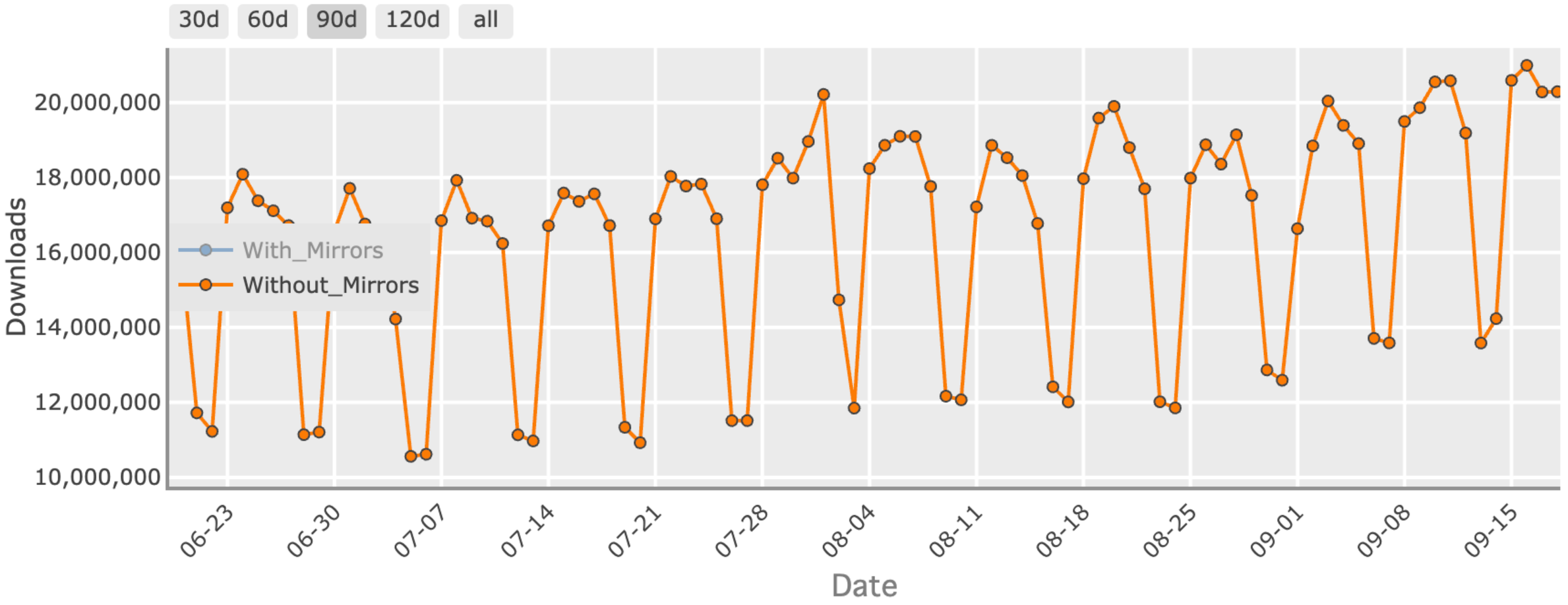
Medvedev *et al.*, *Science* **355**, 49–52 (2017) 6 January 2017

1 of 4

Explore


(b)
rev-vdW-DF2 based IP, heating
rev-vdW-DF2 based IP, cooling
Exp. (Paskevicius M. et al. [31])
cooling
heating
Lattice parameter, Å
T, K
10.2
10.1
10.0
9.9
9.8
9.7
9.6
9.5
9.4
300
400
500
600
700
800

Numpy daily downloads statistics: What are these periods?



Exploratory data analysis pipeline

- Build data
- Clean data
- Explore global features
- Explore group features

Build (read) data in a structured format

- Pandas DataFrame
- One row per variable

```
df = pd.read_csv("eg_data.csv")
```

Clean the data

- Outliers
- NaNs (missing values)
- Constant rows
- Duplicates

```
df.dropna()
```

- Plus visual support: histograms, scatter plots, box plots, etc

Study the global summary statistics

```
df.describe()
```

```
df.aggregeate(
                {
                "column_name": ["min", "max", "median", "skew"]
                }
)
```

Plus visual support: histograms, scatter plots, box plots, etc

Study the summary statistics of the subgroups

```
df[["bandgap", "chemsys"]].groupby("chemsys").mean()
```

Plus visual support: histograms, scatter plots, box plots, bar plots, etc

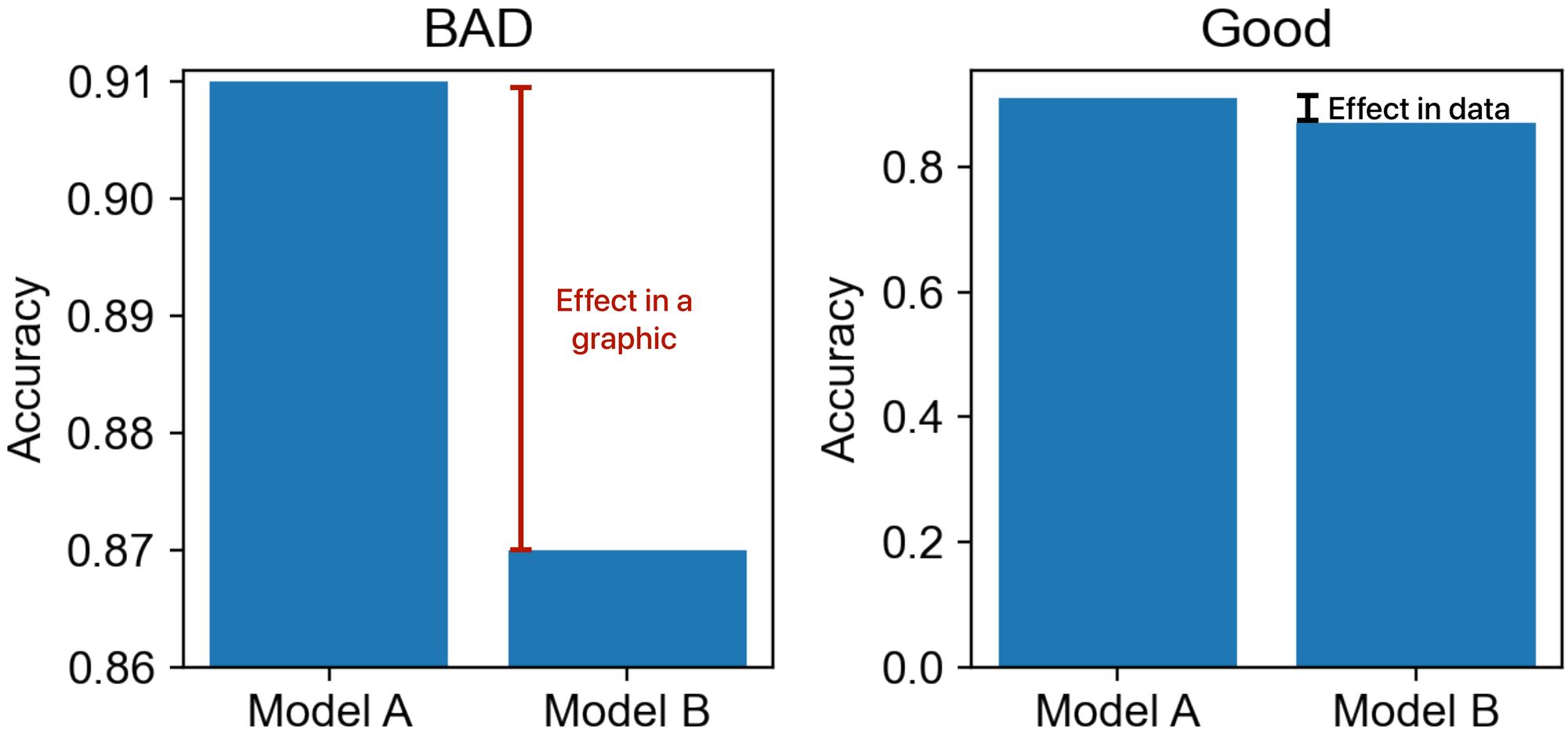
Some principles for effective EDA

Avoid misleading graphs

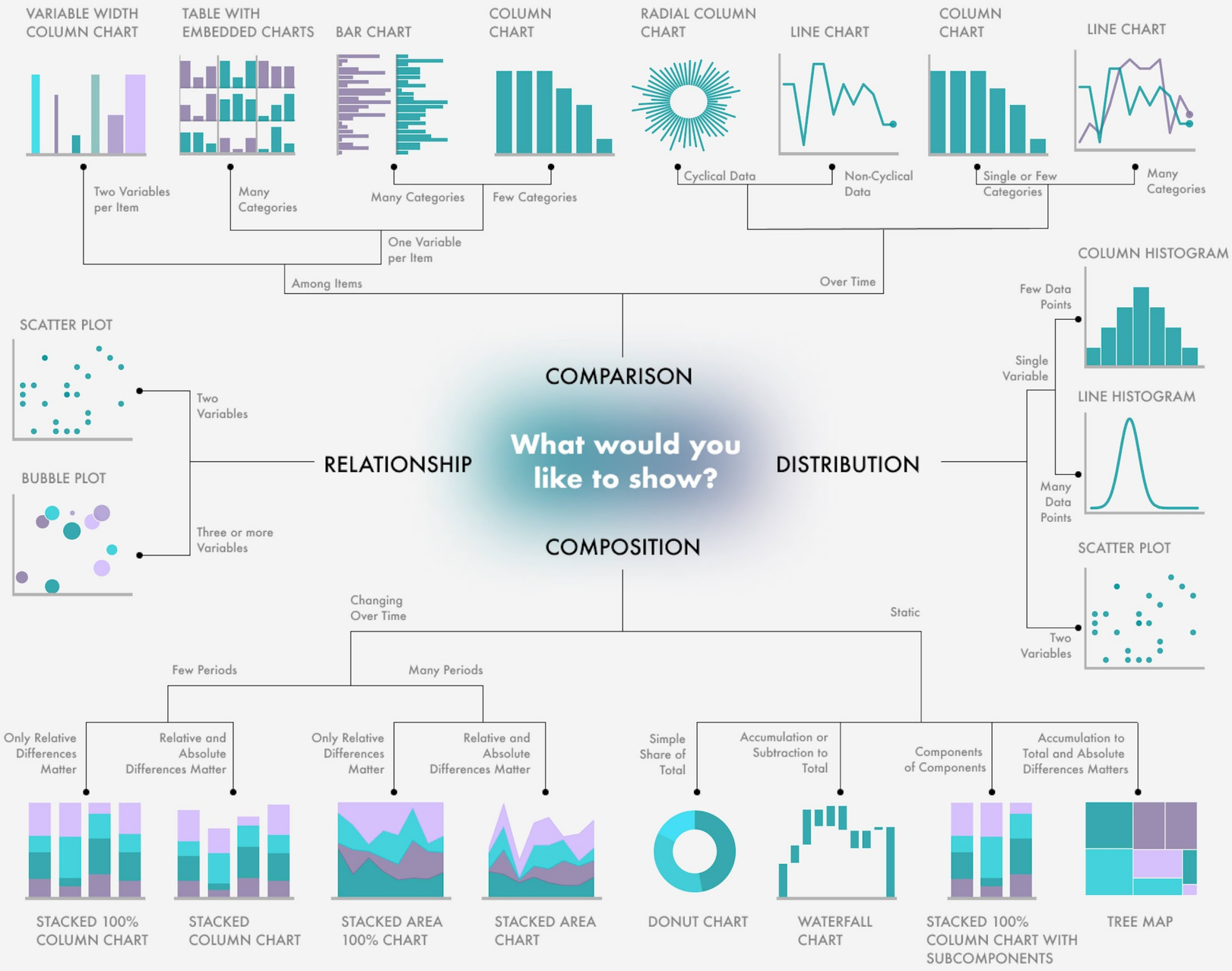
- Do not distort scales
- Do not truncate graph when comparing the data
  - or indicate the truncation
- Avoid 3D charts
- Do not change y(or x)-axis maximum
- Aspect ratio determines the perception of steepness in slope
  - be proportional

Have a look at this page: https://en.wikipedia.org/wiki/Misleading_graph

$$\text{Lie factor} = \frac{\text{Effect in a graphic}}{\text{Effect in data}}$$



Use the right display

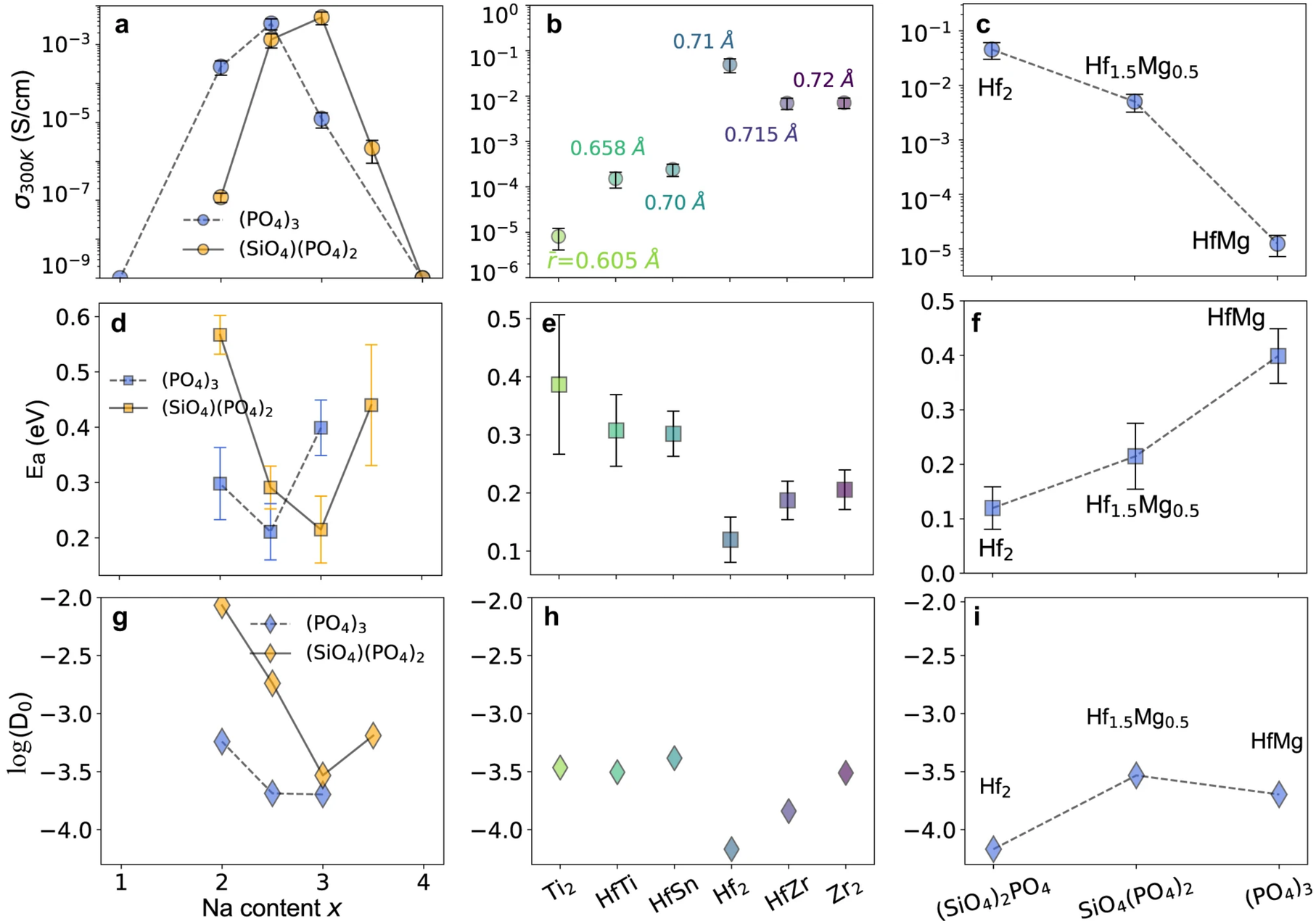


Correlations

- Scatter plot, correlation matrix

Is it a good graph?

Why?

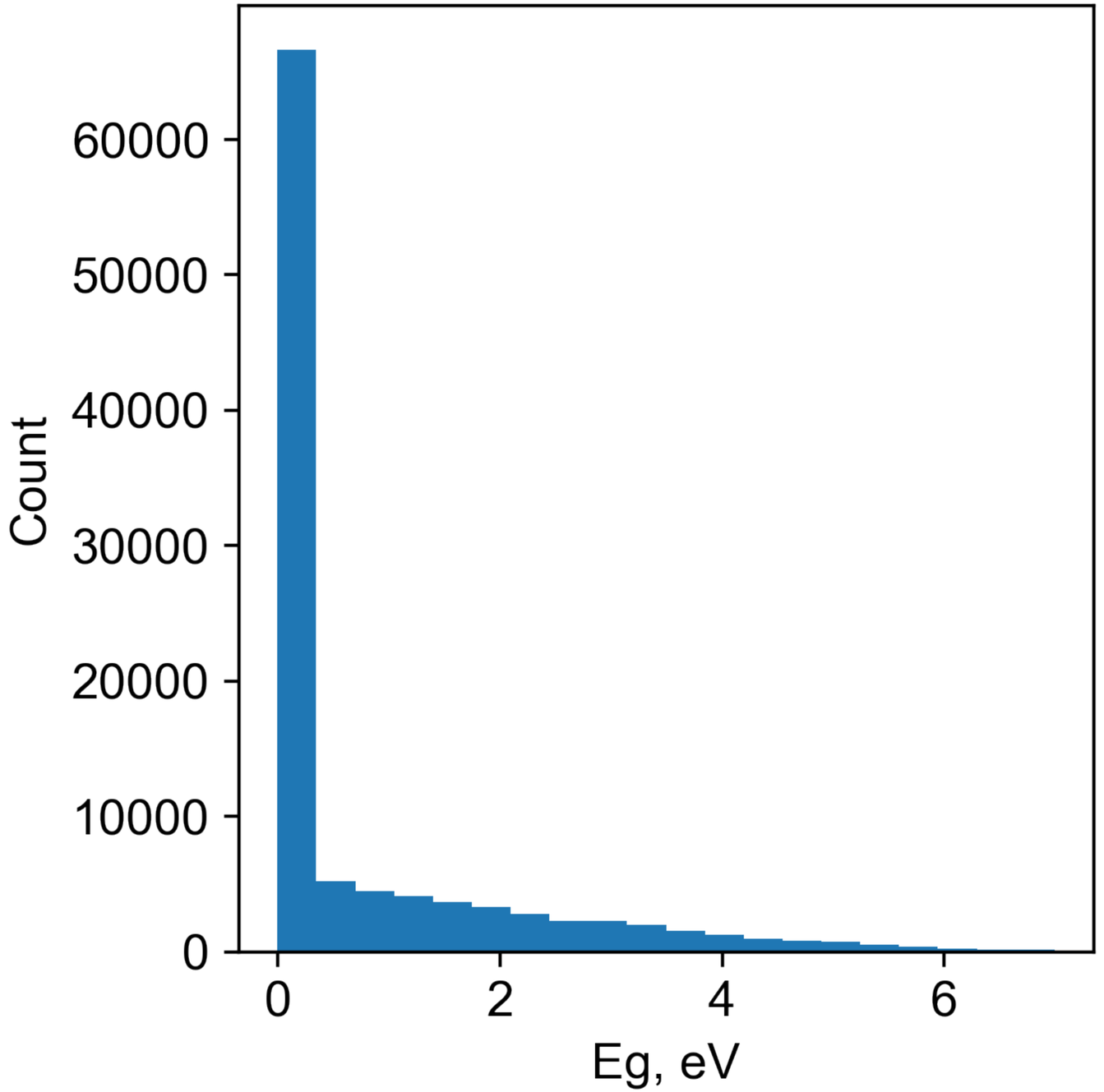


Distribution

- Histogram, density plot

Is it a good graph?

Why?

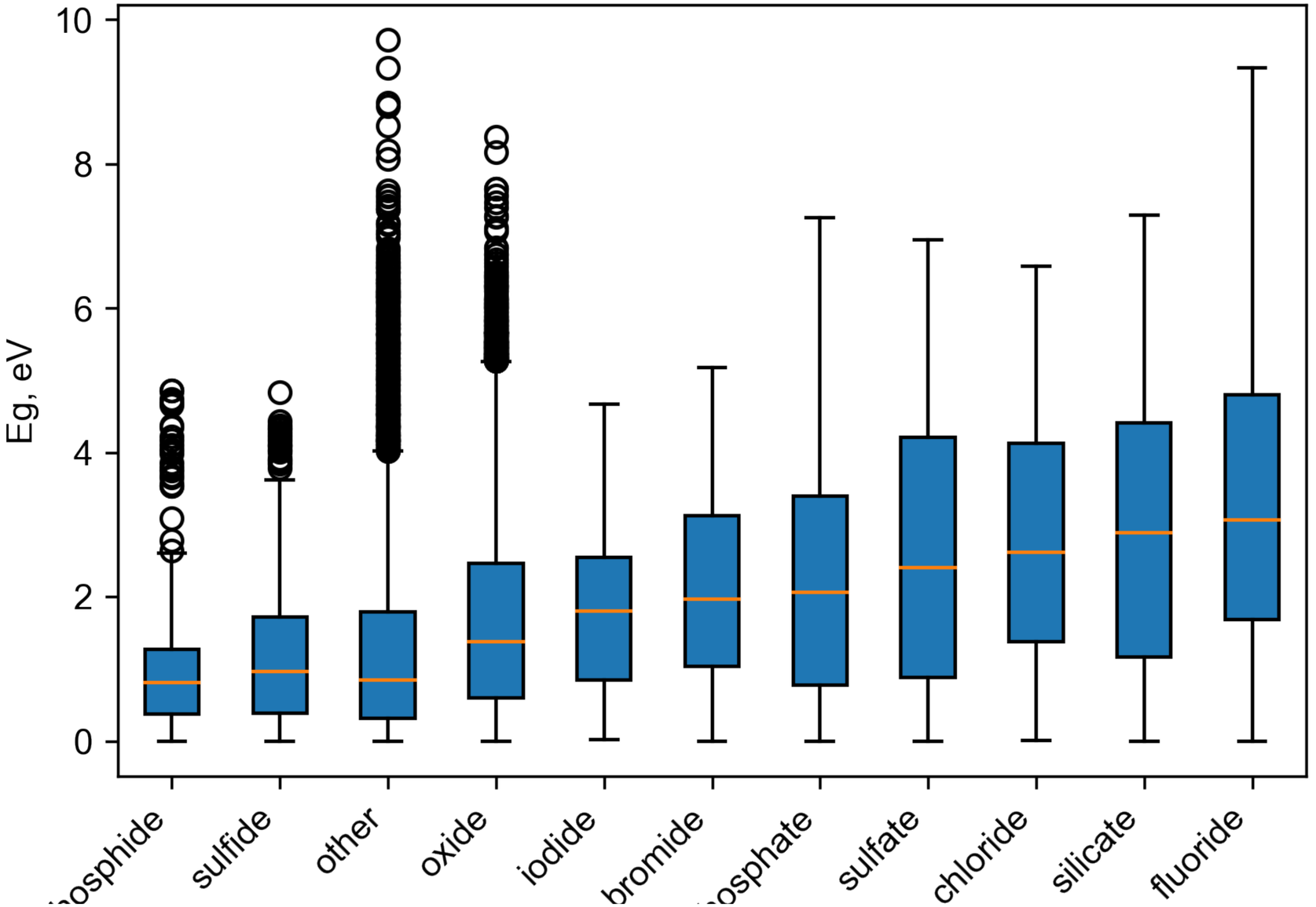


Comparison

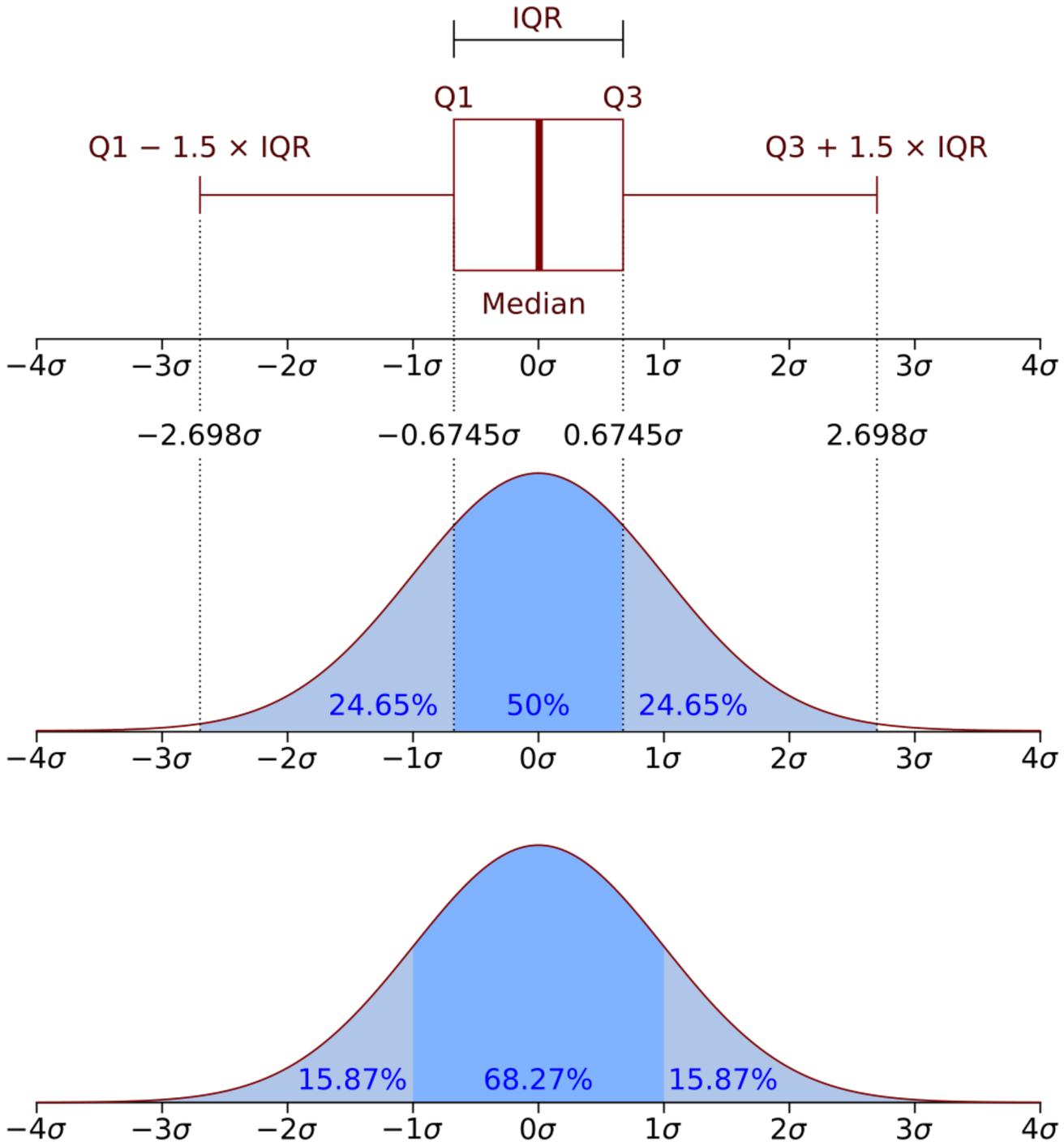
- Bar plot, box plot

Is it a good graph?

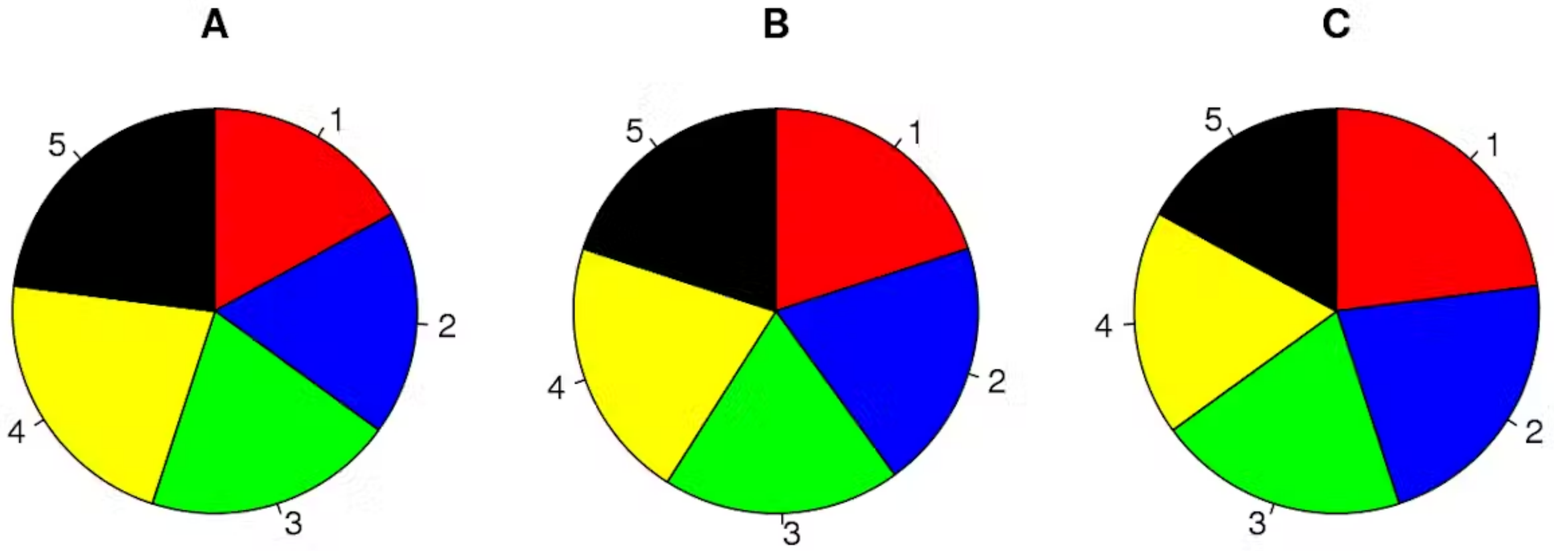
Why?



Box plot


IQR
Q1
Q3
Q1 − 1.5 × IQR
Q3 + 1.5 × IQR
Median
−4σ
−3σ
−2σ
−1σ
0σ
1σ
2σ
3σ
4σ
−2.698σ
−0.6745σ
0.6745σ
2.698σ
24.65%
50%
24.65%
15.87%
68.27%
15.87%

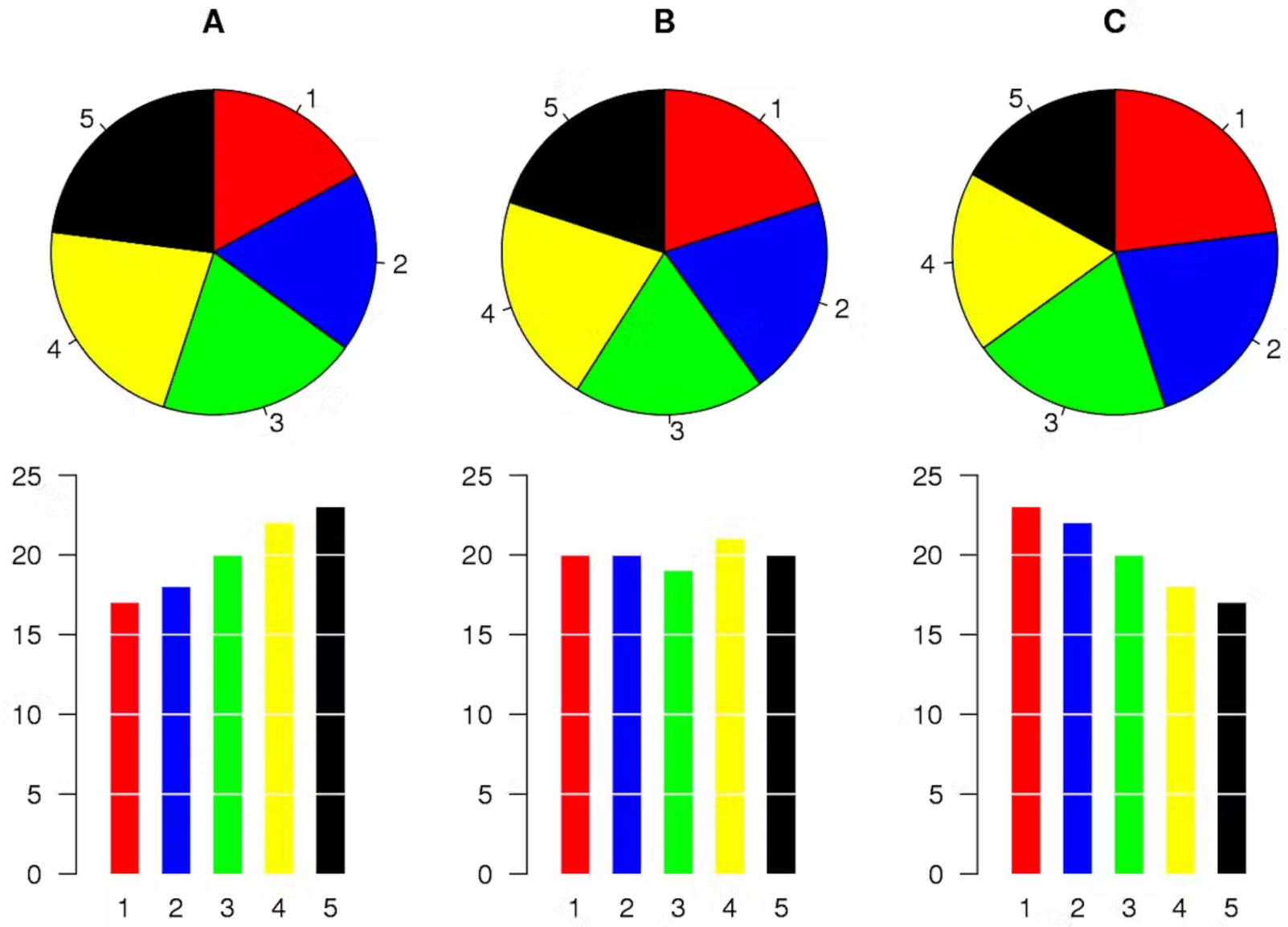
Don’t use pie charts!



Here’s why you should (almost) never use a pie chart for your data

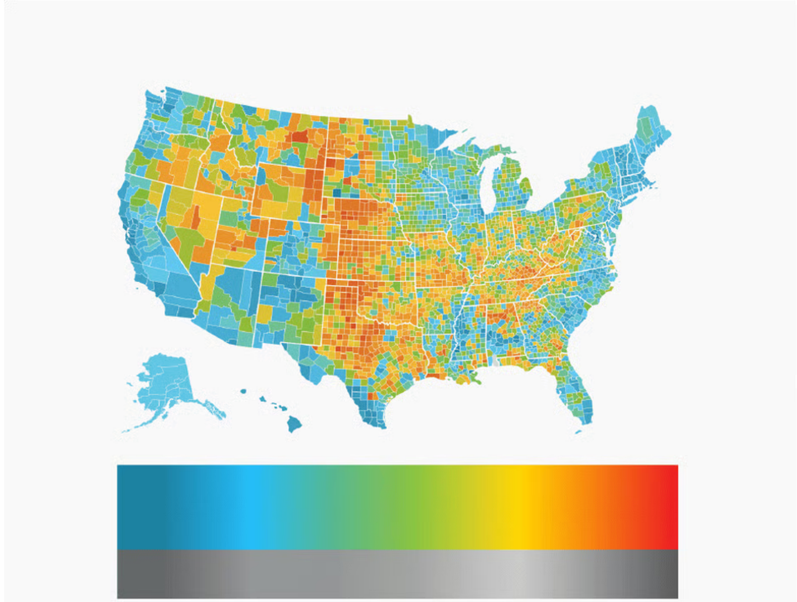
Don’t use pie charts!

Bar plots are easier to compare

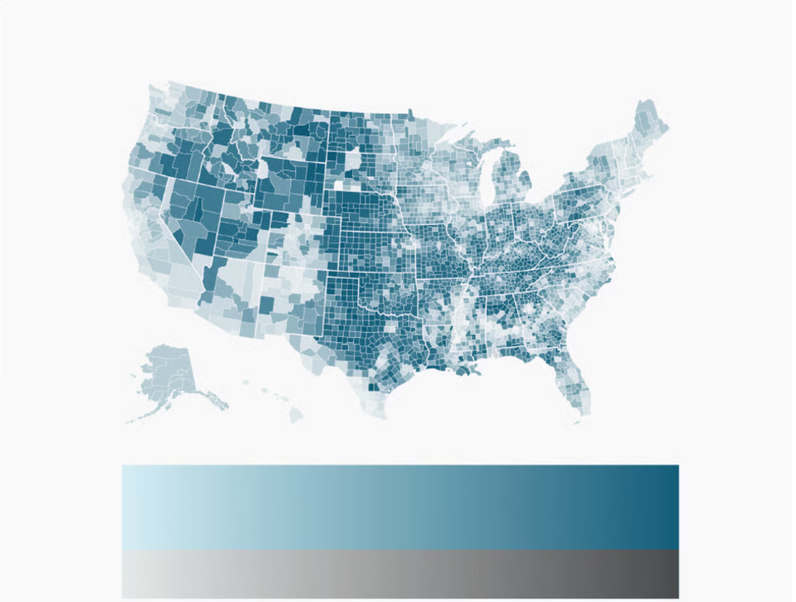


Use color

Have a look at this page: https://www.datawrapper.de/blog/colors



NOT IDEAL

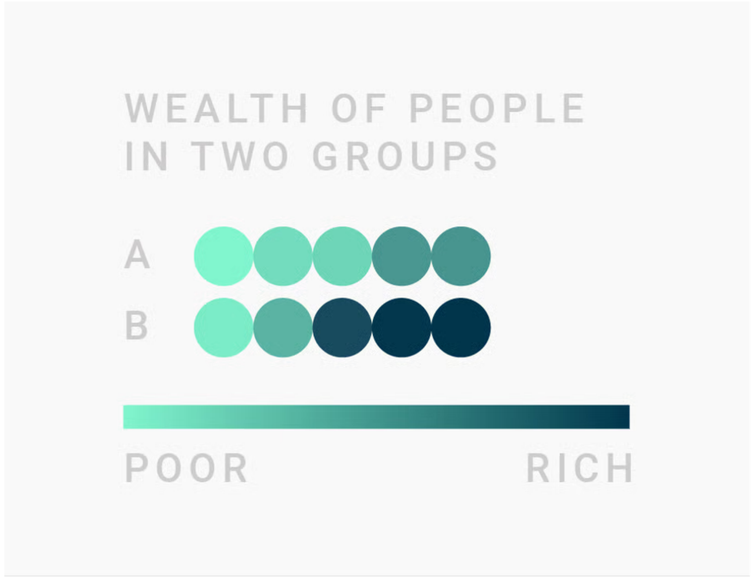


BETTER

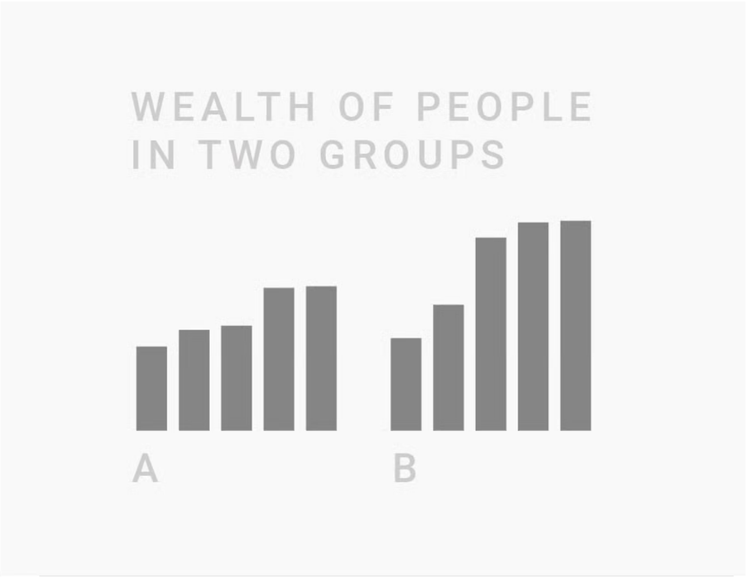
But consider a better alternative if possible

- The simpler is better

Have a look at this page: https://www.datawrapper.de/blog/colors



NOT IDEAL

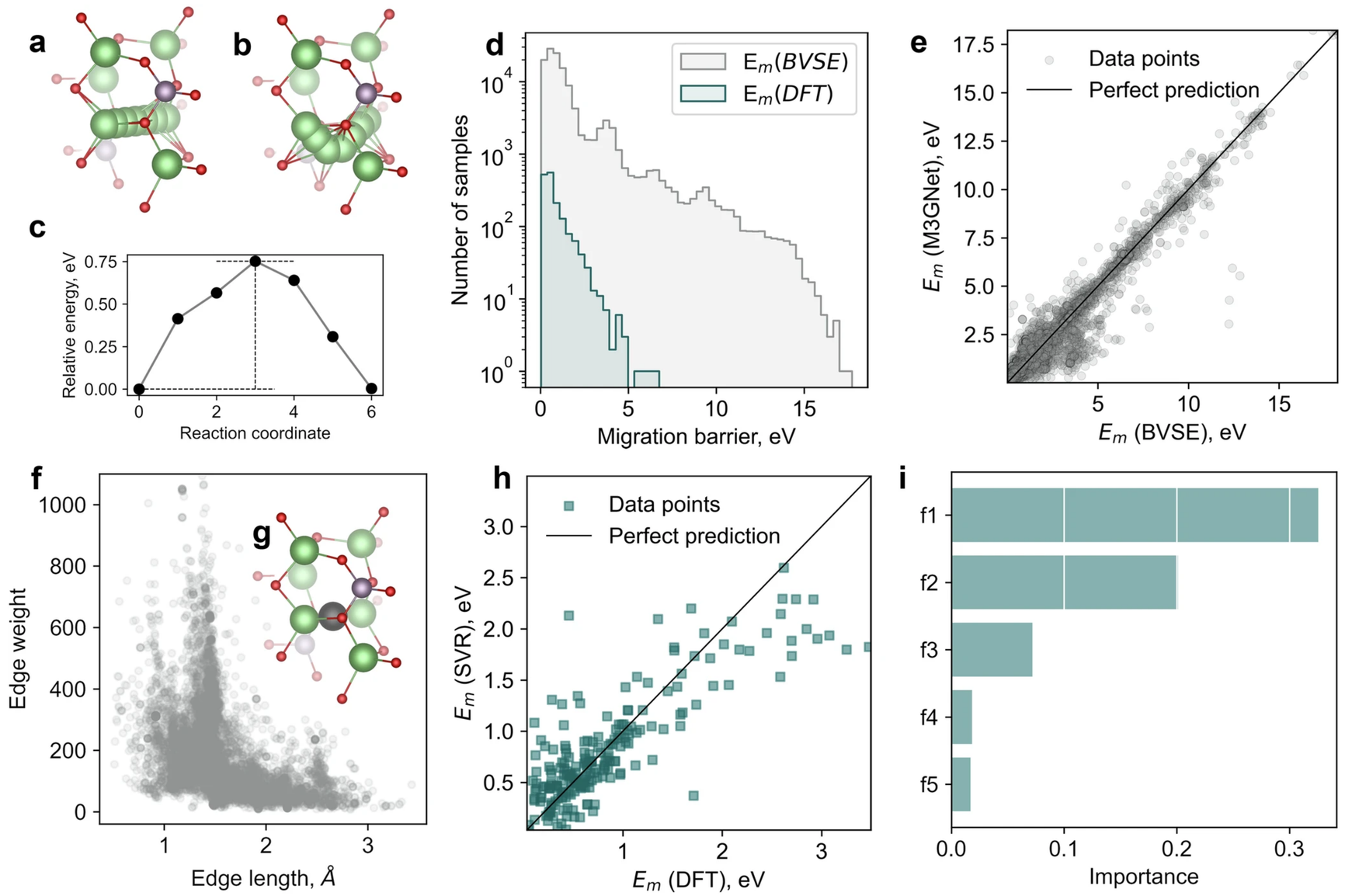


BETTER

Don’t use too many panels

(If possible)

- It is difficult to follow

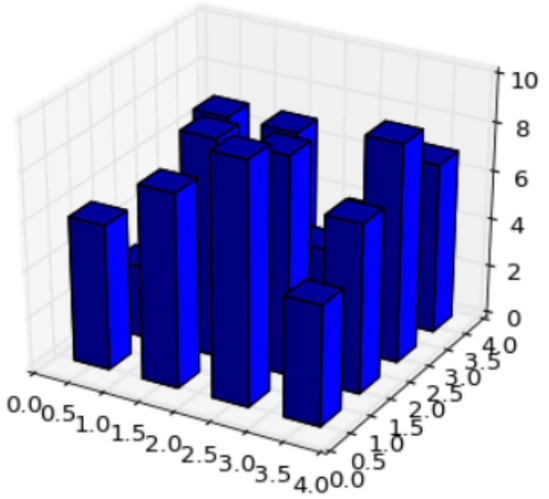


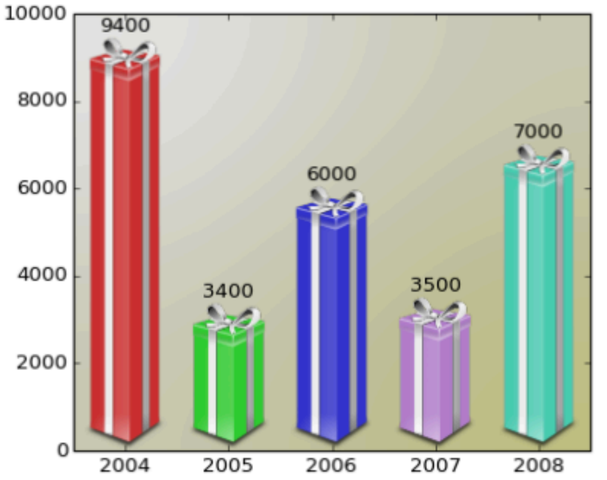
Don't!

My favourite

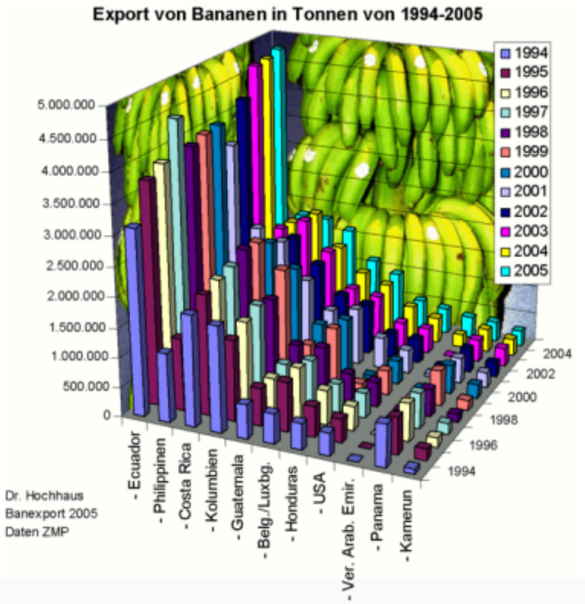
– Don't use 3D plots

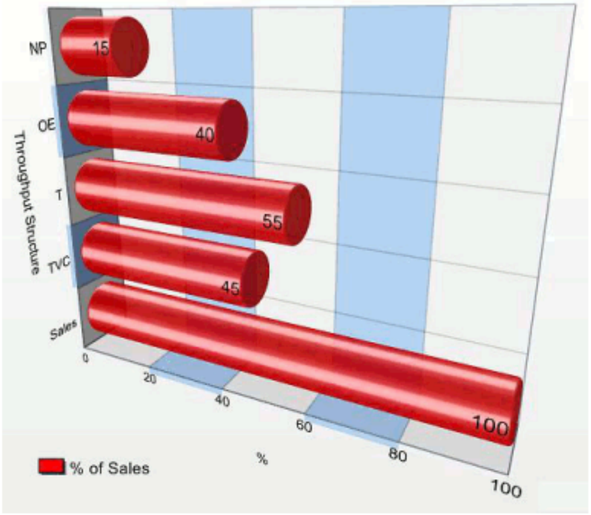
– It's difficult to compare





matplotlib gallery





Excel Charts Blog

Take home message

Visualizing data helps you

- Present data and ideas
- Analyze results
- Define future steps

The data is more important than the design

- Represent the data in a right way
- Avoid misleading graphs

Resources

https://harvard-iacs.github.io/2018-CS109A/lectures/lecture-3/presentation/lecture3.pdf

https://en.wikipedia.org/wiki/Misleading_graph

https://en.wikipedia.org/wiki/Anscombe%27s_quartet

https://blog.datawrapper.de/colors/