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

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

Agenda

- Goals
- Attribution
- Why visual data inspection?
- Tips for plotting the data

Attribution

- Parts of these slides are adopted 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

Descriptive statistics

"...is a summary statistic that quantitatively describes or summarizes features from a collection of information"

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

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

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

"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."

1, 3, 3, **6**, 7, 8, 9

Median = **6**

1, 2, 3, **4**, **5**, 6, 8, 9

Median = (4 + 5) ÷ 2

= **4.5**

Standard deviation

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

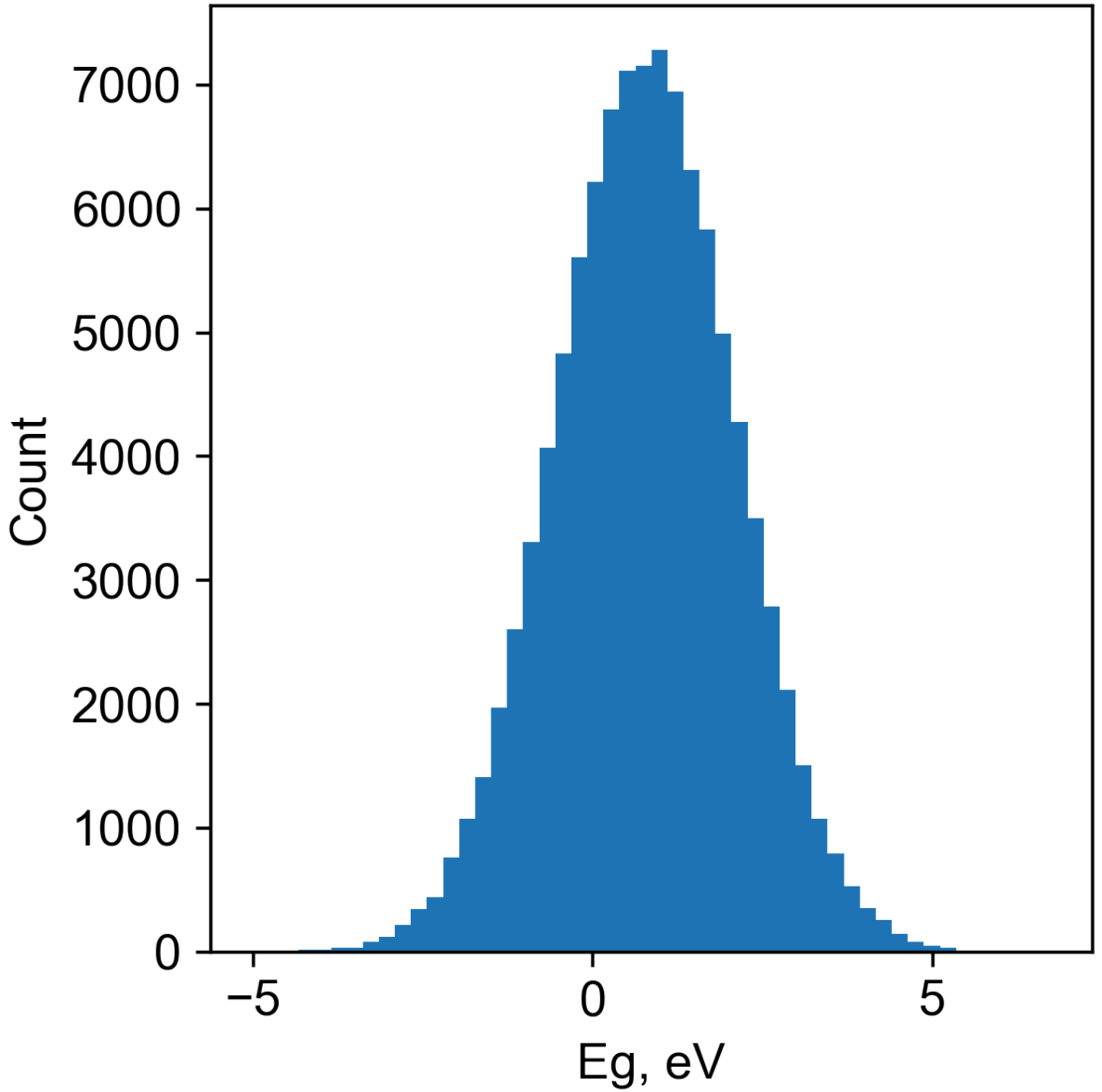
$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}, \text{ where } \mu = \frac{1}{N}\sum_{i=1}^{N} x_i.$$

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

- Sample size
  - 103,217
- Mean of Eg
  - 0.79
- Standard deviation of Eg:
  - 1.37

Is it what you expected?

- What's wrong with this distribution?



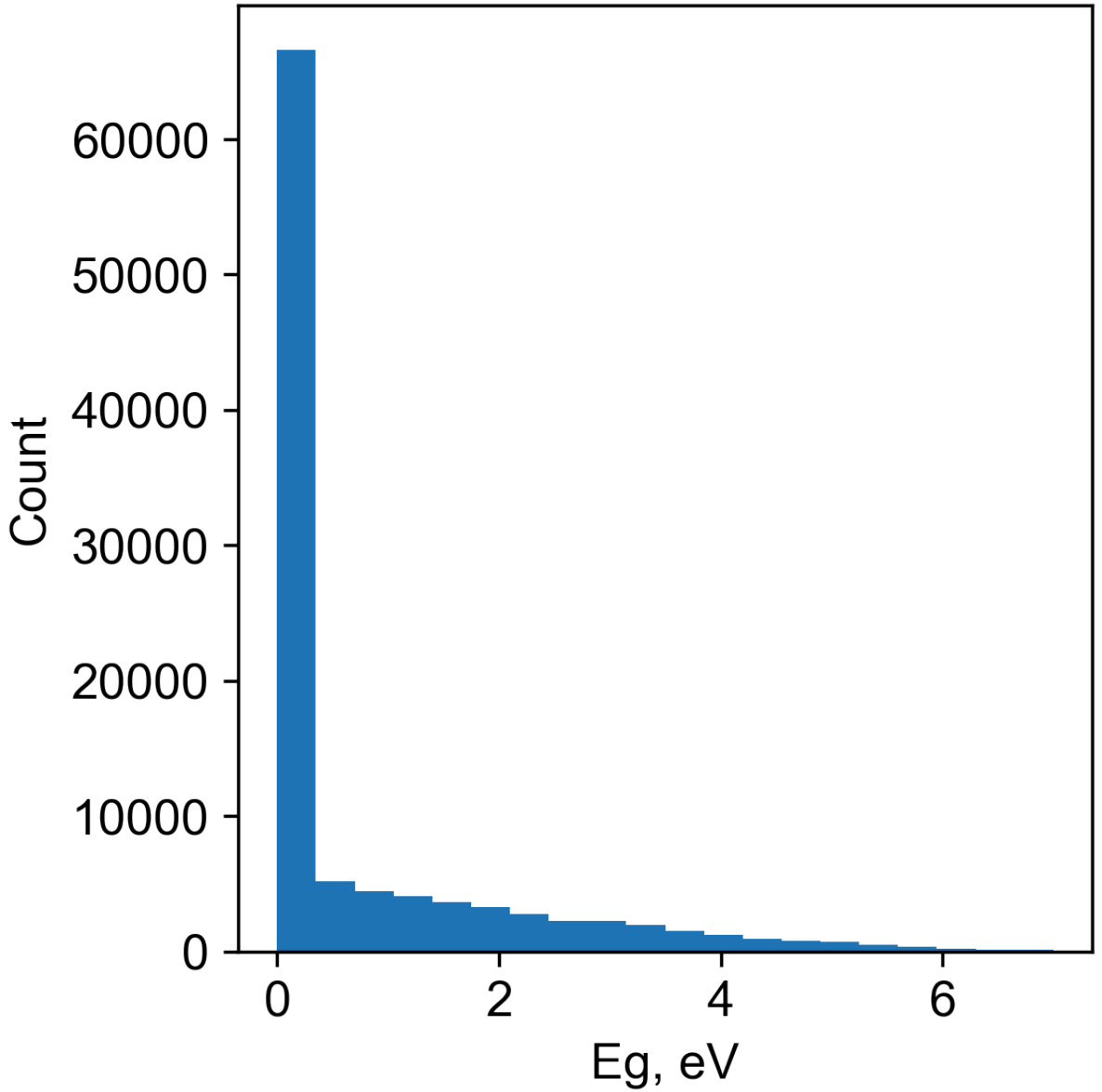
Any ideas?

- Sample size
  - 103,217
- Median of Eg:
  - 0.0 <--- ???

This is the real distribution

- Metals have a zero Eg

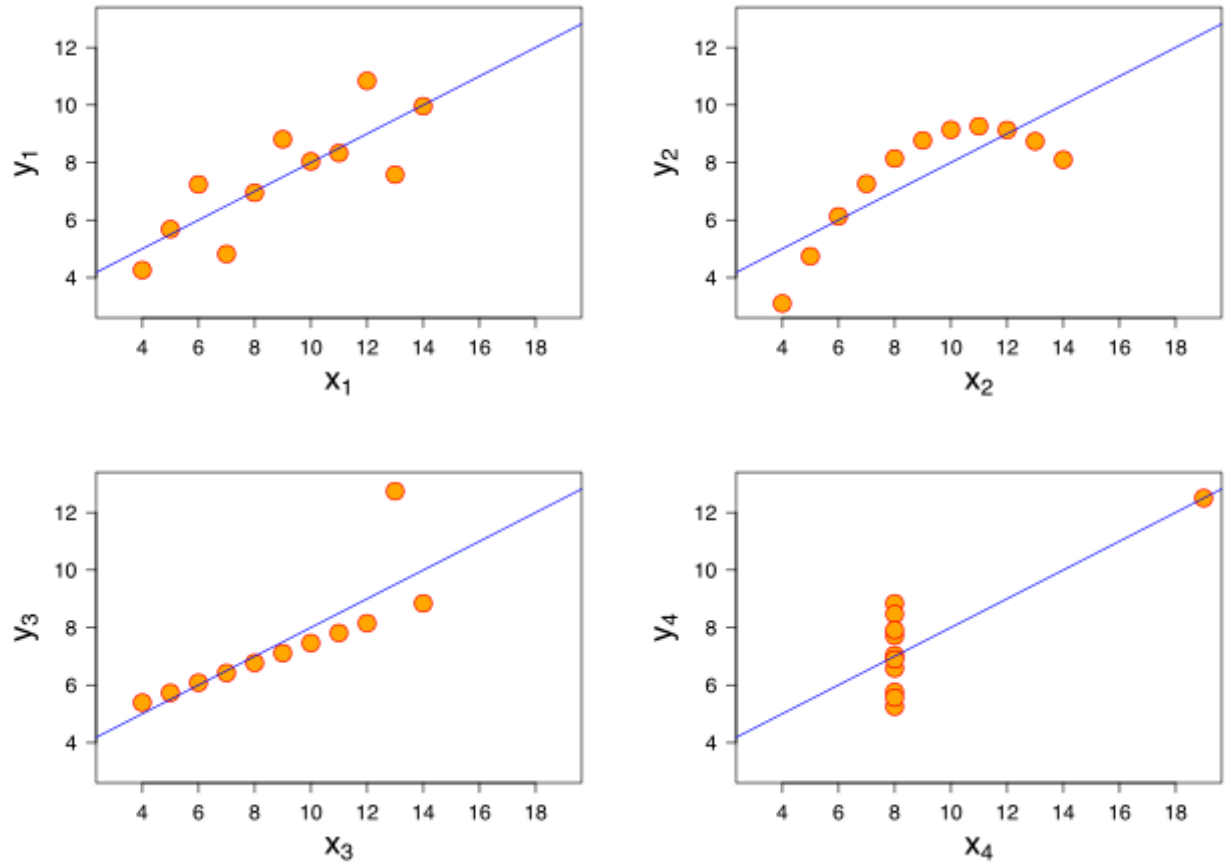
> Median(Eg) = 0.0 says that metals represent at least half of the sample



Why is visual inspection of data important?

- Same descriptive statistics
- Very different distributions

https://en.wikipedia.org/wiki/Anscombe's_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

Communicate

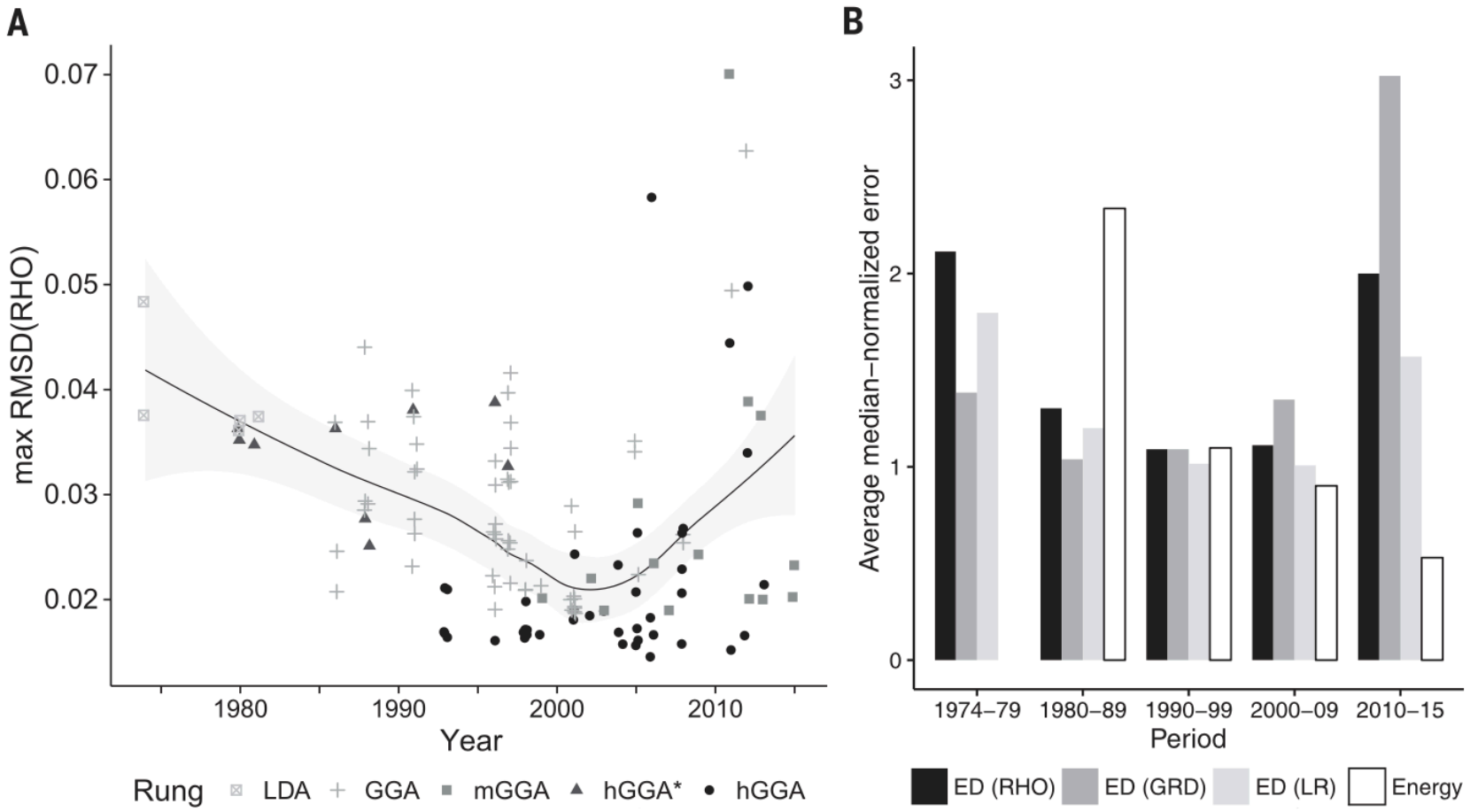


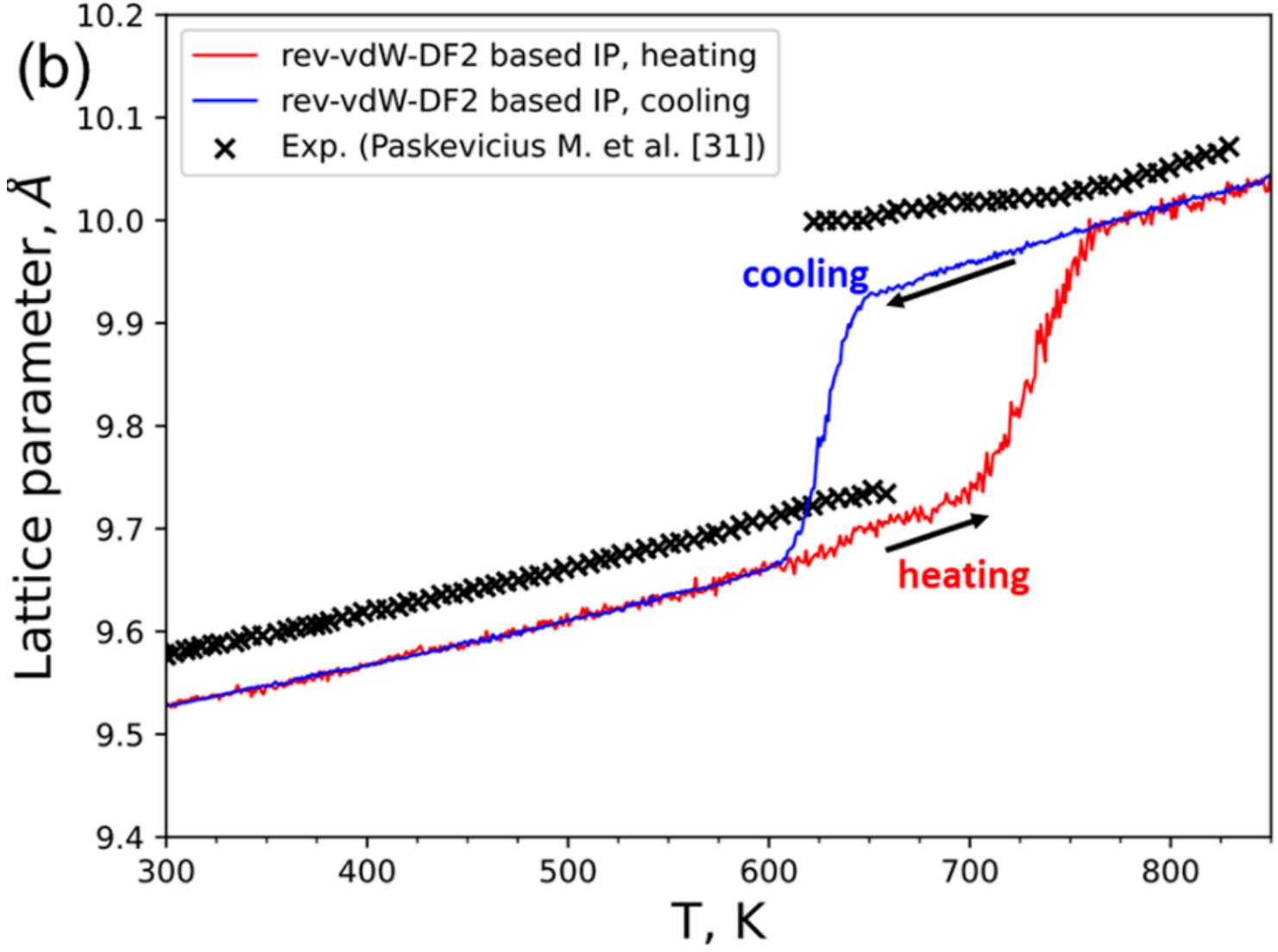
Fig. 1. The historical trends in maximal deviation of the density produced by various DFT methods from the exact one. (**A**) The line shows the average deviation, with the light gray area denoting its 95% confidence interval; hGGA* denotes 100% exact exchange-based methods. (**B**) The bars denote averages 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

Density functional theory is straying from the path toward the exact functional

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

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('ed_data.csv')
```

Clean the data

- outliers
- NaNs (missing values)
- constant rows

```
df.dropna()
```

- plus visual support: histogram, box plot

Study the global summary statistics

```
df.describe()
```

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

- plus visual support: histogram, scatter plot, bar plot

Study the summary statistics of the subgroups

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

- plus visual support: histogram, scatter plot, bar plot

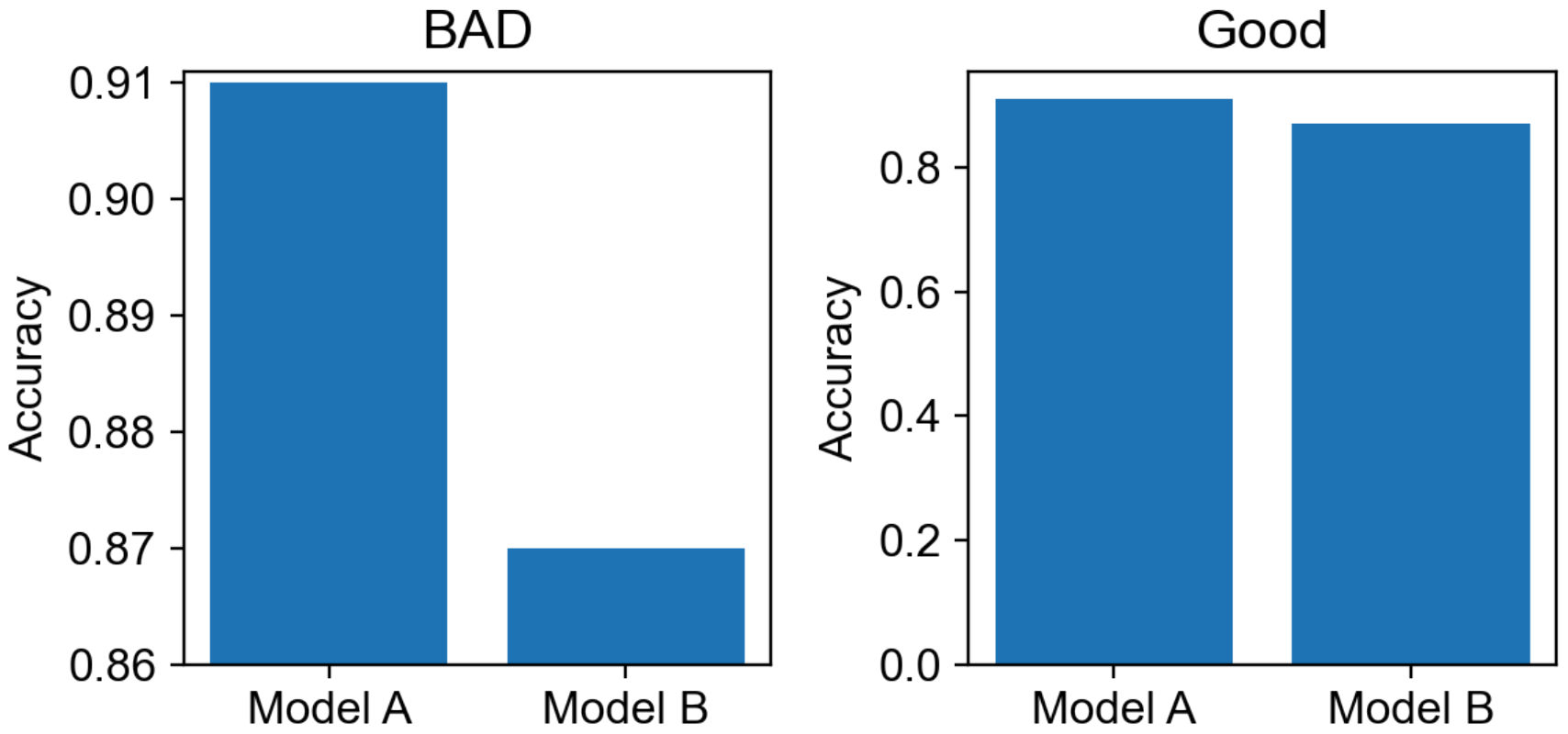
Some principles for effective EDA

Avoid misleading graphs

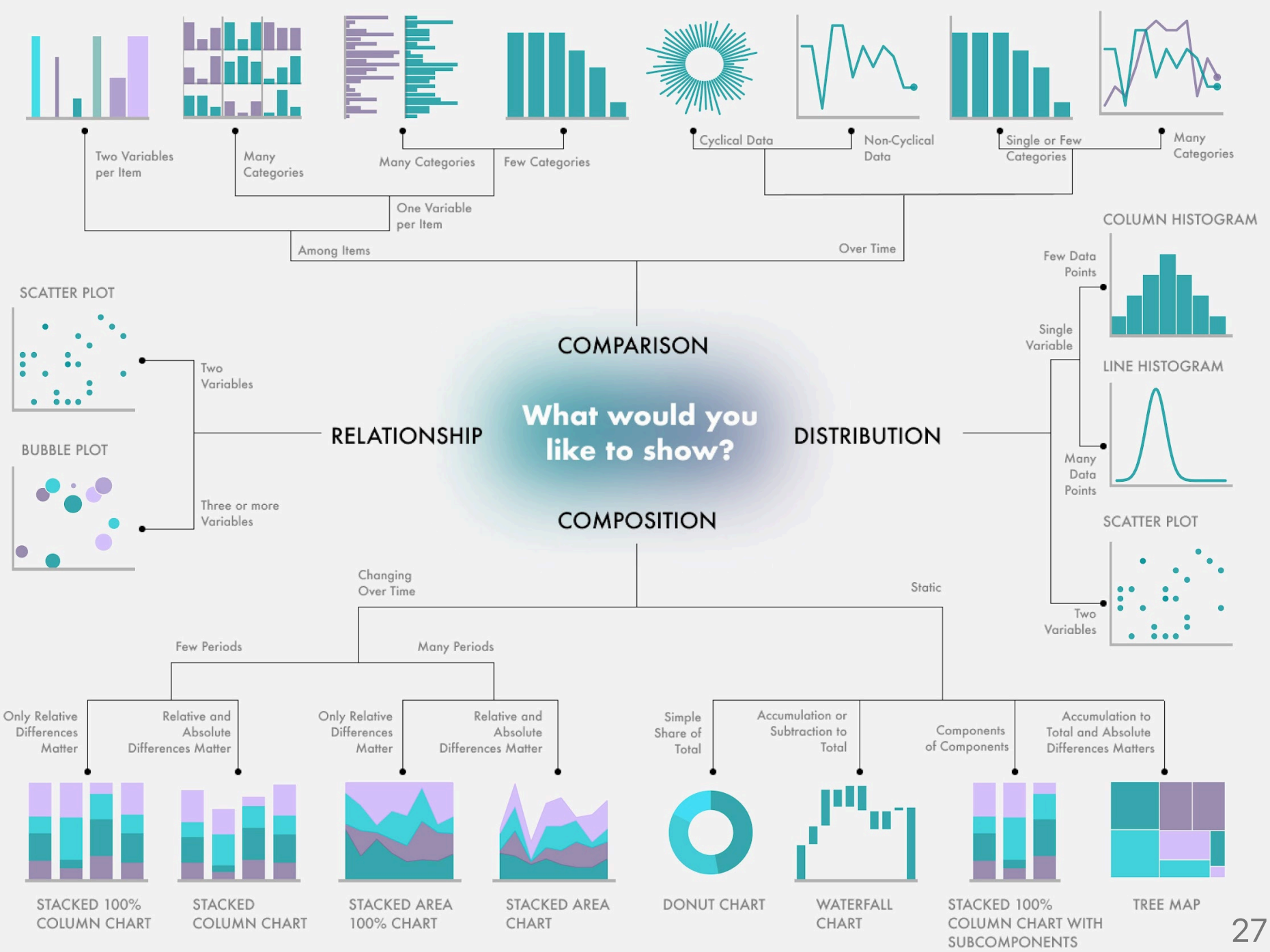
- Do not distort scales
- Do not truncate graph when comparing the data
    - or indicate the truncation
- Avoid 3D charts
- Do not change y(or x)-axis maximum
- Aspect ratio determines the perception of steepness in slope
    - be proportional

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

Lie factor


BAD
Accuracy
0.91
0.90
0.89
0.88
0.87
0.86
Model A
Model B
Good
Accuracy
0.8
0.6
0.4
0.2
0.0
Model A
Model B

Use the right display



Correlations

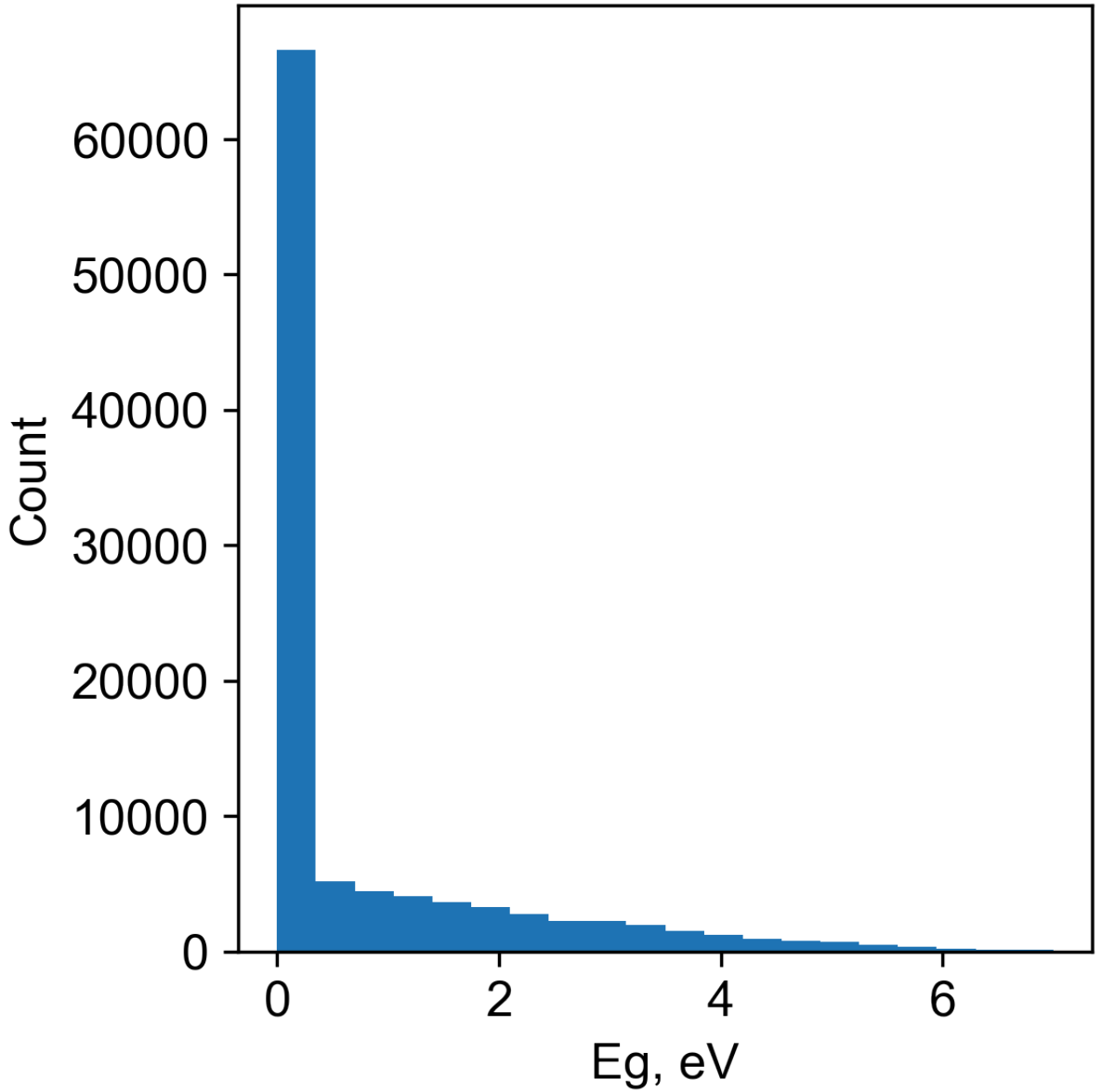
- scatter plot, correlation matrix

Is it a good graph? Why?

Distribution

- histogram, density plot

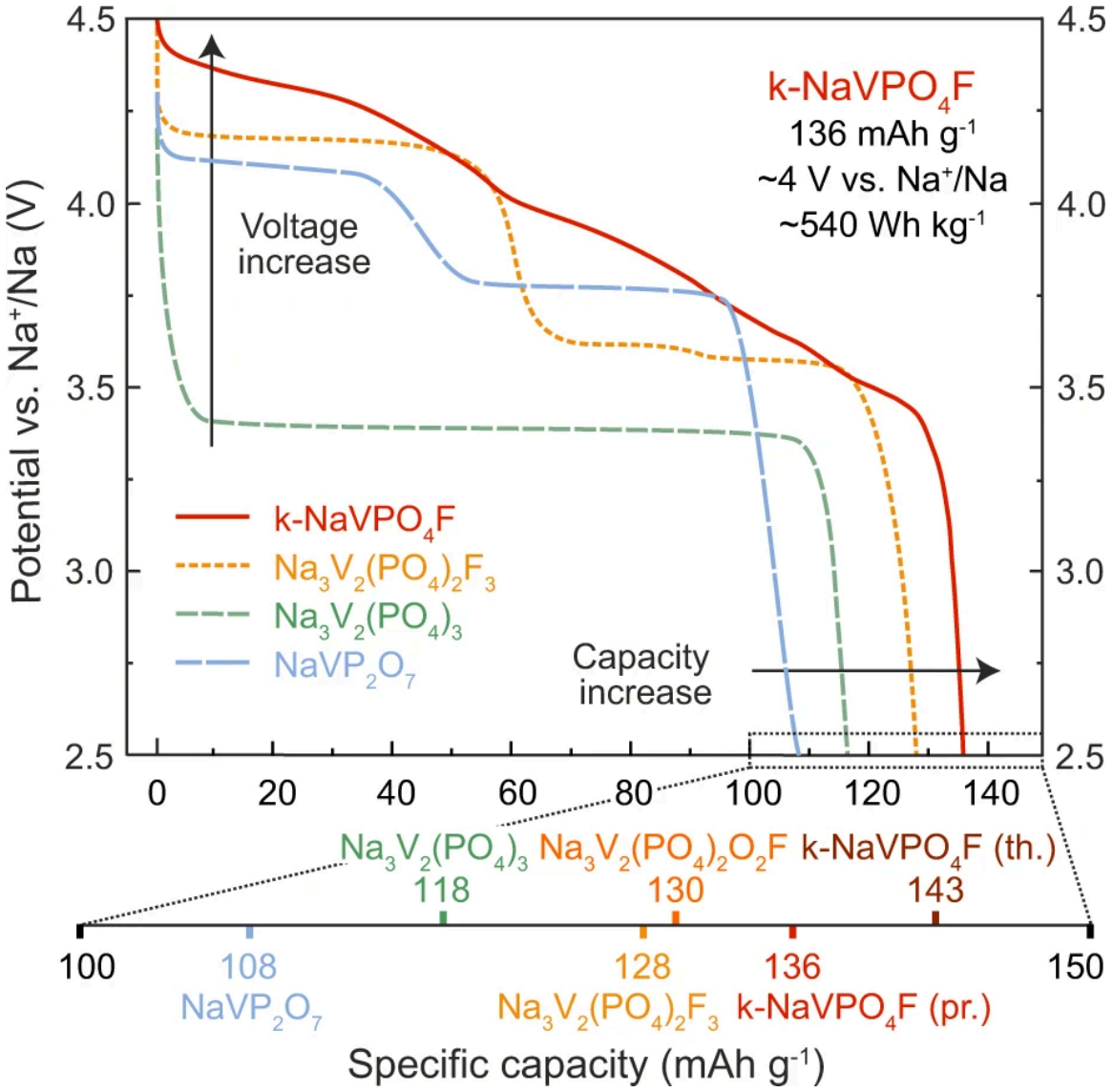
Is it a good graph? Why?



Comparison

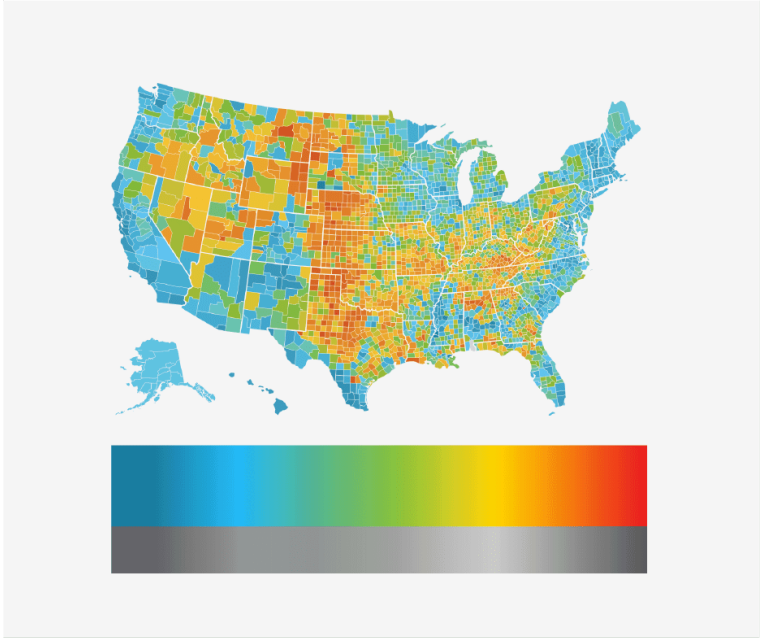
- bar plot

Is it a good graph? Why?

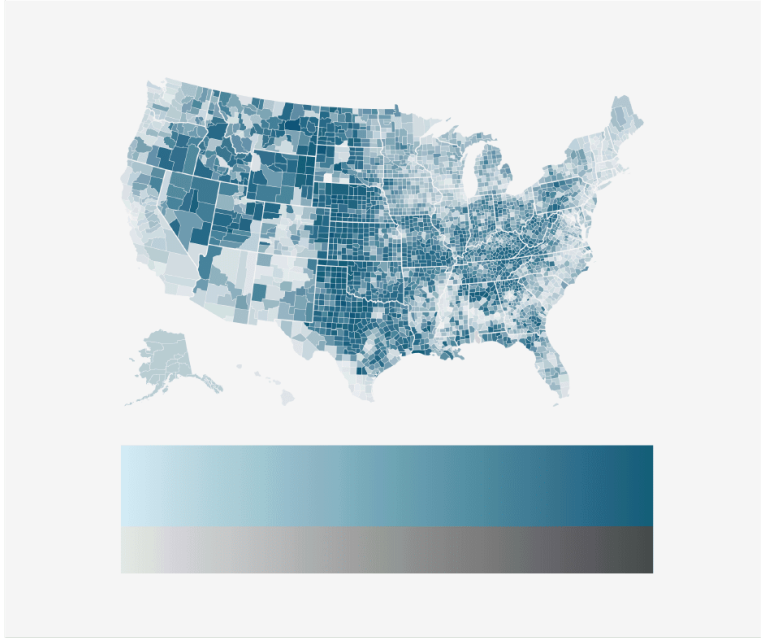


Use color

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



NOT IDEAL

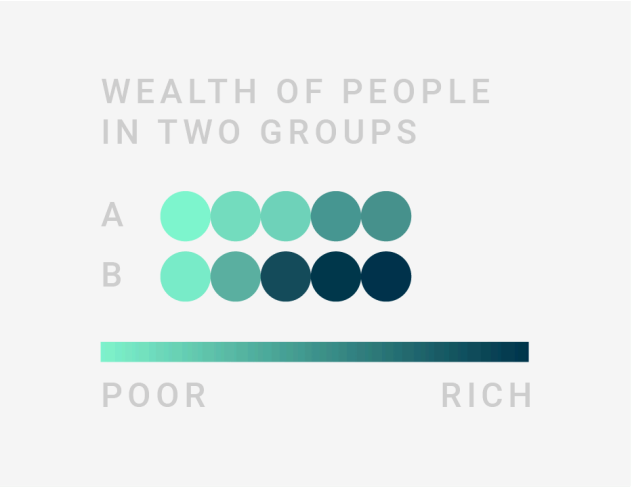


BETTER

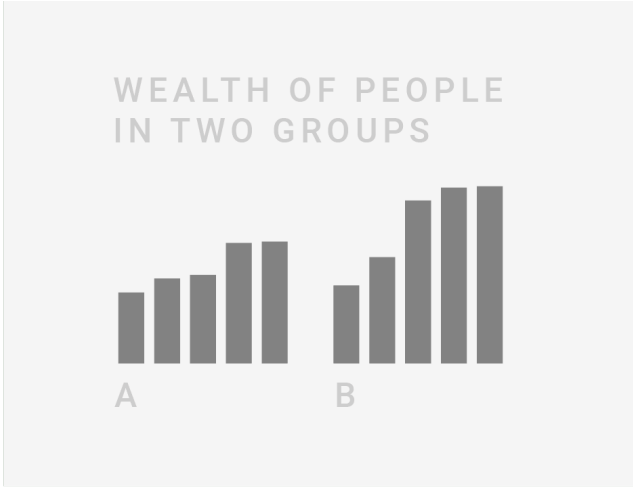
But consider a better alternative if possible

- the simpler the better

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



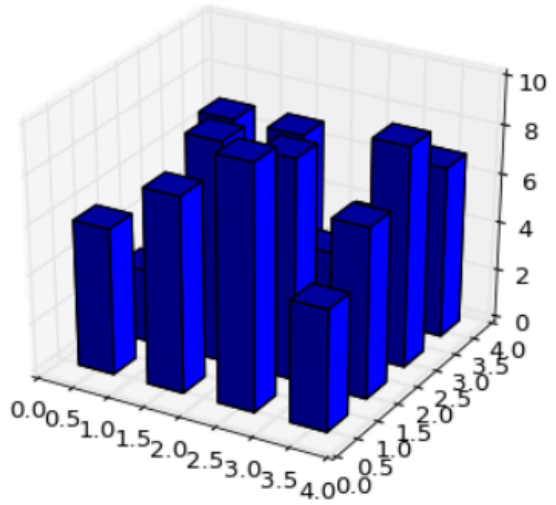
NOT IDEAL

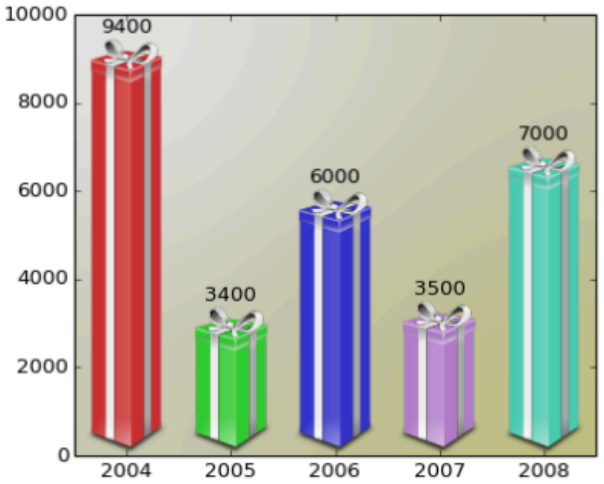


BETTER

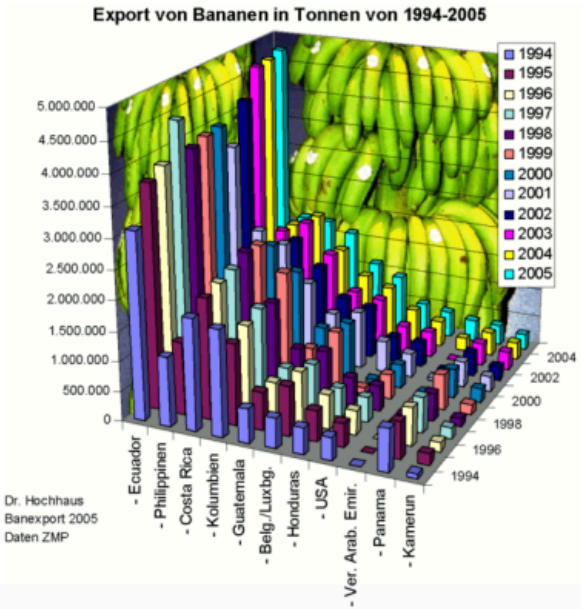
Don't!

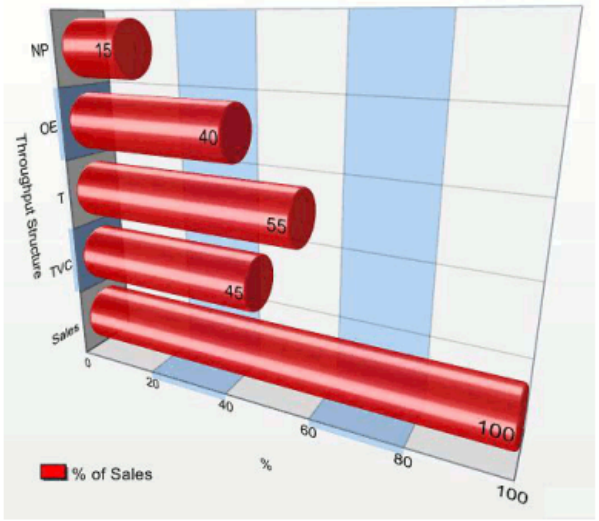
My favorite





matplotlib gallery





Excel Charts Blog

From CS 109a: Data Science, Effective Exploratory Data Analysis and Visualization by Pavlos Protopapas & Kevin Rader slide #55

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's_quartet

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

Thank you for your attention!