

DATA 3464: Fundamentals of Data Processing

Exploratory Data Analysis

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This week's topics

- Exploratory data analysis (EDA)
- Splitting your data

Resources used:

- [Feat.Engineering Chapter 3](#)
- [R for Data Science \(2e\), Chapter 10](#)
- Hands on Machine Learning with Scikit-Learn and Tensorflow/PyTorch, Chapter 2.
Available at [MRU Library](#)

Exploratory data analysis

The goal of EDA is to **Understand your data**

1. Ask questions (e.g. are my data normally distributed?)
2. Look for answers (e.g. by making histograms)
3. Find more questions and return to step 1 (hmm, those are some weird numbers, what do these values represent?)

EDA is not a formal process with a strict set of rules. More than anything, EDA is a state of mind. During the initial phases of EDA you should feel free to investigate every idea that occurs to you. Some of these ideas will pan out, and some will be dead ends. -- Hadley Wickham

Basic things to look at

- Data source - File? Database? API?
- Structured/unstructured
- Assumption 1: relatively small (fits in memory) tabular dataset
 - Data types - numeric/categorical, text, other
 - Assumption 2: numeric data
 - Ranges
 - Summary statistics
 - Missing values
- Next week: categorical data, after reading week unstructured

Example: Anscombe's Quartet

- Very small dataset, constructed by hand in 1973 by [Francis Anscombe](#)

Most textbooks on statistical methods, and most statistical computer programs, pay too little attention to graphs. Few of us escape being indoctrinated with these notions:

(1) numerical calculations are exact, but graphs are rough;

(2) for any particular kind of statistical data there is just one set of calculations constituting a correct statistical analysis;

(3) performing intricate calculations is virtuous, whereas actually looking at the data is cheating.

- Not known exactly how he made it, but Drs. Roberta La Haye and Peter Zizler proposed a [compelling argument](#) for linear algebra

Case Study: Data visualization to the rescue

- A [2012 study about honesty](#) reported that "Signing at the beginning makes ethics salient and decreases dishonest self-reports in comparison to signing at the end"
- In 2020, the authors published a new paper admitting that their original results [could not be replicated](#), and noticed an anomaly in the **summary statistics**
- The 2020 paper also published the original data, which was downloaded and visualized by a team of anonymous researchers working with [Data Colada](#)
- This led to the 2012 paper being retracted, a [\\$25M lawsuit](#), a [data-driven defense](#)

Moral of the story is, look at your data!

Useful starting points

Assuming your data is small enough and well structured:

- `pandas.DataFrame.info`: data type, number of non-null, names, dimensions
- `pandas.DataFrame.head`: return the first `n` rows (default 5). Also `tail`.
- `pandas.DataFrame.describe`: Compute a bunch of summary statistics
- Various aggregation statistics

Next up, visualize!

Where we left off on January 15

Types of exploratory visualizations

- I will not provide an exhaustive list of visualizations!
- Pandas provides a [handy wrapper](#) around [matplotlib](#)
- So does [Seaborn](#) - check out the [example gallery](#)
- Some of my favourites:
 - Histograms
 - Scatter plots/hexbin plots
 - Box plots/violin plots
- But before we get too deep into EDA, it's time to **split your data**

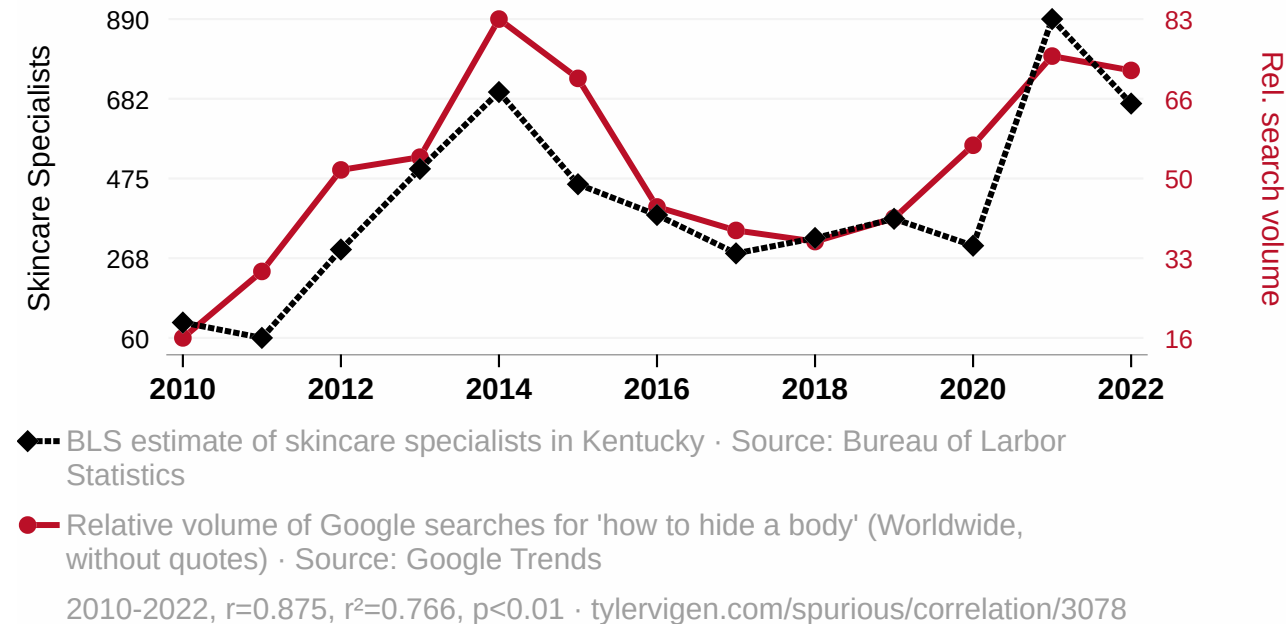
Why split your data?

- We need to set aside a final **test set** to evaluate our final model
- Humans are great at detecting patterns!
- Even looking at test data could influence decisions, causing **data leakage**

The number of skincare specialists in Kentucky

correlates with

Google searches for 'how to hide a body'



When to split your data

How much EDA should you do before splitting? You might need to know:

- Are there any missing values?
- Is there a need for [stratified sampling](#)?
- Do the data have a unique identifier beyond the row label?
- As soon as you have a general sense of the:
 - Data types
 - Missing features
 - Distributions, particularly categorical
- It's time to split the data!

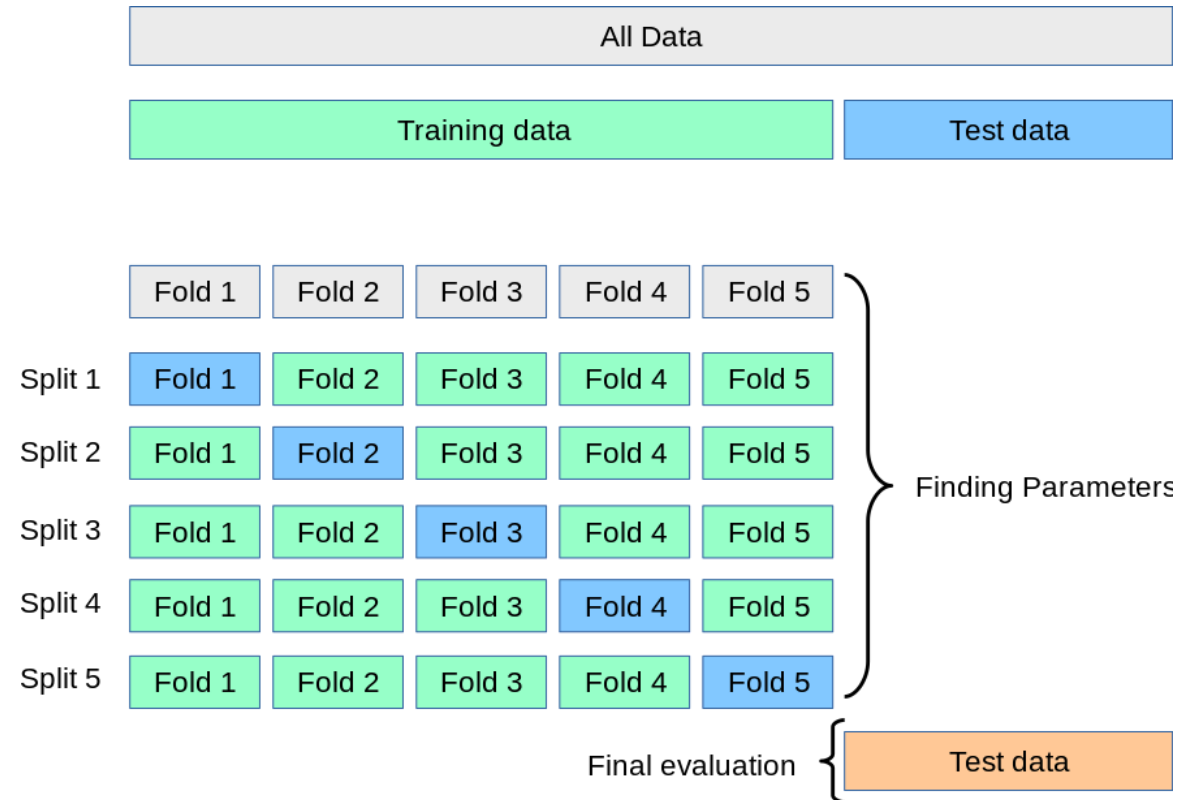
How to split your data

As usual, it depends on the:

- Data set size n
- Relationship between number of predictors p and n
- Nature of the data:
 - Time series?
 - Stratification needed?
- Intended **validation approach**

Side note: validation

- So far we've talked about **training** and **testing** data
- We also need **validation** data
- If the dataset is sufficiently large, this can be a separate split
- We can also use **cross-validation**



Validation

- Validation data is used to make decisions about your model, e.g.
 - Model selection
 - Tuning hyperparameters
 - Monitor training progress
- However, validation data is not used to directly *train* a model
- Think of it like a test-adjacent set where you can repeatedly try stuff on your training set, then evaluate on validation

Cross-validation is a way of checking your model choice and parameters, but final training should be done on the entire training set

How to split your data

- Simple scenario: random sample (typically 70-80% for training)
- **Only works if:**
 - Stratification doesn't matter
 - Data is guaranteed not to change
 - Data is not a time-series (later topic)

How do we know if stratification is necessary?

Sampling bias

Stratification is used to mitigate **sampling bias**

- Simple example: assume 80% of population likes cilantro
- Goal: ensure our sample is representative of the population, $\pm 5\%$

The **binomial distribution** can be used to model the probability of choosing k people who like cilantro from n total participants:

$$P(X = k) = \binom{n}{k} p^k (1 - p)^{n-k}, \text{ where } \binom{n}{k} = \frac{n!}{k!(n - k)!}$$

Sampling bias continued

$P(X = k)$ is the probability mass function, and the corresponding cumulative distribution function is just the sum up to k :

$$P(X \leq k) = \sum_{i=0}^k \binom{n}{i} p^i (1-p)^{n-i}$$

Suppose we **randomly** sample 100 people. What is the probability of fewer than 75 or more than 85 cilantro lovers?

Here we've defined an "unbiased sample" as being $\pm 5\%$

Stratification approach

- The need for stratification depends on sample size, distribution of stratification category, and how much bias you're willing to accept

	Small Sample Size	Large Sample Size
Unbalanced Classes	Stratify	Maybe
Balanced Classes	Maybe	Not necessary

- Stratification categories can be the target variable, or a predictor
- Goal is to have the same class distribution in both testing and training

Repeatable randomness

- At minimum, you should **always set a random seed** so that every time you sample your data it is the same "random sample"
- This isn't enough if your data might get updated! You can:
 - Store the IDs of your split offline, then sample any new data and append to them (ensuring that test/train never mix)
 - Get fancy with a deterministic method like hashing features to create unique IDs, then thresholding based on maximum possible value
 - Example: compute **CRC** to get a 32-bit integer, select $< 0.8 \times 2^{32}$

Back to visualizations

Now that we've got a test set safely stashed, we can **ask questions** about the data and use visualizations and statistics to answer them. Some examples:

- Do any of my features seem to be related to my target?
- Do any of my features seem to be related to each other?
- Why are some values more common than others?
- Do these values make sense in the context of my **domain knowledge**?
- If I group my data together in some way, are there clear trends?

Some handy tricks

A few things to tweak that can make visualizations easier to read:

- Histogram bin sizes
 - Aiming for a smooth distribution that works for your data
- Transparency (`alpha`)
 - Useful for both dense scatter plots and overlapping categories
- "Jitter"
 - Mostly for scatter plot of continuous vs categorical data
 - Add a tiny bit of random noise to spread out samples

Coming up next

- Lab: Accessing the City of Calgary API
- Assignment 1, available soon!
- Categorical data
- Encoding strategies
- Dealing with missing values

Feature Engineering Chapter 5