April 12, 2023 DARTMOUTH





Gentle Introduction to Machine Learning: Statistics

A Reproducible Research Workshop

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About the Reproducible Research Group

- Joint venture of Research Computing @ ITC and Research Data Services @ Library
- Consult with experts on
 - research data management,
 - data visualization,
 - · biomedical research support,
 - spatial data and GIS,
 - · high performance and research computing,
 - statistical analysis,
 - economics and social sciences data
- Meet the people on campus that support your reproducible research lifecycle
- Engage in community discussions to learn from other researchers on campus
- Attend a workshop to learn practical tools and tips



About Research Data Services

Research Data Management

Data Management Plans (DMPs) for sponsored projects

Finding and using 3rd party data

Collection and cleaning of data

Organization and documentation

Publishing and Repositories

Data Analysis/Visualization

Textual, numeric, spatial data

Reproducible research workflows

Scripting in R: tidyverse core package (i.e., ggplot, dplyr, tydr, tibble, etc.)

Scripting in Python: NumPy, SciPy, Pandas, Scikit-learn, Matplotlib, Seaborn, (OpenCV, PyTorch, TensorFlow, Tesseract, NLTK, etc.)

Computational Scholarship

Computational project planning

Collections as Data

Storytelling with data and visualizations

Text and data mining

Digital Humanities support

Computational Pedagogy



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Activity:

Why are you here?

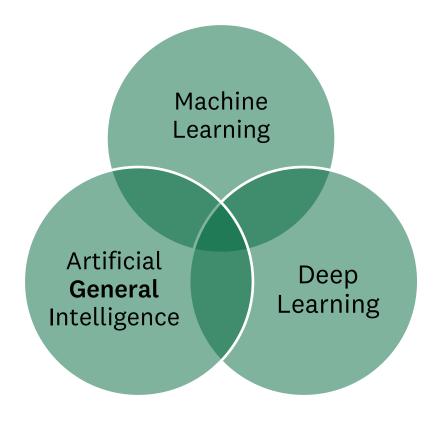
What do you hope to take away from this workshop (series)?



Machine Learning is "the field of study that gives computers the ability to learn without explicitly being programmed."

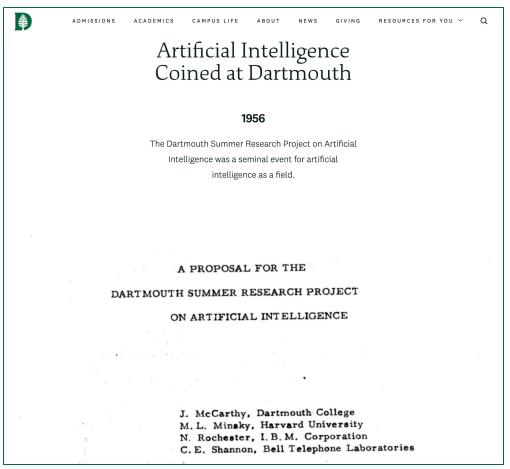
- Arthur Samuel, 1959 (paraphrased)

Machine Learning is what we should call (the current) Artificial Intelligence!





Intro





The New Hork Times

CURRENTS

A.I. Here, There, Everywhere

Many of us already live with artificial intelligence now, but researchers say interactions with the technology will become increasingly personalized.

By Craig S. Smith

Published Feb. 23, 2021 Updated March 9, 2021

5 MIN READ

- Machine Learning is everywhere
- We are interacting with it every day
- But how much do most of us know about our new algorithmic overlords?



Aims of this series:

- Demystify the field a bit and give context to the buzzwords
- P A working mental model how machine learning algorithms think calculate
- To provide enough knowledge to think critically about "A.I."
- To inspire you to confidently use machine learning in your work and personal life



Statistics

- A brief survey of the fundamentals for Machine Learning
- Regression (April 25)
 - How can an algorithm find relationships between two variables?
- Classification (May 9)
 - How can an algorithm put a label on a real-world object?



Basics

Intro

Activity:

Define "Statistics"

One definition (Upton & Cook, 2008):

"The science of collecting, displaying, and analysing data."

In Machine Learning:

"The way that algorithms perceive the world"



Basics

Intro

Two sides of the (fair) coin:

Descriptive Statistics

Q Describing an apparent mess of data

Inferential Statistics

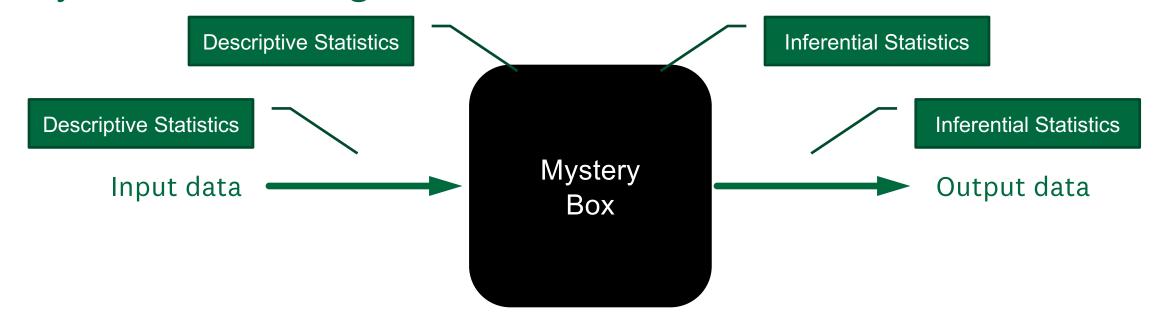
Making **predictions** based on a mess that represents a larger mess



Basics Intro

Descriptive Statistics
Inferential Statistics

Every machine learning model, ever:





Random Process, Variable, Data

Data: Recorded pieces of information

Random Variable: The underlying characteristic or quantity observed through data

Random Process:

- Assigning a value (data) to a variable randomly
- random ≠ arbitrary
- The deterministic internals of the process are not known
- The process is described by how likely it is to observe a specific value



Descriptive Statistics Sample, Population

Population:

The entirety of a group of interest (e.g., everyone at Dartmouth)

Sample:

 The relatively few examples from the population that were observed (e.g., survey respondents)



Types of data

Data: Recorded pieces of information

Variable: The underlying characteristic or quantity observed through data

Activity:

We want to statistically describe the population of people at Dartmouth to a machine learning model.

Pair up and identify some variables that may help us do that



Types of data

- Categorical data (qualitative)
 - Data which can be divided into groups
 - A May have inherent order (ordinal scale) or not (nominal scale)
- Numerical data (quantitative)
 - · Data which is in the form of numbers with mathematical meaning
 - Can be discrete (e.g., the count of books) or continuous (e.g., the cost of books)



Descriptive Statistics Visualizing Data

Example:

- Rolling a six-sided die
- 100 observations (i.e., rolls)
- How can we visualize the results in a diagram?
- What would you expect to see?

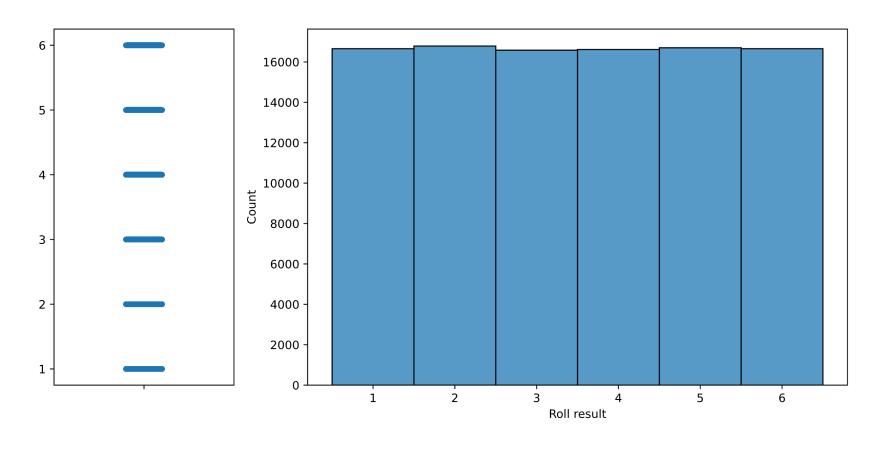


Descriptive Statistics Visualizing Data

Demo



Visualizing Data: Discrete uniform distribution





Descriptive Statistics Visualizing Data

- Example:
 - Rolling multiple six-sided dice
 - 100 observations (i.e., rolls)
- What would you expect to see now?

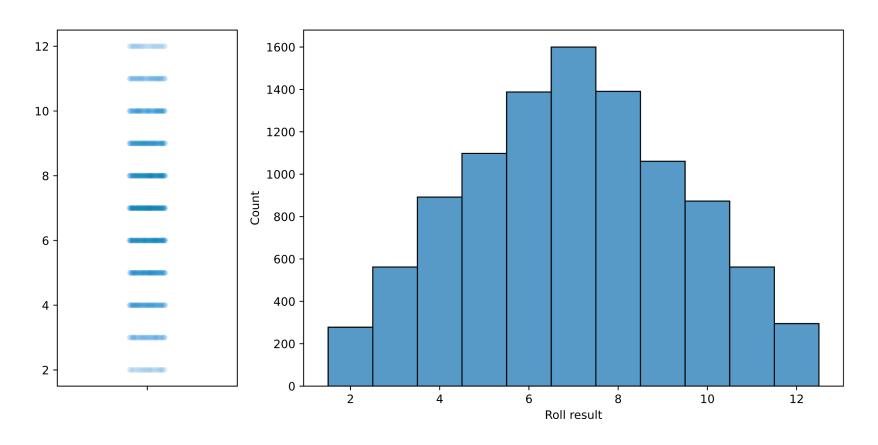


Descriptive Statistics Visualizing Data

Demo

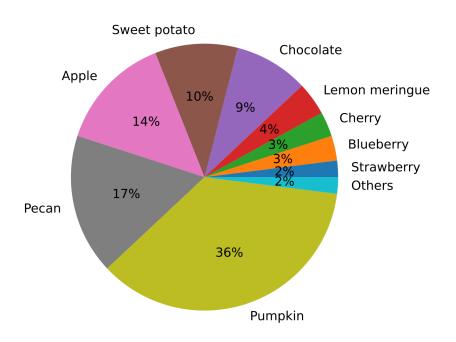


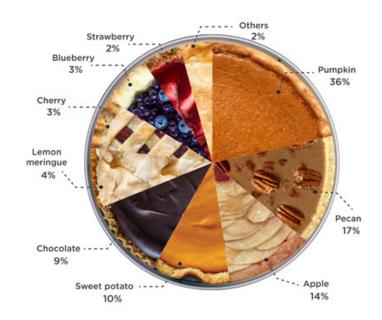
Visualizing Data: Discrete non-uniform distribution





Descriptive Statistics Visualizing Data: Categorical distribution





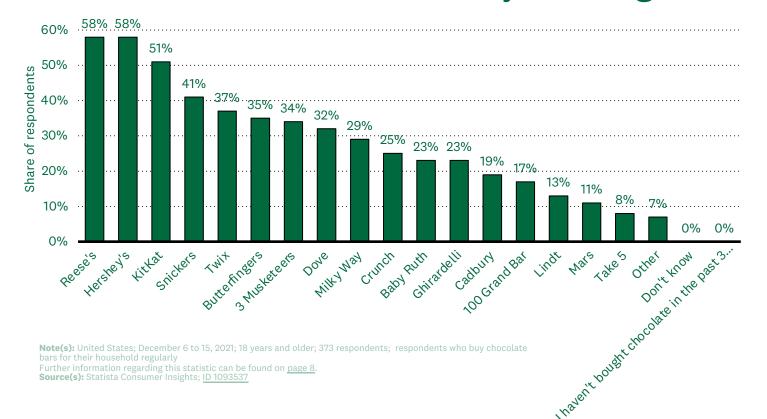
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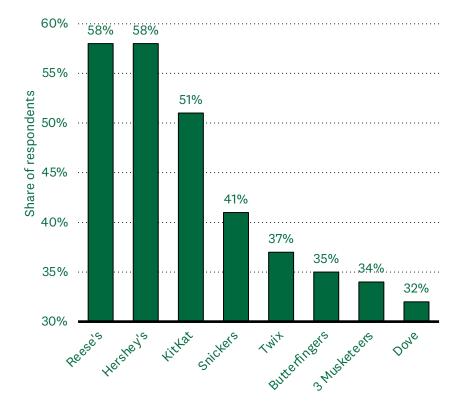
Thanksgiving Pie Survey Breaks Down America's Favorites. (2017). Delta Dental. URL: https://www.deltadental.com/us/en/about-us/press-center/2017/thanksgiving-pie-survey-breaks-down-america-s-favorites.html



Visualizing Data: Categorical distribution

"Which chocolate bars have you bought in the past 3 months?"







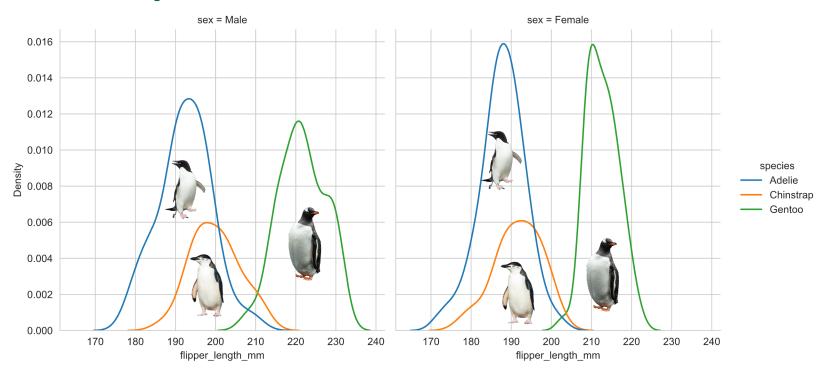
Descriptive Statistics Summarizing data Challenge:

- We cannot define a deterministic function that describes the observed data
- How can we provide a compact representation of the sample?



Descriptive Statistics Summarizing data

Activity: How would you describe these observed distributions?





Descriptive Statistics Summarizing data

- Percentiles
 - How do the observations spread out?
- Measures of Central Tendency
 - What is a "typical" observation?
- Measures of Variability
 - How much do observations vary from the "typical" one?



Summarizing data: Percentiles

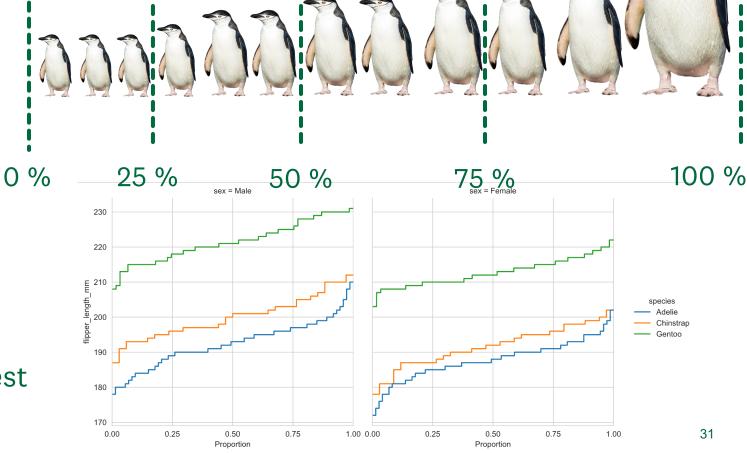
1. Sort the data ascendingly





Summarizing data: Percentiles

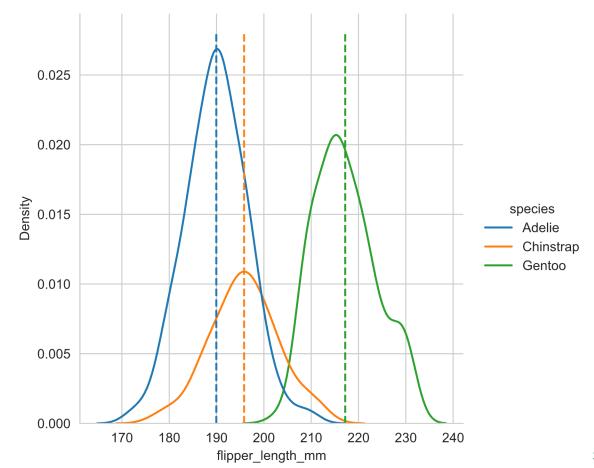
- 1. Sort the data ascendingly
- 2. Divide the data into groups
 - Four groups: quartiles
 - Five groups: quantiles
 - X groups: 1/X percentiles
- 3. The five magic numbers:
 - Lowest, 25 %, 50 %, 75 %, Largest





Summarizing data: Measures of Central Tendency

- Mean:
 - 1. Sum up all observations
 - 2. Divide by number of observations
- Interpretation:
 - Typical observation





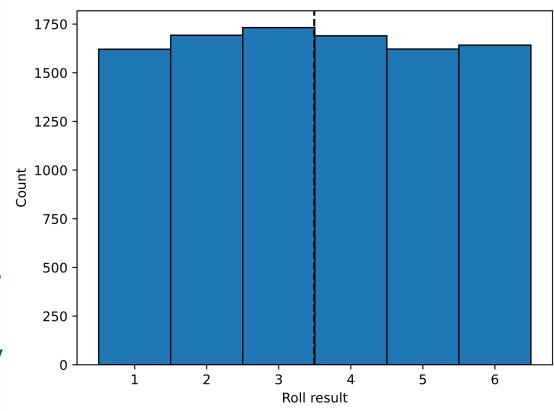
Summarizing data: Measures of Central Tendency

Mean:

- 1. Sum up all observations
- 2. Divide by number of observations

Interpretation:

- Typical observation
- Expected value: "If you expect this value, you are probably the least wrong"
- No guarantee that this value was actually observed!





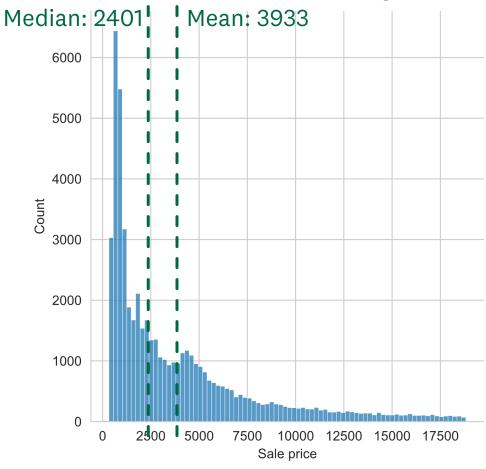
Summarizing data: Measures of Central Tendency

Median:

- 1. Sort all observations
- Pick the one in the middle

Interpretation:

- Typical example from the dataset
- Half of the observations are smaller, half are bigger





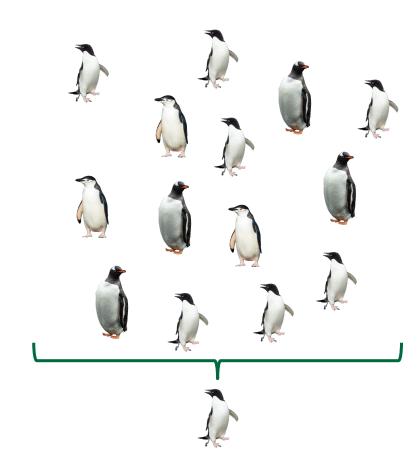
Summarizing data: Measures of Central Tendency

Mode:

- 1. Count each occurrence of a value
- 2. The most frequent one is the 'mode'

Interpretation:

 The value you are most likely to observe if you pick an example from the sample at random





Summarizing data: Measures of Central Tendency

	Mean	Median	Mode
Interpretation:	"Least-error expectation"	Half-way point in the data	Most likely to observe this
Defined for:	Numeric data	Sortable data	Categorical

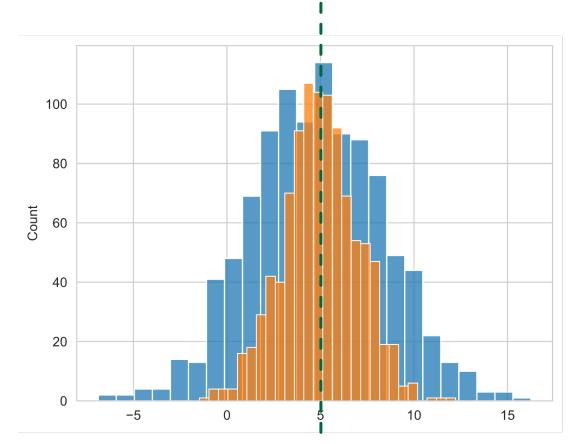


Summarizing data: Measures of Variability

• Two distributions with the same mean ($\mu = 5.0$)

Question:

What makes them different?

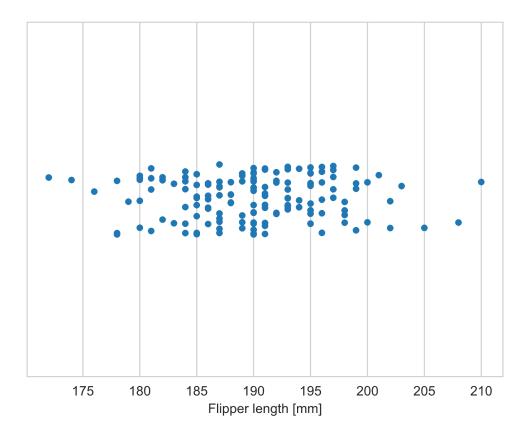




Summarizing data: Measures of Variability

Question:

How would you describe the spread of the data?





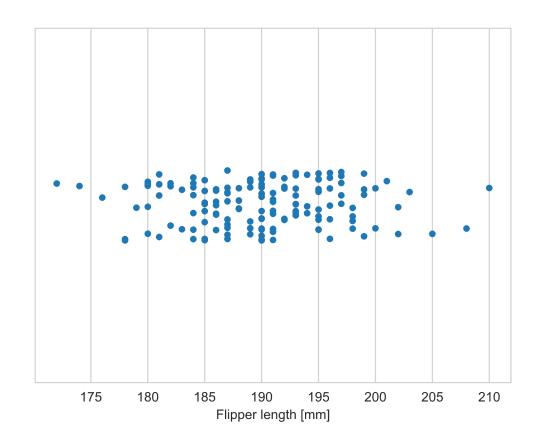
Summarizing data: Measures of Variability

Question:

How would you describe the spread of the data?

Some options:

- Range (largest minus smallest observed value)
 - Spread of the data overall
- Interquartile range (75th percentile 25th percentile)
 - Spread of the middle half of the data





Summarizing data: Measures of Variability

Question:

How would you describe the spread of the data?

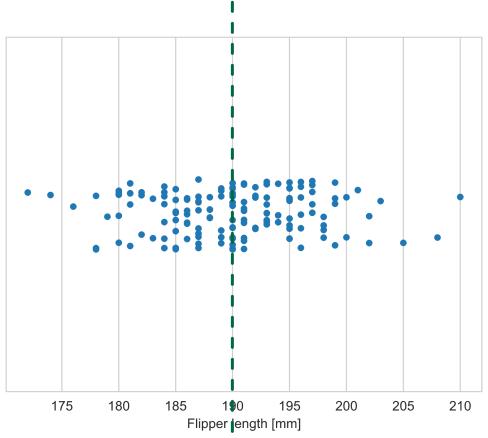
The most popular option:

Average deviation of an observation from the mean

a.k.a.

standard deviation σ

Since we don't want positive and negative differences to cancel out, we calculate the average of the squared difference (the $variance \sigma^2$) and then take the square root again



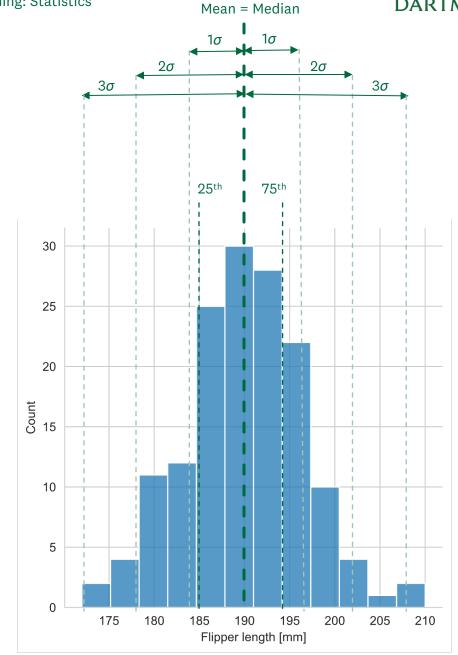
Mean



Descriptive Statistics Normal is special

What makes a distribution "normal"?

- The mean and the median are approximately the same
- The 25th and 75th percentile are approximately the same distance from the mean
- 68 % of data are within 1 standard deviation of the mean,
 95 % of data are within 2 standard deviations of the mean,
 99.7 % of data are within 3 standard deviations of the mean
 - The "68-95-99.7 rule"



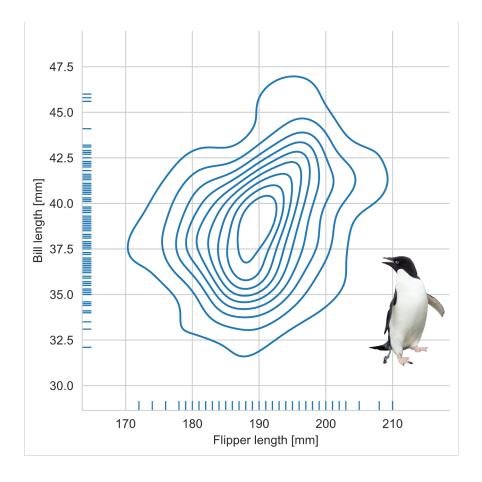


Descriptive Statistics Multivariate distributions

- We usually describe an "object" to a machine learning model using multiple variables
- So far, we have only looked at the properties of a single variable (univariate statistics)
- We can also describe the distribution of multiple variables together (multivariate statistics)

Example:

The distribution of flipper and bill length of Adelie penguins





Basic Ideas

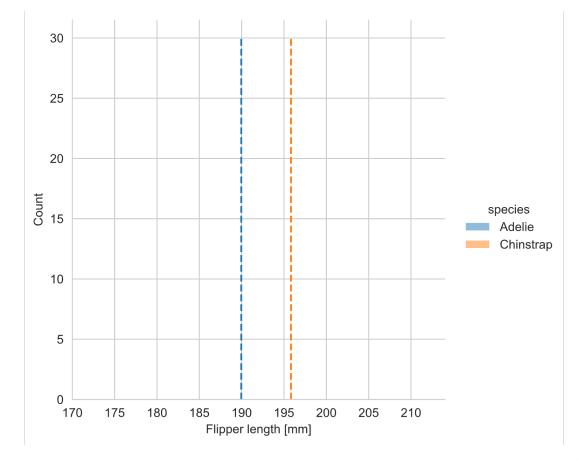
- 1. How can you tell if two samples are different?
 - Hypothesis testing
- 2. How can you make assumptions based on the data you have seen?
 - Extrapolations and predictions
 - Regression and classification

Part of the next two sessions



Inferential Statistics Hypothesis Testing

- You have two samples
- Are they different on average?



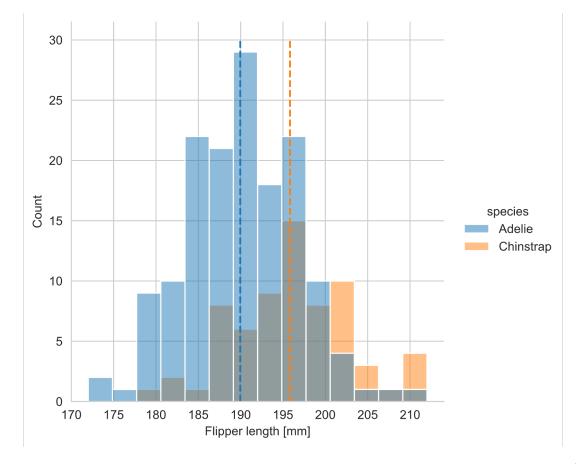


Hypothesis Testing

- You have two samples
- Are they different on average?

Hypothesis testing workflow:

- 1. Formulate a hypothesis
 - "These samples are from the same underlying distribution and just happen to be different because of random chance"
- 2. Calculate the difference between the means
- 3. Take the variance and the number of observations into account
- 4. Calculate how likely it is that the hypothesis is false (p value)
- 5. Compare with a threshold probability *alpha* (e.g., 5 %)
- 6. Call it "significant" if p is less than alpha

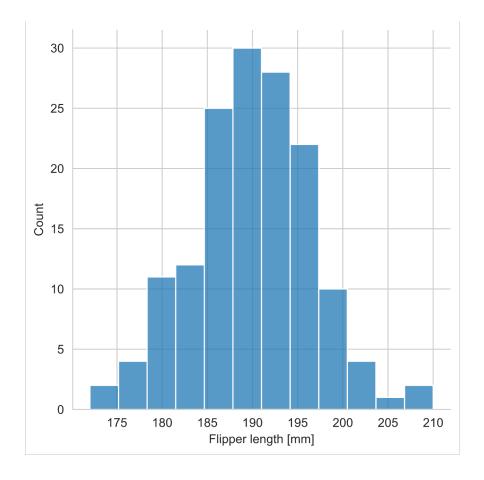




Making predictions

Naïve predictor

- Guess the flipper length of an Adelie penguin!
- Always go with the central tendency -> High bias
- Go with a random value -> High variance
- Fundamental design dilemma in machine learning:
 Bias-variance tradeoff





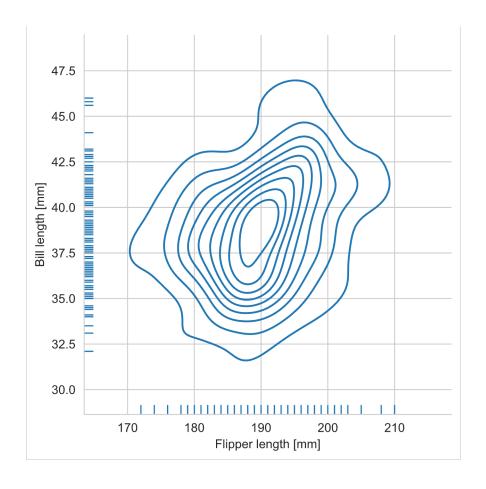
Making predictions

Naïve predictor

- Guess the flipper length of an Adelie penguin!
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- Go with a random value -> High variance
- Fundamental design dilemma in machine learning:
 Bias-variance tradeoff

Conditional predictor

- Given the bill length, guess the flipper length of an Adelie penguin!
- Take a slice through the joint distribution





Critical thinking about statistics

Visualizations

Pie charts:

- Do the percentages add up to (about) 100 %?
- Watch for distortions!
- Check the sample size!

Bar charts:

- Do the units make sense when comparing bars (e.g., number of crimes versus crimes per capita)
- Is the scale appropriate or are small differences visually amplified?



Critical thinking about statistics

Biased Data

Activity:

What may cause the data or the analysis to be biased?

Some ideas:

- Is the measurement technique sufficiently precise?
- Is the observed sample representative of the population?
- Are the researchers objective? Can the analysis be "blinded"?



Critical thinking about statistics

Pitfalls in descriptive statistics

Activity:

How could a sample's statistics be misrepresented?

Some options:

- Small sample size
- Using an unsuitable measure of central tendency
- Not taking the variability into account
- Not checking for significance when comparing samples
- Normal is special!



Summary

Key take-aways

- When you cannot define a deterministic formula to explain a relationship between two variables, we need statistics
- There is no absolute certainty in statistics
- Statistics let us describe a complex object or process in simple terms
- Statistics let us extrapolate from observed and quantified data to "unseen" data



References

Upton, G., & Cook, I. (2008). *A dictionary of statistics*. Oxford University Press. DOI: 10.1093/acref/9780199541454.001.000

Rumsey, Deborah J. (2019). *Statistics Essentials*. 1st edition. Hoboken, NJ: For Dummies.