```
In [1]: from dsc80_utils import *
```

Lecture 13 – Linear Regression

DSC 80, Fall 2025

Agenda 📆

- Last bits of TF-IDF.
- Modeling.
- Case study: Restaurant tips 🧑‍🍳 .
- Regression in `sklearn`.
- Announcement about HDSI career services.

Conceptually, today will mostly be review from DSC 40A, but we'll introduce a few new practical tools that we'll build upon next week.

TF-IDF

The importance of words

Issue: The bag of words model doesn't know which words are "important" in a document. Consider the following document:

"my brother has a friend named **billy** who has an uncle named **billy**"

How do we determine which words are important?

- The most common words ("the", "has") often **don't** have much meaning!
- The very rare words are also less important!

Goal: Find a way of quantifying the importance of a word in a document by **balancing the above two factors**, i.e. find the word that **best summarizes/represents** a document.

```
In [2]: sentences = [
    "It is a book. A book is good.",
    "A computer is not a book. It is a computer.",
    "A car is a car. A car is good and bad.",
    "The universe is everything. The universe is a book, a computer, and a c
]
```

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...quency

- The **term frequency** of a word (term) t in a document d, denoted $\text{tf}(t, d)$ is the proportion of words in document d that are equal to t.

$$ \text{tf}(t, d)= \frac{\text{\# of occurrences of t in d}}{\text{total \# of words in d}} $$

- **Example**: What is the term frequency of "computer" in the following document?

"A **computer** is not a book. It is a **computer**."

- **Answer**: $\frac{2}{10}$.

- Intuition: Words that occur often within a document are important to the document's meaning.
  - If $\text{tf}(t, d)$ is large, then word t occurs often in d.
  - If $\text{tf}(t, d)$ is small, then word t does not occur often d.

- Issue: "is" also has a TF of $\frac{2}{10}$, but it seems less "important" than "computer".

Computing TF (Term Frequency)

It is good to canonicalize first by removing punctuation and lower-casing.

In [3]:
```python
import re

def canonicalize(text: str):
    text = text.lower()

    # replace special characters with spaces
    text = re.sub('[^A-z0-9]', ' ', text)

    # collapse multiple spaces into one space
    text = re.sub(' +', ' ', text)

    return text.strip()
```

In [4]:
```python
canonicalize("This is a test! Does this work?")
```

Out[4]: 'this is a test does this work'

In [5]:
```python
def tf(term: str, document: str) -> float:
    term = term.lower()
    document_words = canonicalize(document).split()

           sum(term == word for word in document_words) / len(document_words
```

In [6]:
```
tf("foo", "Foo! Bar! Foo, bar, baz!")
```

Out[6]: 0.4

Inverse document frequency

- The **inverse document frequency** of a word t in a set of documents $d_1, d_2, ...$ is

$$\text{idf}(t) = \log \left(\frac{\text{total \# of documents}}{\text{\# of documents in which t appears}} \right)$$

- **Example**: What is the inverse document frequency of "computer" in the following four documents?
  - "It is a book. A book is good.",
  - "A computer is not a book. It is a computer.",
  - "A car is a car. A car is good and bad.",
  - "The universe is everything. The universe is a book, a computer, and a car."

- **Answer**: $\log \left(\frac{4}{2}\right) \approx 0.6931$.

- **Example**: What is the inverse document frequency of "is" in the following four documents?
  - "It is a book. A book is good.",
  - "A computer is not a book. It is a computer.",
  - "A car is a car. A car is good and bad.",
  - "The universe is everything. The universe is a book, a computer, and a car."

- **Answer**: $\log \left(\frac{4}{4}\right) =0$.

- Intuition: If a word appears in every document (like "the" or "has"), it is probably not a good summary of any one document.
  - If $\text{idf}(t)$ is large, then t is rarely found in documents.
  - If $\text{idf}(t)$ is small, then t is commonly found in documents.
  - Think of $\text{idf}(t)$ as the "rarity factor" of t across documents – the larger $\text{idf}(t)$ is, the more rare t is.

Computing IDF (Inverse Document Frequency)

In [7]:
```
def document_contains_term(term: str, document: str) -> bool:
    """Returns True if document contains the term, otherwise False."""
    return term.lower() in canonicalize(document).split()
```

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```
def idf(term: str, documents: list[str]) -> float:
    n_documents_containing_term = sum(document_contains_term(term, document)
    return np.log(len(documents) / n_documents_containing_term)
```

In [8]:
```
idf('computer', sentences)
```

Out[8]:
```
np.float64(0.6931471805599453)
```

In [9]:
```
idf('is', sentences)
```

Out[9]:
```
np.float64(0.0)
```

Intuition

$$\text{tf}(t, d) = \frac{\text{\# of occurrences of t in d}}{\text{total \# of words in d}}$$$$\text{idf}(t) = \log \left(\frac{\text{total \# of documents}}{\text{\# of documents in which t appears}} \right)$$

Goal: Quantify how well word t **summarizes** document d.

- If $\text{tf}(t, d)$ is small, then t doesn't occur very often in d, so t can't be a good summary of d.
- If $\text{idf}(t)$ is small, then t occurs often amongst all documents, and so it is not a good summary of any one document.
- If $\text{tf}(t, d)$ and $\text{idf}(t)$ are both large, then **t occurs often in d but rarely overall**. This makes t **a good summary** of document d.

In [10]:
```
def show_tf_idf_for_sentence(sentence_number: int, test_terms: list[str], sh
    import IPython.display
    import matplotlib.colors as mcolors

    document = sentences[sentence_number]
    df = pd.DataFrame({
            'Terms': test_terms,
            'TF(t,d)': [tf(term, document) for term in test_terms],
            'IDF(t)': [idf(term, sentences) for term in test_terms]
    }).set_index('Terms')
    if show_product:
        df['TF-IDF(t,d)'] = df['TF(t,d)'] * df['IDF(t)']

    print()
    print(f'Document: "{document}".')
    print()

    num_cols = df.select_dtypes(include='number').columns
    styled = (
```

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```
        df.style
          .format({col: '{:.4f}' for col in num_cols})
          .background_gradient(cmap='Greens', subset=num_cols, vmin=0)
    )

    if show_product:
        best_summary_word = df['TF-IDF(t,d)'].idxmax()
        print(f"Best summary term: {best_summary_word}")
        print()

    IPython.display.display(styled)
```

In [11]:
```
show_tf_idf_for_sentence(3, test_terms=['computer', 'book', 'car', 'universe
```

```
Document: "The universe is everything. The universe is a book, a computer, a
nd a car.".
```

Terms	TF(t,d)	IDF(t)
computer	0.0714	0.6931
book	0.0714	0.2877
car	0.0714	0.6931
universe	0.1429	1.3863
is	0.1429	0.0000
a	0.2143	0.0000

Term frequency-inverse document frequency

The **term frequency-inverse document frequency (TF-IDF)** of word t in document d is the product:

$$ \begin{align*} \text{tfidf}(t, d) &= \text{tf}(t, d) \cdot \text{idf}(t) \\\ &= \frac{\text{\# of occurrences of t in d}}{\text{total \# of words in d}} \cdot \log \left(\frac{\text{total \# of documents}}{\text{\# of documents in which t appears}} \right) \end{align*} $$

- If $\text{tfidf}(t, d)$ is large, then t is a good summary of d, because t occurs often in d but rarely across all documents.

- TF-IDF is a **heuristic** – it has no probabilistic justification.

- To know if $\text{tfidf}(t, d)$ is large for one particular word t, we need to compare it to $\text{tfidf}(t_i, d)$, for several different words t_i.

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In [12]:
```
show_tf_idf_for_sentence(
    3,
    test_terms=['computer', 'book', 'car', 'universe', 'is', 'a'],
    show_product=True
)
```

```
Document: "The universe is everything. The universe is a book, a computer, a
nd a car.".

Best summary term: universe
```

Terms	TF(t,d)	IDF(t)	TF-IDF(t,d)
computer	0.0714	0.6931	0.0495
book	0.0714	0.2877	0.0205
car	0.0714	0.6931	0.0495
universe	0.1429	1.3863	0.1980
is	0.1429	0.0000	0.0000
a	0.2143	0.0000	0.0000

In [13]:
```
show_tf_idf_for_sentence(
    3,
    test_terms=['computer', 'book', 'car', 'universe', 'is', 'a', 'the'],
    show_product=True
)
```

```
Document: "The universe is everything. The universe is a book, a computer, a
nd a car.".

Best summary term: universe
```

Terms	TF(t,d)	IDF(t)	TF-IDF(t,d)
computer	0.0714	0.6931	0.0495
book	0.0714	0.2877	0.0205
car	0.0714	0.6931	0.0495
universe	0.1429	1.3863	0.1980
is	0.1429	0.0000	0.0000
a	0.2143	0.0000	0.0000
the	0.1429	1.3863	0.1980

TF-IDF of all words in all documents

On its own, the TF-IDF of a word in a document doesn't really tell us anything; we must compare it to TF-IDFs of other words in that same document.

In [14]:
```
sentences
```

Out[14]:
```
['It is a book. A book is good.',
 'A computer is not a book. It is a computer.',
 'A car is a car. A car is good and bad.',
 'The universe is everything. The universe is a book, a computer, and a ca
r.']
```

In [15]:
```
show_tf_idf_for_sentence(
    2,
    test_terms=list(set(canonicalize(sentences[2]).split())),
    show_product=True
)
```

```
Document: "A car is a car. A car is good and bad.".

Best summary term: car
```

Terms	TF(t,d)	IDF(t)	TF-IDF(t,d)
car	0.2727	0.6931	0.1890
good	0.0909	0.6931	0.0630
a	0.2727	0.0000	0.0000
and	0.0909	0.6931	0.0630
is	0.1818	0.0000	0.0000
bad	0.0909	1.3863	0.1260

Interpreting TF-IDFs

Note that there are two ways that $\text{tfidf}(t, d) = \text{tf}(t, d) \cdot \text{idf}(t)$ can be 0:

- If t appears in every document, because then $\text{idf}(t) = \log (\frac{\text{\# documents}}{\text{\# documents}}) = \log(1) = 0$.
- If t does not appear in document d, because then $\text{tf}(t, d) = \frac{0}{\text{len}(d)} = 0$.

The word that **best summarizes** a document is the word with the highest TF-IDF for that document:

In [16]:
```
show_tf_idf_for_sentence(
    2,
    test_terms=list(set(canonicalize(sentences[2]).split())),
```

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```
    show_product=True
)
```

```
Document: "A car is a car. A car is good and bad.".

Best summary term: car
```

Terms	TF(t,d)	IDF(t)	TF-IDF(t,d)
car	0.2727	0.6931	0.1890
good	0.0909	0.6931	0.0630
a	0.2727	0.0000	0.0000
and	0.0909	0.6931	0.0630
is	0.1818	0.0000	0.0000
bad	0.0909	1.3863	0.1260

In [17]:
```
show_tf_idf_for_sentence(
    3,
    test_terms=list(set(canonicalize(sentences[2]).split())),
    show_product=True
)
```

```
Document: "The universe is everything. The universe is a book, a computer, a
nd a car.".

Best summary term: car
```

Terms	TF(t,d)	IDF(t)	TF-IDF(t,d)
car	0.0714	0.6931	0.0495
good	0.0000	0.6931	0.0000
a	0.2143	0.0000	0.0000
and	0.0714	0.6931	0.0495
is	0.1429	0.0000	0.0000
bad	0.0000	1.3863	0.0000

Look closely at the rows of `tfidf` – in documents 2 and 3, the max TF-IDF is not unique!

State of the Union addresses

In [18]:
```
from pathlib import Path
sotu_txt = Path('data') / 'stateoftheunion1790-2023.txt'
```

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```
sotu = sotu_txt.read_text()
speeches = sotu.split('\n***\n')[1:]
```

In [19]:
```
import re
def extract_struct(speech):
    L = speech.strip().split('\n', maxsplit=3)
    L[3] = re.sub(r"[^A-Za-z' ]", ' ', L[3]).lower()
    return dict(zip(['speech', 'president', 'date', 'contents'], L))
```

In [20]:
```
speeches_df = pd.DataFrame(list(map(extract_struct, speeches)))
speeches_df
```

Out[20]:

	speech	president	date	contents
0	State of the Union Address	George Washington	January 8, 1790	fellow citizens of the senate and house of re...
1	State of the Union Address	George Washington	December 8, 1790	fellow citizens of the senate and house of re...
2	State of the Union Address	George Washington	October 25, 1791	fellow citizens of the senate and house of re...
...	...	...	...	...
230	State of the Union Address	Joseph R. Biden Jr.	April 28, 2021	thank you thank you thank you good to be b...
231	State of the Union Address	Joseph R. Biden Jr.	March 1, 2022	madam speaker madam vice president and our ...
232	State of the Union Address	Joseph R. Biden Jr.	February 7, 2023	mr speaker madam vice president our firs...

233 rows × 4 columns

Finding the most important words in each speech

Here, a "document" is a speech. We have 233 documents.

In [21]:
```
speeches_df
```

Out[21]:

	speech	president	date	contents
0	State of the Union Address	George Washington	January 8, 1790	fellow citizens of the senate and house of re...
1	State of the Union Address	George Washington	December 8, 1790	fellow citizens of the senate and house of re...
2	State of the Union Address	George Washington	October 25, 1791	fellow citizens of the senate and house of re...
...	...	...	...	...
230	State of the Union Address	Joseph R. Biden Jr.	April 28, 2021	thank you thank you thank you good to be b...
231	State of the Union Address	Joseph R. Biden Jr.	March 1, 2022	madam speaker madam vice president and our ...
232	State of the Union Address	Joseph R. Biden Jr.	February 7, 2023	mr speaker madam vice president our firs...

233 rows × 4 columns

A rough sketch of what we'll compute:

```
for each word t:
    for each speech d:
        compute tfidf(t, d)
```

In [22]:
```
unique_words = speeches_df['contents'].str.split().explode().value_counts()
# Take the top 500 most common words for speed
unique_words = unique_words.iloc[:500].index
unique_words
```

Out[22]:
```
Index(['the', 'of', 'to', 'and', 'in', 'a', 'that', 'for', 'be', 'our',
       ...
       'desire', 'call', 'submitted', 'increasing', 'months', 'point', 'tru
st',
       'throughout', 'set', 'object'],
      dtype='object', name='contents', length=500)
```

💡 Pro-Tip: Using `tqdm`

This code takes a while to run, so we'll use the `tdqm` package to track its progress. (Install with `mamba install tqdm` if needed).

In [23]:
```
from tqdm.notebook import tqdm

tfidf_dict = {}
tf_denom = speeches_df['contents'].str.split().str.len()

# Wrap the sequence with `tqdm()` to display a progress bar
n tqdm(unique_words):
```

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```
    re_pat = fr' {word} ' # Imperfect pattern for speed.
    tf = speeches_df['contents'].str.count(re_pat) / tf_denom
    idf = np.log(len(speeches_df) / speeches_df['contents'].str.contains(re_
    tfidf_dict[word] =  tf * idf
```

```
 0%|          | 0/500 [00:00<?, ?it/s]
```

In [24]:
```
tfidf = pd.DataFrame(tfidf_dict)
tfidf.head()
```

Out[24]:

	the	of	to	and	...	trust	throughout	set	object
0	0.0	0.0	0.0	0.0	...	4.29e-04	0.00e+00	0.00e+00	2.04e-03
1	0.0	0.0	0.0	0.0	...	0.00e+00	0.00e+00	0.00e+00	1.06e-03
2	0.0	0.0	0.0	0.0	...	4.06e-04	0.00e+00	3.48e-04	6.44e-04
3	0.0	0.0	0.0	0.0	...	6.70e-04	2.17e-04	0.00e+00	7.09e-04
4	0.0	0.0	0.0	0.0	...	2.38e-04	4.62e-04	0.00e+00	3.77e-04

5 rows × 500 columns

Note that the TF-IDFs of many common words are all 0!

Summarizing speeches

By using `idxmax`, we can find the word with the highest TF-IDF in each speech.

In [25]:
```
summaries = tfidf.idxmax(axis=1)
summaries
```

Out[25]:
```
0          object
1      convention
2       provision
          ...
230          it's
231       tonight
232          it's
Length: 233, dtype: object
```

What if we want to see the 5 words with the highest TF-IDFs, for each speech?

In [26]:
```
def five_largest(row):
    return ', '.join(row.index[row.argsort()][-5:])
```

In [27]:
```
keywords = tfidf.apply(five_largest, axis=1)
keywords_df = pd.concat([
    speeches_df['president'],
    speeches_df['date'],
    keywords
], axis=1)
```

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In [28]:
```
keywords_df
```

Out[28]:

	president	date	0
0	George Washington	January 8, 1790	your, proper, regard, ought, object
1	George Washington	December 8, 1790	case, established, object, commerce, convention
2	George Washington	October 25, 1791	community, upon, lands, proper, provision
...	...	...	...
230	Joseph R. Biden Jr.	April 28, 2021	get, americans, percent, jobs, it's
231	Joseph R. Biden Jr.	March 1, 2022	let, jobs, americans, get, tonight
232	Joseph R. Biden Jr.	February 7, 2023	down, percent, jobs, tonight, it's

233 rows × 3 columns

Uncomment the cell below to see every single row of `keywords_df`.

In [29]:
```
# display_df(keywords_df, rows=233)
```

Aside: What if we remove the $\log$ from $\text{idf}(t)$?

Let's try it and see what happens.

In [30]:
```
tfidf_nl_dict = {}
tf_denom = speeches_df['contents'].str.split().str.len()

for word in tqdm(unique_words):
    re_pat = fr' {word} ' # Imperfect pattern for speed.
    tf = speeches_df['contents'].str.count(re_pat) / tf_denom
    idf_nl = len(speeches_df) / speeches_df['contents'].str.contains(re_pat)
    tfidf_nl_dict[word] =  tf * idf_nl
```

```
 0%|          | 0/500 [00:00<?, ?it/s]
```

In [31]:
```
tfidf_nl = pd.DataFrame(tfidf_nl_dict)
tfidf_nl.head()
```

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Out [31]:

	the	of	to	and	...	trust	throughout	set	object
0	0.09	0.06	0.05	0.04	...	1.47e-03	0.00e+00	0.00e+00	5.78e-03
1	0.09	0.06	0.03	0.03	...	0.00e+00	0.00e+00	0.00e+00	2.99e-03
2	0.11	0.07	0.04	0.03	...	1.39e-03	0.00e+00	1.30e-03	1.82e-03
3	0.09	0.07	0.04	0.03	...	2.29e-03	7.53e-04	0.00e+00	2.01e-03
4	0.09	0.07	0.04	0.02	...	8.12e-04	1.60e-03	0.00e+00	1.07e-03

5 rows × 500 columns

In [32]:

```
keywords_nl = tfidf_nl.apply(five_largest, axis=1)
keywords_nl_df = pd.concat([
    speeches_df['president'],
    speeches_df['date'],
    keywords_nl
], axis=1)
keywords_nl_df
```

Out [32]:

	president	date	0
0	George Washington	January 8, 1790	a, and, to, of, the
1	George Washington	December 8, 1790	in, and, to, of, the
2	George Washington	October 25, 1791	a, and, to, of, the
...	...	...	...
230	Joseph R. Biden Jr.	April 28, 2021	of, it's, and, to, the
231	Joseph R. Biden Jr.	March 1, 2022	we, of, to, and, the
232	Joseph R. Biden Jr.	February 7, 2023	a, of, and, to, the

233 rows × 3 columns

The role of $\log$ in $\text{idf}(t)$

$$ \begin{align*} \text{tfidf}(t, d) &= \text{tf}(t, d) \cdot \text{idf}(t) \\ &= \frac{\text{\# of occurrences of t in d}}{\text{total \# of words in d}} \cdot \log \left(\frac{\text{total \# of documents}}{\text{\# of documents in which t appears}} \right) \end{align*} $$

- Remember, for any positive input x, $\log(x)$ is (much) smaller than x.
- In $\text{idf}(t)$, the $\log$ "dampens" the impact of the ratio $\frac{\text{\# documents}}{\text{\# documents with t}}$.

- If a word is very common, the ratio will be close to 1. The log of the ratio will be close to 0.

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In [33]:
```
(1000 / 999)
```

Out[33]:
```
1.001001001001001
```

In [34]:
```
np.log(1000 / 999)
```

Out[34]:
```
np.float64(0.0010005003335835622)
```

- If a word is very common (e.g. 'the'), removing the log multiplies the statistic by a large factor.
- If a word is very rare, the ratio will be very large. However, for instance, a word being seen in **2 out of 50** documents is not very different than being seen in **2 out of 500** documents (it is very rare in both cases), and so $\text{idf}(t)$ should be similar in both cases.

In [35]:
```
(50 / 2)
```

Out[35]:
```
25.0
```

In [36]:
```
(500 / 2)
```

Out[36]:
```
250.0
```

In [37]:
```
np.log(50 / 2)
```

Out[37]:
```
np.float64(3.2188758248682006)
```

In [38]:
```
np.log(500 / 2)
```

Out[38]:
```
np.float64(5.521460917862246)
```

Question 🤔

From the Fa23 final:

Consider the following corpus:

```
Document number Content
1               yesterday rainy today sunny
2               yesterday sunny today sunny
3               today rainy yesterday today
4               yesterday yesterday today today
```

Which words have a TF-IDF score of 0 for all four documents?

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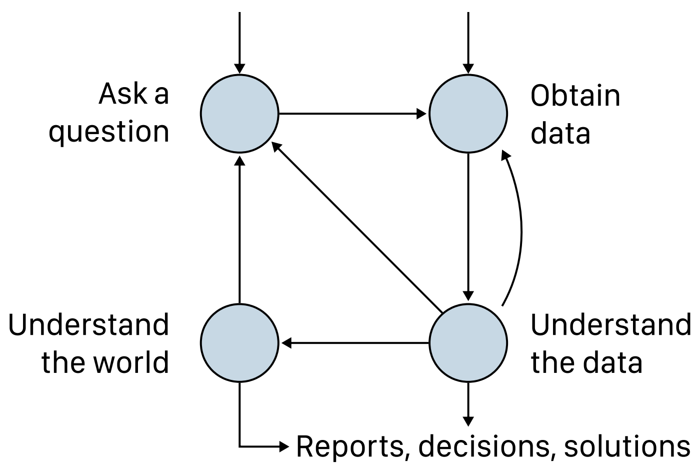
Modeling

Reflection

So far this quarter, we've learned how to:

- Extract information from tabular data using `pandas` and regular expressions.
- Clean data so that it best represents an underlying data generating process.
  - Missingness analyses and imputation.
- Collect data from the internet through scraping and APIs, and parse it using BeautifulSoup.
- Perform exploratory data analysis through aggregation, visualization, and the computation of summary statistics like TF-IDF.
- Infer about the relationships between samples and populations through hypothesis and permutation testing.
- **Now, let's make predictions.**



Modeling

- **A model is a set of assumptions about how data were generated.**
- George Box, a famous statistician, once said "All models are wrong, but some are useful." What did he mean?

Philosophy

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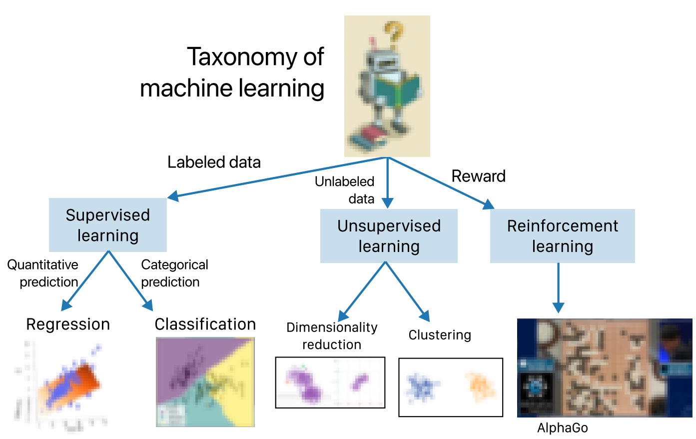
> "It has been said that "all models are wrong but some models are useful." In other words, any model is at best a useful fiction—there never was, or ever will be, an exactly normal distribution or an exact linear relationship. Nevertheless, enormous progress has been made by entertaining such fictions and using them as approximations."

> "Since all models are wrong the scientist cannot obtain a "correct" one by excessive elaboration. On the contrary following William of Occam he should **seek an economical description of natural phenomena**. Just as the ability to devise simple but evocative models is the signature of the great scientist so overelaboration and overparameterization is often the mark of mediocrity."

Goals of modeling

1. To make accurate **predictions** regarding **unseen data**.
   - Given this dataset of past UCSD data science students' salaries, can we predict your future salary? (regression)
   - Given this dataset of images, can we predict if this new image is of a dog, cat, or zebra? (classification)

2. To make **inferences** about complex phenomena in nature.
   - Is there a linear relationship between the heights of children and the heights of their biological mothers?
   - The weights of smoking and non-smoking mothers' babies babies in my *sample* are different – how *confident* am I that this difference exists in the *population*?



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- Of the two focuses of models, we will focus on **prediction**.
- In the above taxonomy, we will focus on **supervised learning**.
- We'll start with **regression** before moving to classification.

Features

- A **feature** is a measurable property of a phenomenon being observed.
  - Other terms for "feature" include "(explanatory) variable" and "attribute".
  - Typically, features are the *inputs* to models.
- In DataFrames, features typically correspond to **columns**, while rows typically correspond to different individuals.
- Some features come as part of a dataset, e.g. weight and height, but others we need to create given existing features, for example:

$$\text{BMI} = \frac{\text{weight (kg)}}{\text{[height (m)]}^2}$$

- Example: TF-IDF creates **features** that summarize documents!

Example: Restaurant tips 🧑‍🍳

About the data

What features does the dataset contain? Is this likely a recent dataset, or an older one?

In [39]:
```
# The dataset is built into plotly!
tips = px.data.tips()
tips
```

Out[39]:

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
...	...	...	...	...	...	...	...
241	22.67	2.00	Male	Yes	Sat	Dinner	2
242	17.82	1.75	Male	No	Sat	Dinner	2
243	18.78	3.00	Female	No	Thur	Dinner	2

244 rows × 7 columns

Predicting tips

- **Goal**: Given various information about a table at a restaurant, we want to predict the **tip** that a server will earn.

- **Why** might a server be interested in doing this?
  - To determine which tables are likely to tip the most (inference).
  - To predict earnings over the next month (prediction).

Exploratory data analysis

- The most natural feature to look at first is total bills.

- As such, we should explore the relationship between total bills and tips. Moving forward:
  - x: Total bills.
  - y: Tips.

In [40]:
```
fig = tips.plot(kind='scatter', x='total_bill', y='tip', title='Tip vs. Tota
fig.update_layout(xaxis_title='Total Bill', yaxis_title='Tip')
```

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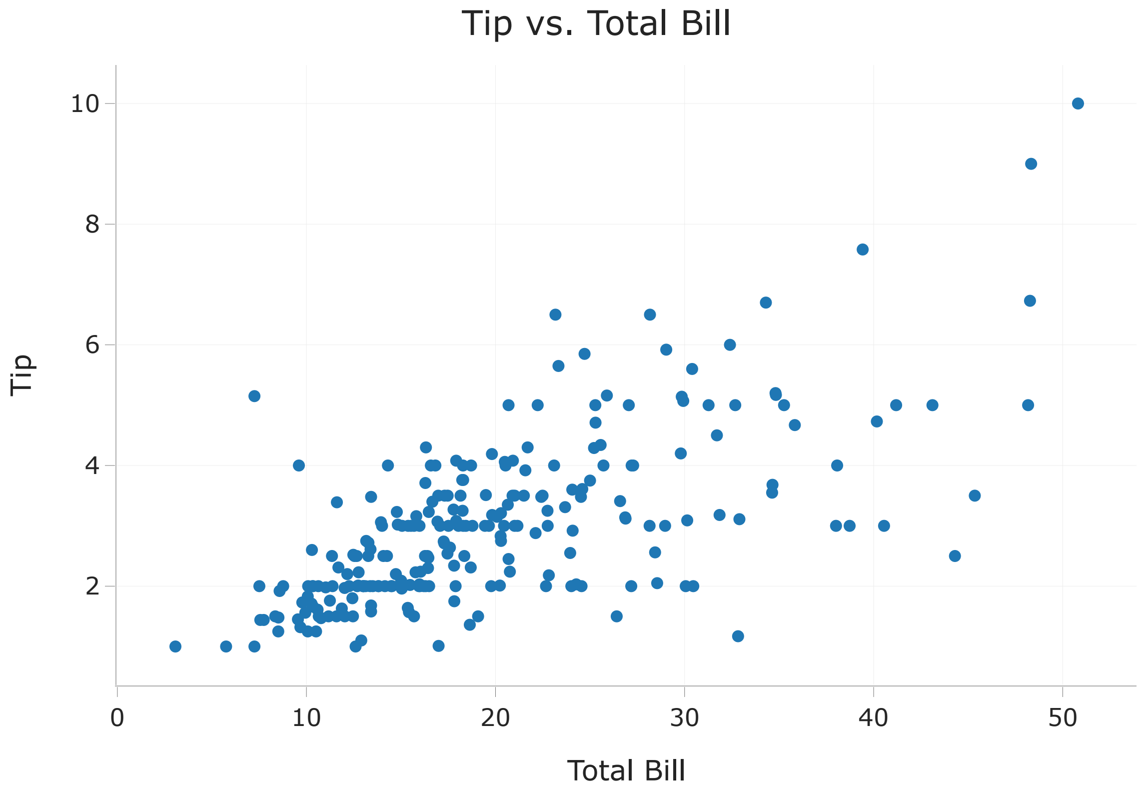


Model #1: Constant

- Let's start simple, by ignoring all features. Suppose our model assumes every tip is given by a constant dollar amount:

$$\text{tip} = h^{\text{true}}$$

- **Model**: There is a single tip amount h^{true} that all customers pay.
  - Correct? No!
  - Useful? Perhaps. An estimate of h^{true}, denoted by h^*, can allow us to predict future tips.

Estimating h^{true}

- The true **parameter** h^{true} is determined by the universe. We'll never get to see it, so we need to **estimate** it.

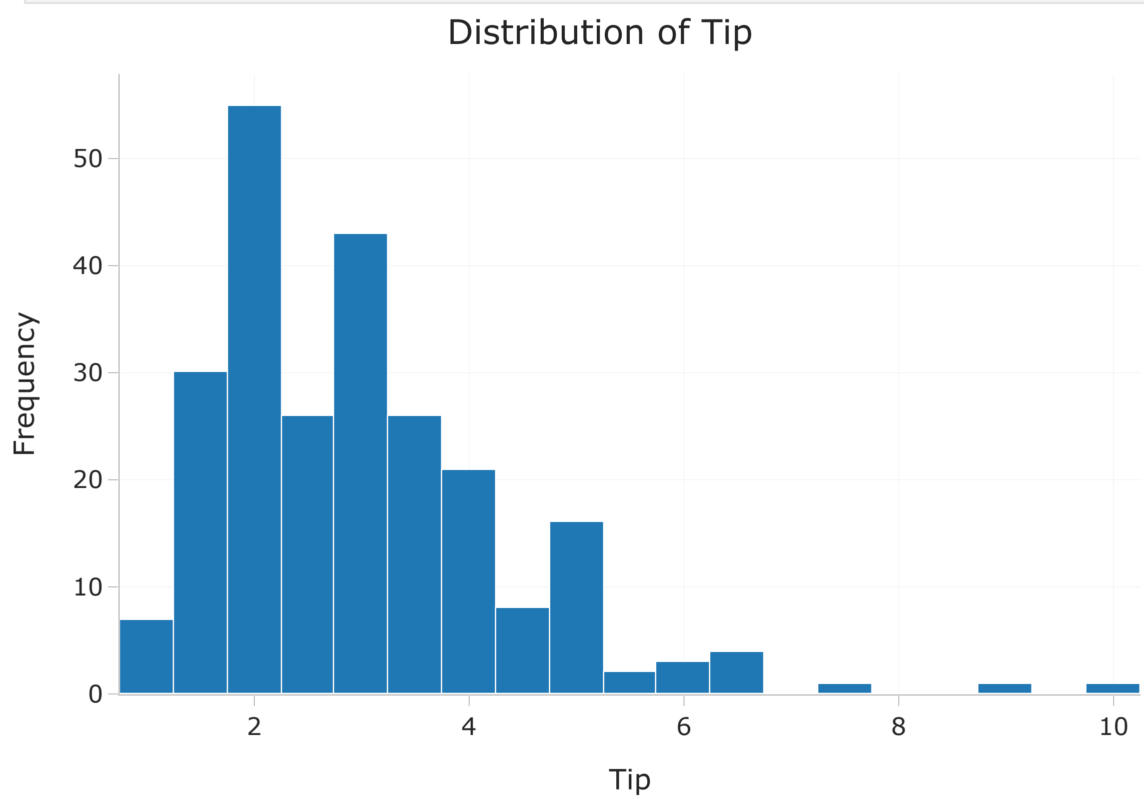
- There are several ways we *could* estimate h^{true}. For instance, we *could* use domain knowledge: for instance, assume that everyone clicks the $1 tip option when buying coffee.

- But, perhaps, we should look at the tips that we've already seen in our dataset to estimate h^{true}.

Looking at the data

Our estimate for h^{true} should be a good **summary statistic** of the distribution of tips.

In [41]:
```
fig = tips.plot(kind='hist', x='tip', title='Distribution of Tip', nbins=20)
fig.update_layout(xaxis_title='Tip', yaxis_title='Frequency')
```



Empirical risk minimization

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- In DSC 40A, we established a framework for estimating model parameters:
  - **Choose a loss function**, which measures how "good" a single prediction is.
  - **Minimize empirical risk**, to find the best estimate for the dataset that we have.

- Depending on which loss function we choose, we will end up with different h^* (which are estimates of $h^{\text{true}})$.

- If we choose **squared loss**, then our empirical risk is **mean squared error**:

$$\text{MSE} = \frac{1}{n} \sum_{i = 1}^n (y_i - h)^2 \overset{\text{calculus}}\implies h^* = \text{mean}(y)$$

Remember, tips are our y variable.

- If we choose **absolute loss**, then our empirical risk is **mean absolute error**:

$$\text{MAE} = \frac{1}{n} \sum_{i = 1}^n | y_i - h | \overset{\text{algebra}}\implies h^* = \text{median}(y)$$

The mean tip

Let's suppose we choose squared loss, meaning that $h^* = \text{mean}(y)$.

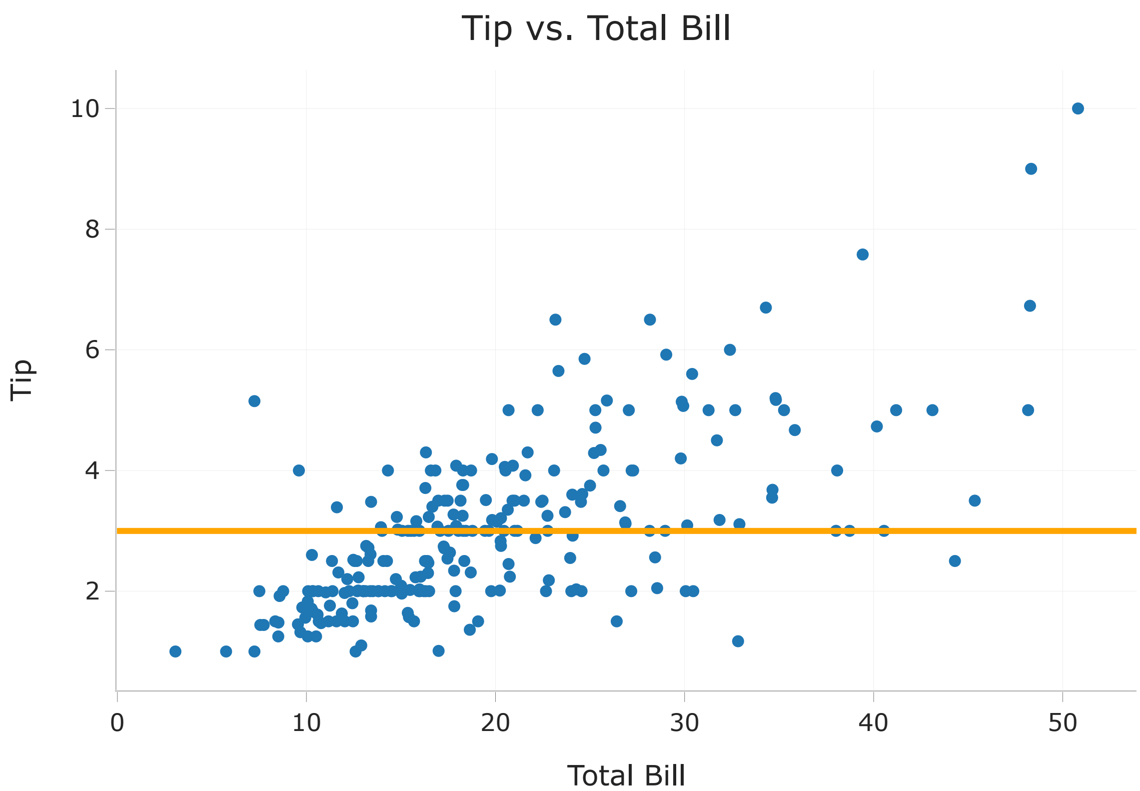
In [42]:
```
mean_tip = tips['tip'].mean()
mean_tip
```

Out[42]:
```
np.float64(2.99827868852459)
```

$h^* = 2.998$ is our **fit model** – it was fit to our **training data** (the data we have available to learn from).

Let's visualize this prediction.

In [43]:
```
fig = px.scatter(tips, x='total_bill', y='tip')
fig.add_hline(mean_tip, line_width=3, line_color='orange', opacity=1)
fig.update_layout(title='Tip vs. Total Bill',
                  xaxis_title='Total Bill', yaxis_title='Tip')
```



Note that to make predictions, this model ignores total bill (and all other features), and predicts the same tip for all tables.

The quality of predictions

- **Question**: How can we quantify how **good** this constant prediction is at predicting tips in our **training data** – that is, the data we used to **fit** the model?

- **One answer**: use the mean squared error. If y_i represents the ith actual value and $H(x_i)$ represents the ith predicted value, then:

$$\text{MSE} = \frac{1}{n} \sum_{i = 1}^n \big(y_i - H(x_i) \big)^2$$

In [44]:
```
np.mean((tips['tip'] - mean_tip) ** 2)
```

Out[44]: `np.float64(1.9066085124966412)`

In [45]:
```
# The same! A fact from 40A.
np.var(tips['tip'])
```

Out[45]: `np.float64(1.9066085124966412)`

- Issue: The units of MSE are "dollars squared", which are a little hard to interpret.

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Root mean squared error

- Often, to measure the quality of a regression model's predictions, we will use the **root mean squared error (RMSE)**:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i = 1}^n \big(y_i - H(x_i) \big)^2}$$

- The units of the RMSE are the same as the units of the original y values – dollars, in this case.

- **Important**: Minimizing MSE is the same as minimizing RMSE; the constant tip h^* that minimizes MSE is the same h^* that minimizes RMSE. (Why?)

Computing and storing the RMSE

Since we'll compute the RMSE for our future models too, we'll define a function that can compute it for us.

In [46]:
```
def rmse(actual, pred):
    return np.sqrt(np.mean((actual - pred) ** 2))
```

Let's compute the RMSE of our constant tip's predictions, and store it in a dictionary that we can refer to later on.

In [47]:
```
rmse(tips['tip'], mean_tip)
```

Out[47]:
```
np.float64(1.3807999538298954)
```

In [48]:
```
rmse_dict = {}
rmse_dict['constant tip amount'] = rmse(tips['tip'], mean_tip)
rmse_dict
```

Out[48]:
```
{'constant tip amount': np.float64(1.3807999538298954)}
```

Key idea: Since the mean minimizes RMSE for the constant model, it is **impossible** to change the `mean_tip` argument above to another number and yield a **lower** RMSE.

Model #2: Simple linear regression using total bill

- We haven't yet used any of the **features** in the dataset. The first natural feature to look at is `'total_bill'`.

In [49]:
```
tips.head()
```

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Out[49]:

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4

- We can fit a **simple linear model** to predict tips as a function of total bills:

$$\text{predicted tip} = w_0 + w_1 \cdot \text{total bill}$$

- This is a reasonable thing to do, because total bills and tips appeared to be linearly associated when we visualized them on a scatter plot a few slides ago.

Recap: Simple linear regression

A simple linear regression model is a linear model with a single feature, as we have here. For any total bill x_i, the predicted tip $H(x_i)$ is given by

$$H(x_i) = w_0 + w_1x_i$$

- **Question**: How do we determine which intercept, w_0, and slope, w_1, to use?

- **One answer**: Pick the w_0 and w_1 that minimize **mean squared error**. If x_i and y_i correspond to the ith total bill and tip, respectively, then:

$$\begin{align*}\text{MSE} &= \frac{1}{n} \sum_{i = 1}^n \big(y_i - H(x_i) \big)^2 \\ &= \frac{1}{n} \sum_{i = 1}^n \big(y_i - w_0 - w_1x_i \big)^2\end{align*}$$

- **Key idea: The lower the MSE on our training data is, the "better" the model fits the training data**.
  - Lower MSE = better **predictions**.
  - But lower MSE ≠ more reflective of reality!

Empirical risk minimization, by hand

$$\begin{align*}\text{MSE} &= \frac{1}{n} \sum_{i = 1}^n \big(y_i - w_0 - w_1x_i \big)^2\end{align*}$$

- In DSC 40A, you found the formulas for the best intercept, w_0^*, and the best slope, w_1^*, through calculus.

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- The resulting line, $H(x_i) = w_0^* + w_1^* x_i$, is called the **line of best fit**, or the **regression line**.

- Specifically, if r is the correlation coefficient, σ_x and σ_y are the standard deviations of x and y, and $\bar{x}$ and $\bar{y}$ are the means of x and y, then:

$$w_1^* = r \cdot \frac{\sigma_y}{\sigma_x}$$$$w_0^* = \bar{y} - w_1^* \bar{x}$$

Regression in `sklearn`

`sklearn`

- `sklearn` (scikit-learn) implements many common steps in the feature and model creation pipeline.
  - It is **widely** used throughout industry and academia.

- It interfaces with `numpy` arrays, and to an extent, `pandas` DataFrames.

- Huge benefit: the documentation online is excellent.

The `LinearRegression` class

- `sklearn` comes with several subpackages, including `linear_model` and `tree`, each of which contains several classes of models.

- We'll start with the `LinearRegression` class from `linear_model`.

In [50]:
```
from sklearn.linear_model import LinearRegression
```

- **Important**: From the documentation, we have:

> LinearRegression fits a linear model with coefficients w = (w1, ..., wp) to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation.

In other words, **`LinearRegression` minimizes mean squared error by default**! (Per the documentation, it also includes an intercept term by default.)

In [51]:
```
LinearRegression?
```

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```
Init signature:
LinearRegression(
    *,
    fit_intercept=True,
    copy_X=True,
    n_jobs=None,
    positive=False,
)
Docstring:
Ordinary least squares Linear Regression.

LinearRegression fits a linear model with coefficients w = (w1, ..., wp)
to minimize the residual sum of squares between the observed targets in
the dataset, and the targets predicted by the linear approximation.

Parameters
----------
fit_intercept : bool, default=True
    Whether to calculate the intercept for this model. If set
    to False, no intercept will be used in calculations
    (i.e. data is expected to be centered).

copy_X : bool, default=True
    If True, X will be copied; else, it may be overwritten.

n_jobs : int, default=None
    The number of jobs to use for the computation. This will only provide
    speedup in case of sufficiently large problems, that is if firstly
    `n_targets > 1` and secondly `X` is sparse or if `positive` is set
    to `True`. ``None`` means 1 unless in a
    :obj:`joblib.parallel_backend` context. ``-1`` means using all
    processors. See :term:`Glossary <n_jobs>` for more details.

positive : bool, default=False
    When set to ``True``, forces the coefficients to be positive. This
    option is only supported for dense arrays.

    .. versionadded:: 0.24

Attributes
----------
coef_ : array of shape (n_features, ) or (n_targets, n_features)
    Estimated coefficients for the linear regression problem.
    If multiple targets are passed during the fit (y 2D), this
    is a 2D array of shape (n_targets, n_features), while if only
    one target is passed, this is a 1D array of length n_features.

rank_ : int
    Rank of matrix `X`. Only available when `X` is dense.

singular_ : array of shape (min(X, y),)
    Singular values of `X`. Only available when `X` is dense.

intercept_ : float or array of shape (n_targets,)
    Independent term in the linear model. Set to 0.0 if
    `fit_intercept = False`.
```

```
n_features_in_ : int
    Number of features seen during :term:`fit`.

    .. versionadded:: 0.24

feature_names_in_ : ndarray of shape (`n_features_in_`,)
    Names of features seen during :term:`fit`. Defined only when `X`
    has feature names that are all strings.

    .. versionadded:: 1.0

See Also
--------
Ridge : Ridge regression addresses some of the
    problems of Ordinary Least Squares by imposing a penalty on the
    size of the coefficients with l2 regularization.
Lasso : The Lasso is a linear model that estimates
    sparse coefficients with l1 regularization.
ElasticNet : Elastic-Net is a linear regression
    model trained with both l1 and l2 -norm regularization of the
    coefficients.

Notes
-----
From the implementation point of view, this is just plain Ordinary
Least Squares (scipy.linalg.lstsq) or Non Negative Least Squares
(scipy.optimize.nnls) wrapped as a predictor object.

Examples
--------
>>> import numpy as np
>>> from sklearn.linear_model import LinearRegression
>>> X = np.array([[1, 1], [1, 2], [2, 2], [2, 3]])
>>> # y = 1 * x_0 + 2 * x_1 + 3
>>> y = np.dot(X, np.array([1, 2])) + 3
>>> reg = LinearRegression().fit(X, y)
>>> reg.score(X, y)
1.0
>>> reg.coef_
array([1., 2.])
>>> reg.intercept_
np.float64(3.0...)
>>> reg.predict(np.array([[3, 5]]))
array([16.])
File:           ~/workbench/dsc80/.venv/lib/python3.12/site-packages/sklear
n/linear_model/_base.py
Type:           ABCMeta
Subclasses:
```

Fitting a simple linear model

First, we must instantiate a `LinearRegression` object and fit it. By calling `fit`, we are saying "minimize mean squared error on this dataset and find w^*."

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In [52]:
```
model = LinearRegression()

# Note that there are two arguments to fit – X and y!
# (It is not necessary to write X= and y=)
model.fit(X=tips[['total_bill']], y=tips['tip'])
```

Out[52]:
```
▾ LinearRegression
LinearRegression()
```

After fitting, we can access w^* – that is, the best slope and intercept.

In [53]:
```
model.intercept_, model.coef_[0]
```

Out[53]:
```
(np.float64(0.9202696135546744), np.float64(0.1050245173843533))
```

These coefficients tell us that the "best way" (according to squared loss) to make tip predictions using a linear model is using:

$$\text{predicted tip} = 0.92 + 0.105 \cdot \text{total bill}$$

This model **predicts** that people tip by:

- Tipping a constant 92 cents.
- Tipping 10.5% for every dollar spent.

This is the best "linear" pattern in the dataset – it doesn't mean this is actually how people tip!

Let's visualize this model, along with our previous model.

In [54]:
```
line_pts = pd.DataFrame({'total_bill': [0, 60]})

fig = px.scatter(tips, x='total_bill', y='tip')
fig.add_trace(go.Scatter(
    x=line_pts['total_bill'],
    y=[mean_tip, mean_tip],
    mode='lines',
    name='Constant Model (Mean Tip)'
))
fig.add_trace(go.Scatter(
    x=line_pts['total_bill'],
    y=model.predict(line_pts),
    mode='lines',
    name='Linear Model: Total Bill Only'
))
fig.update_layout(title='Tip vs. Total Bill',
                  xaxis_title='Total Bill',
                  yaxis_title='Tip')
```

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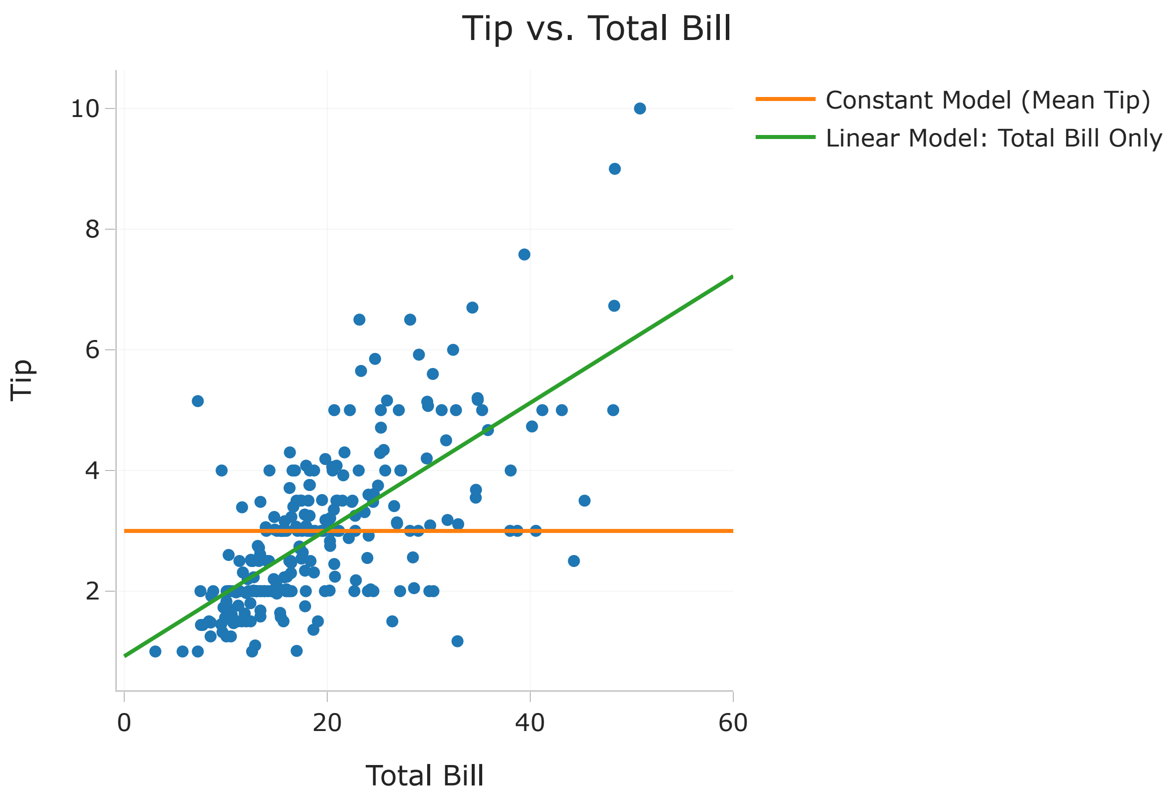

Visually, our linear model *seems* to be a better fit for our dataset than our constant model.

Can we quantify whether or not it is better?

Making predictions

Fit `LinearRegression` objects also have a `predict` method, which can be used to predict tips for any total bill, new or old.

In [55]:
```
model.predict([[15]])
```

```
/Users/eldridge/workbench/dsc80/.venv/lib/python3.12/site-packages/sklearn/b
ase.py:493: UserWarning:

X does not have valid feature names, but LinearRegression was fitted with fe
ature names
```

Out[55]:
```
array([2.5])
```

In [56]:
```
# Since we trained on a DataFrame, the input to model.predict should also
# be a DataFrame. To avoid having to do this, we can use .to_numpy()
# when specifying X= and y=.
test_points = pd.DataFrame({'total_bill': [15, 4, 100]})
model.predict(test_points)
```

Out[56]:
```
array([ 2.5 ,  1.34, 11.42])
```

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Comparing models

If we want to compute the RMSE of our model on the training data, we need to find its predictions on every row in the training data, `tips`.

In [57]:
```
all_preds = model.predict(tips[['total_bill']])
```

In [58]:
```
rmse_dict['one feature: total bill'] = rmse(tips['tip'], all_preds)
rmse_dict
```

Out[58]:
```
{'constant tip amount': np.float64(1.3807999538298954),
 'one feature: total bill': np.float64(1.0178504025697377)}
```

- The RMSE of our simple linear model is **lower** than that of our constant model, which means it does a **better job** at predicting tips in our training data than our constant model.

- Theory tells us it's impossible for the RMSE **on the training data** to increase as we add more features to the same model. However, the RMSE may increase on **unseen data** by adding more features; we'll discuss this idea more soon.

💡 Pro-Tip: Making a DF just to display

Sometimes it's nice to put your values into a dataframe just to make them display nicely:

In [59]:
```
rmse_dict
```

Out[59]:
```
{'constant tip amount': np.float64(1.3807999538298954),
 'one feature: total bill': np.float64(1.0178504025697377)}
```

In [60]:
```
pd.DataFrame({'rmse': rmse_dict.values()}, index=rmse_dict.keys())
```

Out[60]:

	rmse
constant tip amount	1.38
one feature: total bill	1.02

Model #3: Multiple linear regression using total bill and table size

- There are still many features in `tips` we haven't touched:

In [61]:
```
tips.head()
```

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Out[61]:

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4

- Let's try using another feature – table size. Such a model would predict tips using:

$$\text{predicted tip} = w_0 + w_1 \cdot \text{total bill} + w_2 \cdot \text{table size}$$

Multiple linear regression

To find the optimal parameters w^*, we will again use `sklearn`'s `LinearRegression` class. The code is not all that different!

In [62]:
```
model_two = LinearRegression()
model_two.fit(X=tips[['total_bill', 'size']], y=tips['tip'])
```

Out[62]:
```
▾ LinearRegression
LinearRegression()
```

In [63]:
```
model_two.intercept_, model_two.coef_
```

Out[63]:
```
(np.float64(0.668944740812504), array([0.09, 0.19]))
```

In [64]:
```
test_pts = pd.DataFrame({'total_bill': [25], 'size': [4]})
model_two.predict(test_pts)
```

Out[64]:
```
array([3.76])
```

What does this model *look* like?

Plane of best fit ✈️

Here, we must draw a 3D scatter plot and plane, with one axis for total bill, one axis for table size, and one axis for tip. The code below does this.

In [65]:
```
XX, YY = np.mgrid[0:50:2, 0:8:1]
Z = model_two.intercept_ + model_two.coef_[0] * XX + model_two.coef_[1] * YY
plane = go.Surface(x=XX, y=YY, z=Z, colorscale='Oranges')

fig = go.Figure(data=[plane])
fig.add_trace(go.Scatter3d(x=tips['total_bill'],
```

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```
                           y=tips['size'],
                           z=tips['tip'], mode='markers',
                           marker={'color': '#656DF1', 'size': 5}))

fig.update_layout(scene=dict(xaxis_title='Total Bill',
                             yaxis_title='Table Size',
                             zaxis_title='Tip'),
                  title='Tip vs. Total Bill and Table Size',
                  width=500, height=500)
```

WebGL is not supported by your browser - visit https://get.webgl.org for more info

Comparing models, again

How does our two-feature linear model stack up to our single feature linear model and our constant model?

In [66]:

```
rmse_dict['two features'] = rmse(
    tips['tip'], model_two.predict(tips[['total_bill', 'size']])
)
```

In [67]:

```
pd.DataFrame({'rmse': rmse_dict.values()}, index=rmse_dict.keys())
```

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Out[67]:

	rmse
constant tip amount	1.38
one feature: total bill	1.02
two features	1.01

- The RMSE of our two-feature model is the lowest of the three models we've looked at so far, but not by much. We didn't **gain** much by adding table size to our linear model.

- It's also not clear whether table sizes are practically useful in predicting tips.
  - We already have the total amount the table spent; why do we need to know how many people were there?

Residual plots

- From DSC 10: one important technique for diagnosing model fit is the **residual plot**.

- The ith residual is $ y_i - H(x_i) $.

- A residual plot has
  - **predicted values $H(x)$** on the x-axis, and
  - **residuals $ y - H(x) $** on the y-axis.

In [68]:
```
# Let's start with the single-variable model:
with_resid = tips.assign(**{
    'Predicted Tip': model.predict(tips[['total_bill']]),
    'Residual': tips['tip'] - model.predict(tips[['total_bill']]),
})
fig = px.scatter(with_resid, x='Predicted Tip', y='Residual')
fig.add_hline(0, line_width=2, opacity=1).update_layout(title='Residual Plot
```

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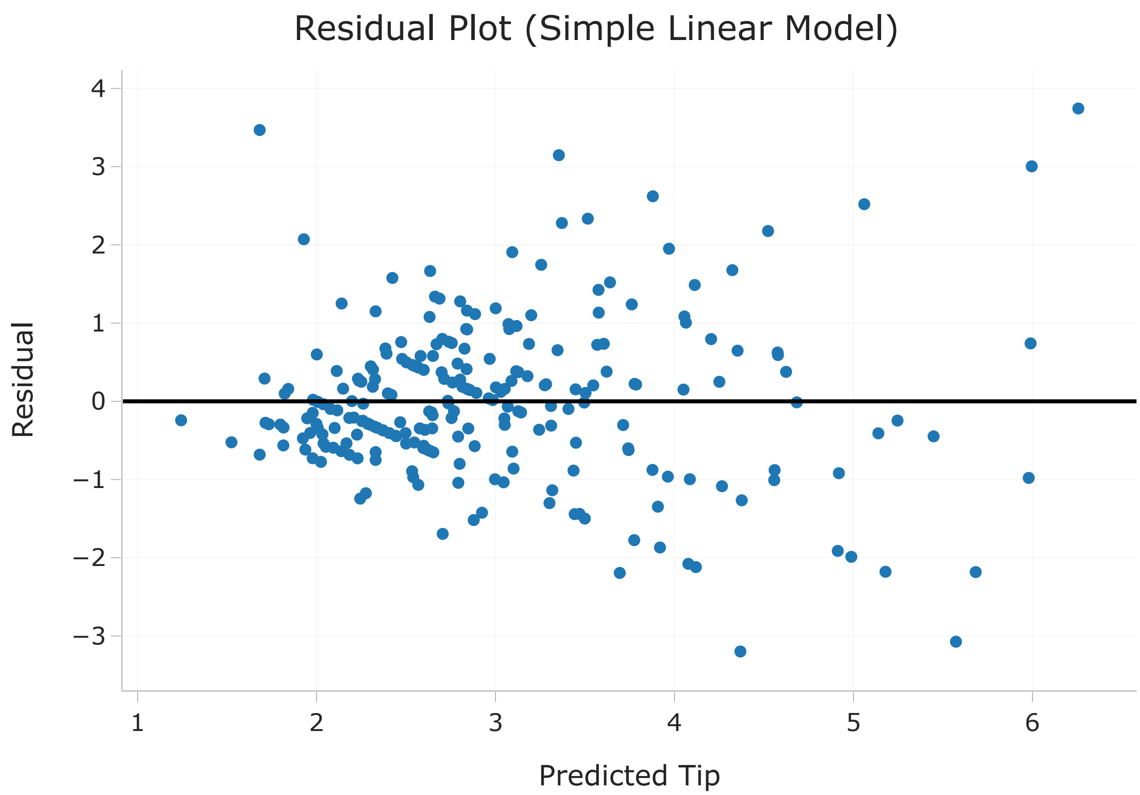

- If all assumptions about linear regression hold, then residual plot should look randomly scattered around the horizontal line $y = 0$.

- Here, we see that the model makes bigger mistakes for larger predicted values. But overall, there's no apparent trend, so a linear model seems appropriate.

In [69]:
```
# What about the two-variable model?
with_resid = tips.assign(**{
    'Predicted Tip': model_two.predict(tips[['total_bill', 'size']]),
    'Residual': tips['tip'] - model_two.predict(tips[['total_bill', 'size']]
})
fig = px.scatter(with_resid, x='Predicted Tip', y='Residual')
fig.add_hline(0, line_width=2, opacity=1).update_layout(title='Residual Plot
```

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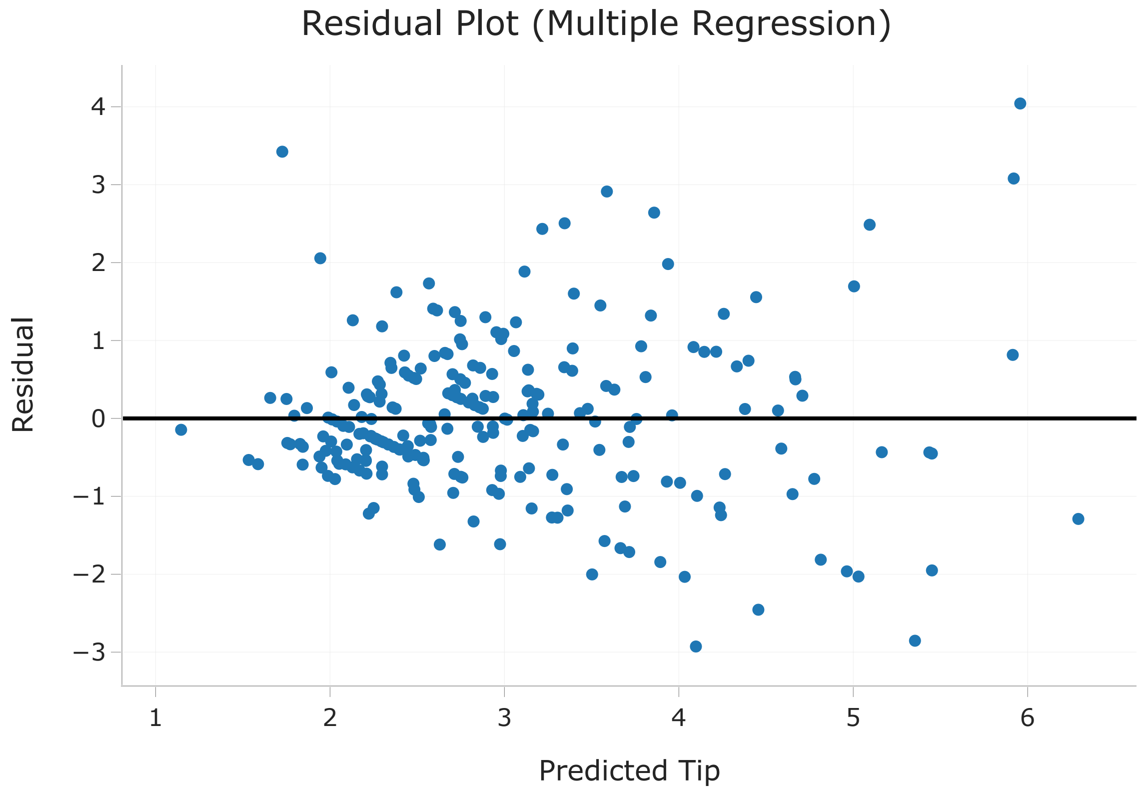

Looks about the same as the previous plot!

Summary, next time

Summary

- We built three models:
  - A constant model: $\text{predicted tip} = h^*$.
  - A simple linear regression model: $\text{predicted tip} = w_0^* + w_1^* \cdot \text{total bill}$.
  - A multiple linear regression model: $\text{predicted tip} = w_0^* + w_1^* \cdot \text{total bill} + w_2^* \cdot \text{table size}$.
- As we added more features, our RMSEs decreased.
  - This was guaranteed to happen, since we were only looking at our training data.
- It is not clear that the final linear model is actually "better"; it doesn't seem to **reflect reality** better than the previous models.

`LinearRegression` summary

Property	Example	Description
Initialize model parameters	`lr = LinearRegression()`	Create (empty) linear regression model

Property	Example	Description
Fit the model to the data	`lr.fit(X, y)`	Determines regression coefficients
Use model for prediction	`lr.predict(X_new)`	Uses regression line to make predictions
Evaluate the model	`lr.score(X, y)`	Calculates the R^2 of the LR model
Access model attributes	`lr.coef_`, `lr.intercept_`	Accesses the regression coefficients and intercept

Next time

In [70]:
```
tips.head()
```

Out[70]:

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4

- So far, in our journey to predict `'tip'`, we've only used the existing numerical features in our dataset, `'total_bill'` and `'size'`.
- There's a lot of information in tips that we didn't use – `'sex'`, `'smoker'`, `'day'`, and `'time'`, for example. We can't use these features in their current form, because they're non-numeric.
- **How do we use categorical features in a regression model?**

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