Data Science: Principles and Practice

Lecture 1: Introduction

Ekaterina Kochmar[1]

[1] Based on slides by Marek Rei

Data Science: Principles and Practice

01 Introduction and motivation

02 Practical basics

03 Course logistics

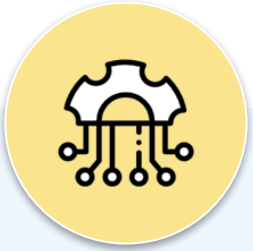
What is Data Science?

Data Processing

crawling
cleaning
connecting

Statistics

measuring
analyzing
exploring



Machine Learning

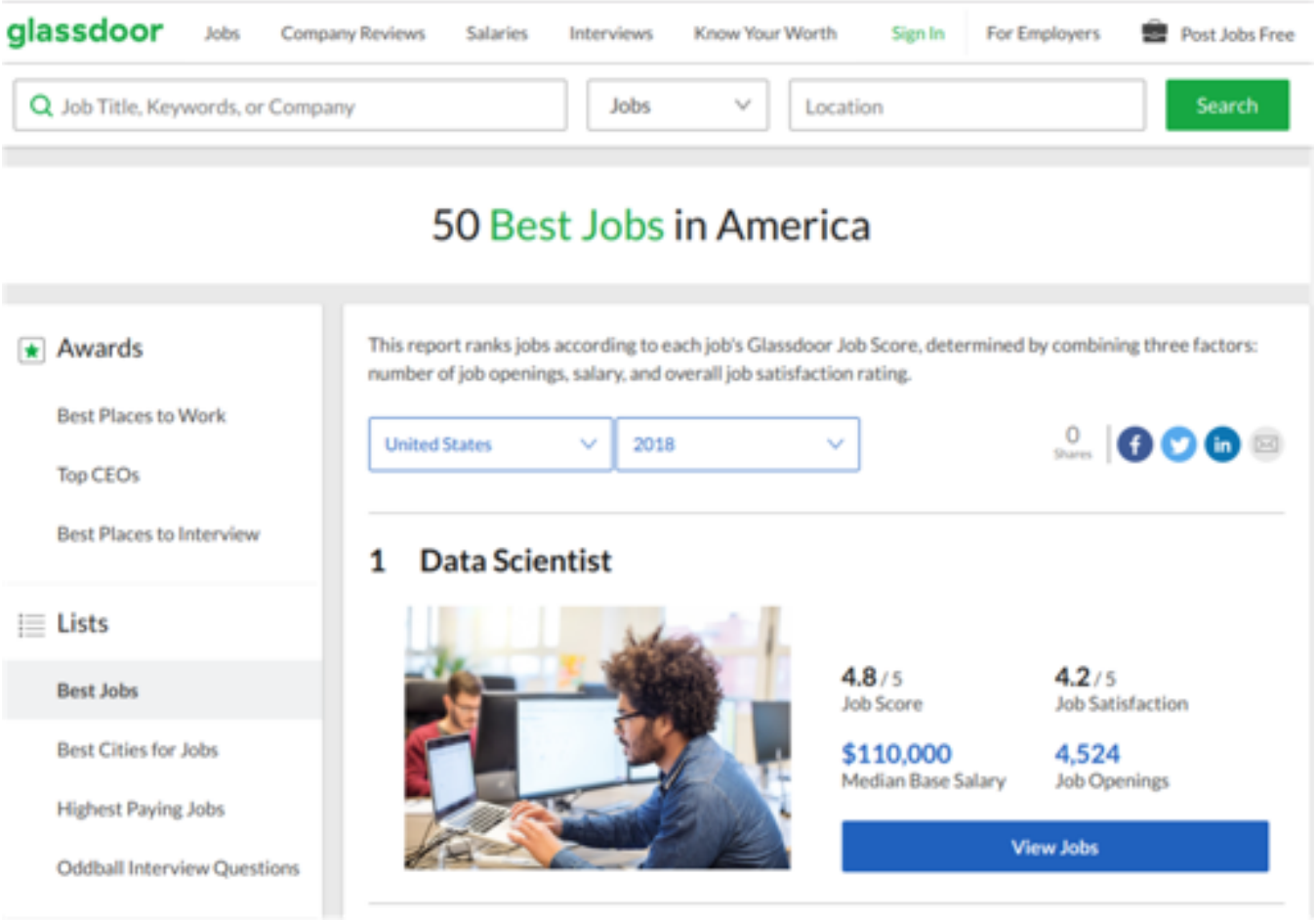
modeling
predicting
simulating

Visuali-zation

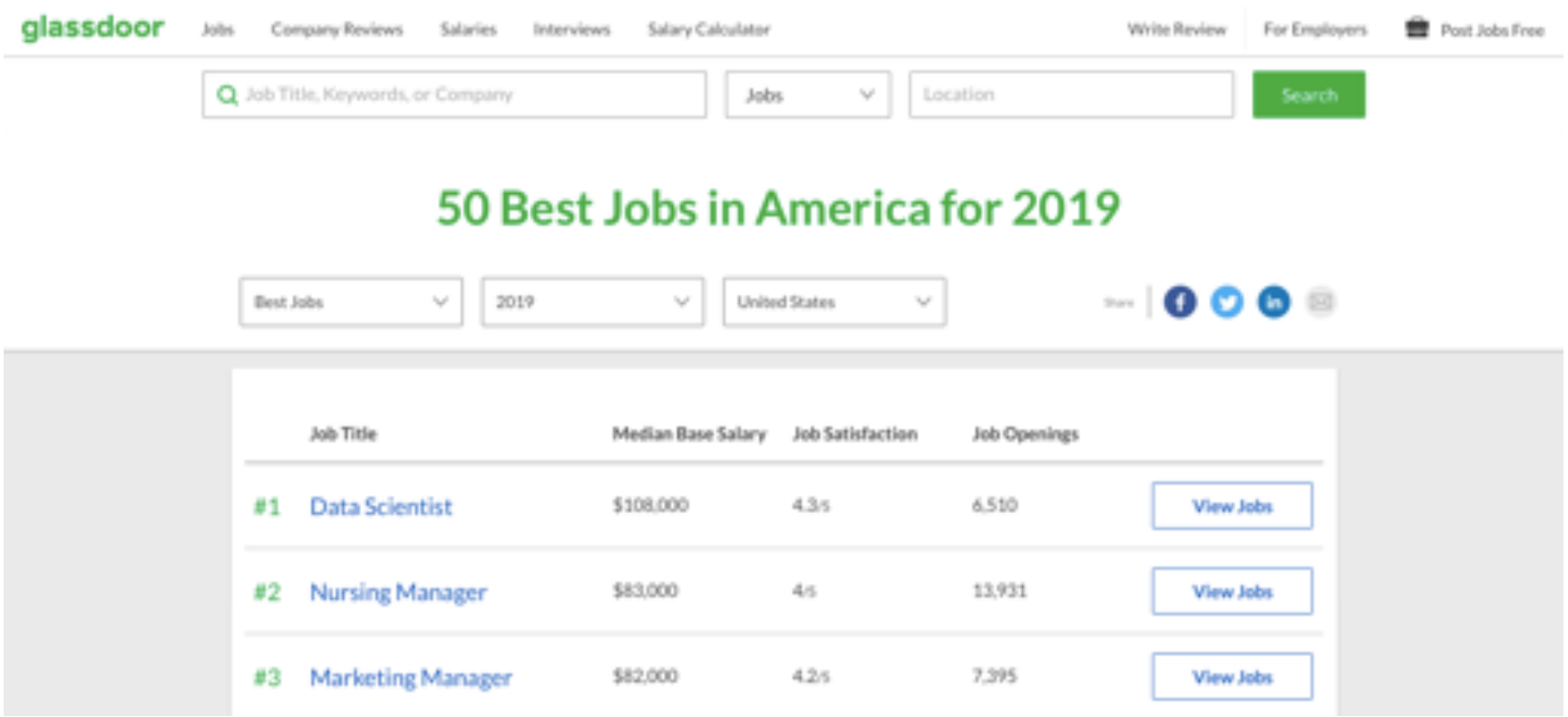
investigating
structuring
presenting

Big Data

processing
parallelizing
optimizing



https://www.glassdoor.com/List/Best-Jobs-in-America-LST_KQ0,20.htm



https://www.glassdoor.com/List/Best-Jobs-in-America-LST_KQ0,20.htm

DATA

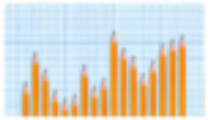
Data Scientist: The Sexiest Job of the 21st Century

by Thomas H. Davenport and D.J. Patil

FROM THE OCTOBER 2012 ISSUE

When Jonathan Goldman arrived for work in June 2006 at LinkedIn, the business networking site, the place still felt like a start-up. The company had just under 8 million accounts, and the number was growing quickly as existing members invited their friends and colleagues to join. But users weren't seeking out connections with the people who were already on the site at the rate executives had expected. Something was apparently missing in the social experience. As one LinkedIn manager put it, "It was like arriving at a conference reception and realizing you don't know anyone. So you just stand in the corner sipping your drink—and you probably leave early."

WHAT TO READ NEXT



What Data Scientists Really Do, According to 35 Data Scientists

VIEW MORE FROM THE
October 2012 Issue

https://hbr.org/2012/10/data-scientist-the-sexiest-job-of-the-21st-century

Data Science as a Field

- In 2006, LinkedIn had just under 8 mln accounts
- **Problem:** people can use their address books (i.e. connect to people they are already in touch with) => further linking opportunities unexplored
- **Solution:** present users with names of people they hadn't yet connected with but are likely to know (e.g., shared their tenures at schools and workplaces)
- **As a result,** the new "People You May Know" feature achieves a click-through rate 30% higher than other prompts on the platform + generates millions of new page views

Regulating the internet giants

The world's most valuable resource is no longer oil, but data

The data economy demands a new approach to antitrust rules

https://www.economist.com/leaders/2017/05/06/the-worlds-most-valuable-resource-is-no-longer-oil-but-data

Case studies

01 Sports

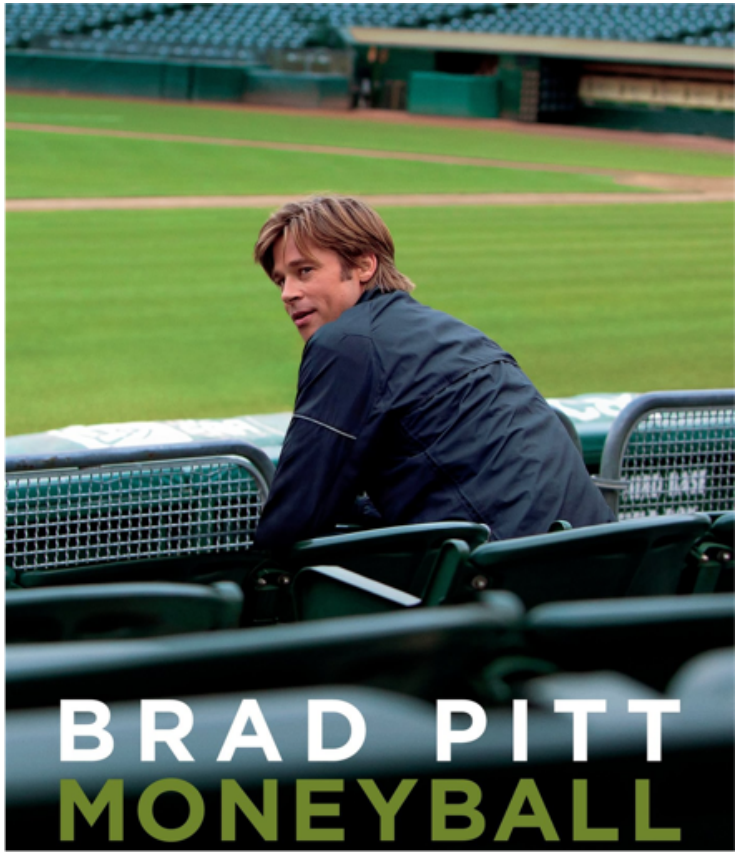
02 Medicine

03 Politics

04 Commerce

05 Climate control

Data Science in Sports



The market for baseball players was so inefficient...
that superior management could run circles around taller piles of cash.
- Michael Lewis

Legendary 2002 season for Oakland Athletics.

Manager Billy Beane put together an unexpected team using data science.

Data Science in Sports

http://adilmoujahid.com/posts/2014/07/baseball-analytics/

Data Science in Drug Discovery

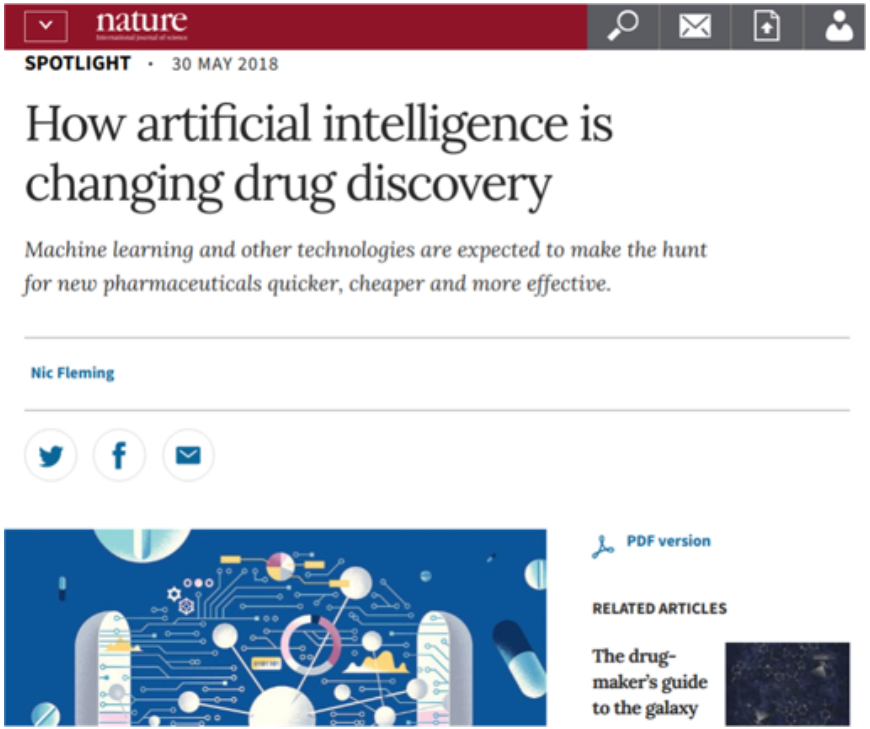
1:10,000 success rate

1:10 success rate

$350M to $5.5B cost

http://sitn.hms.harvard.edu/flash/2017/make-fda-great-trump-future-drug-approval-process/
https://en.wikipedia.org/wiki/Cost_of_drug_development

Data Science in Drug Discovery



nature

SPOTLIGHT · 30 MAY 2018

How artificial intelligence is changing drug discovery

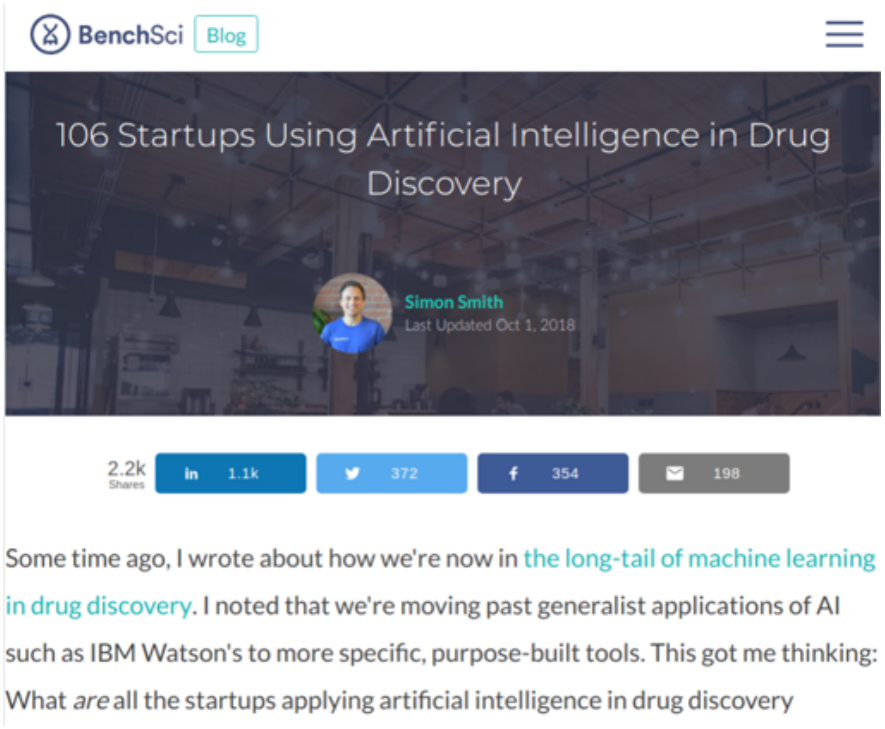
Machine learning and other technologies are expected to make the hunt for new pharmaceuticals quicker, cheaper and more effective.

Nic Fleming

PDF version

RELATED ARTICLES

The drug-maker's guide to the galaxy



BenchSci Blog

106 Startups Using Artificial Intelligence in Drug Discovery

Simon Smith

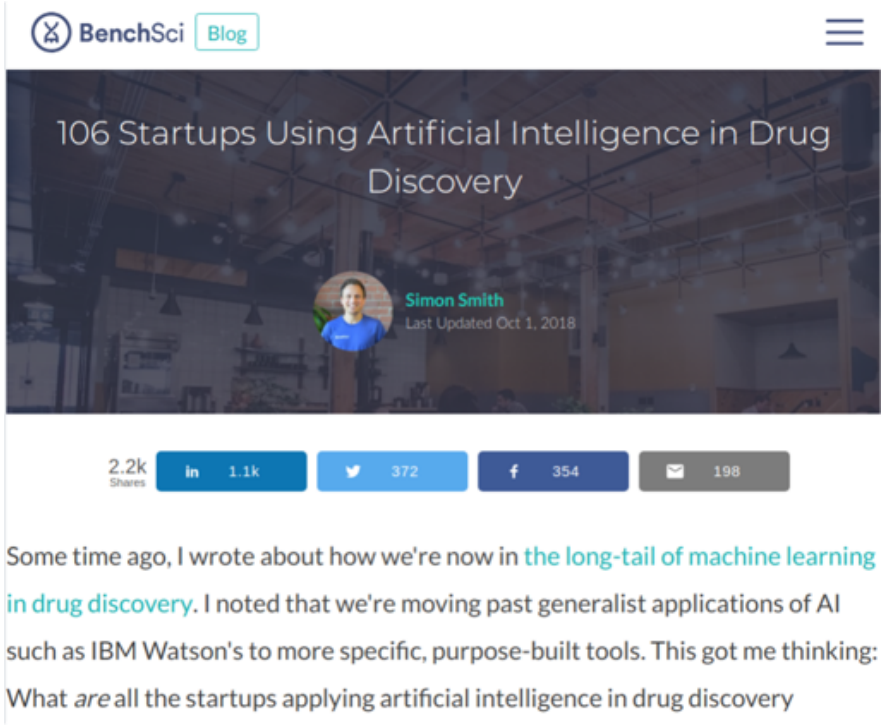
Last Updated Oct 1, 2018

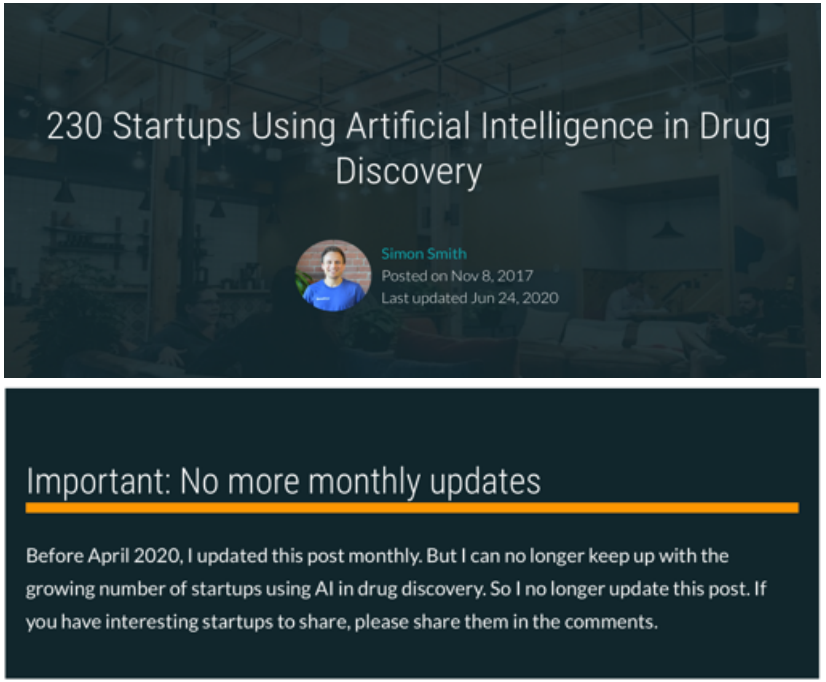
2.2k Shares | in 1.1k | 372 | 354 | 198

Some time ago, I wrote about how we're now in the long-tail of machine learning in drug discovery. I noted that we're moving past generalist applications of AI such as IBM Watson's to more specific, purpose-built tools. This got me thinking: What *are* all the startups applying artificial intelligence in drug discovery

https://www.nature.com/articles/d41586-018-05267-x
https://blog.benchsci.com/startups-using-artificial-intelligence-in-drug-discovery

DS in Drug Discovery: 2018 vs 2020





https://blog.benchsci.com/startups-using-artificial-intelligence-in-drug-discovery

NOV. 4, 2008, AT 6:16 PM

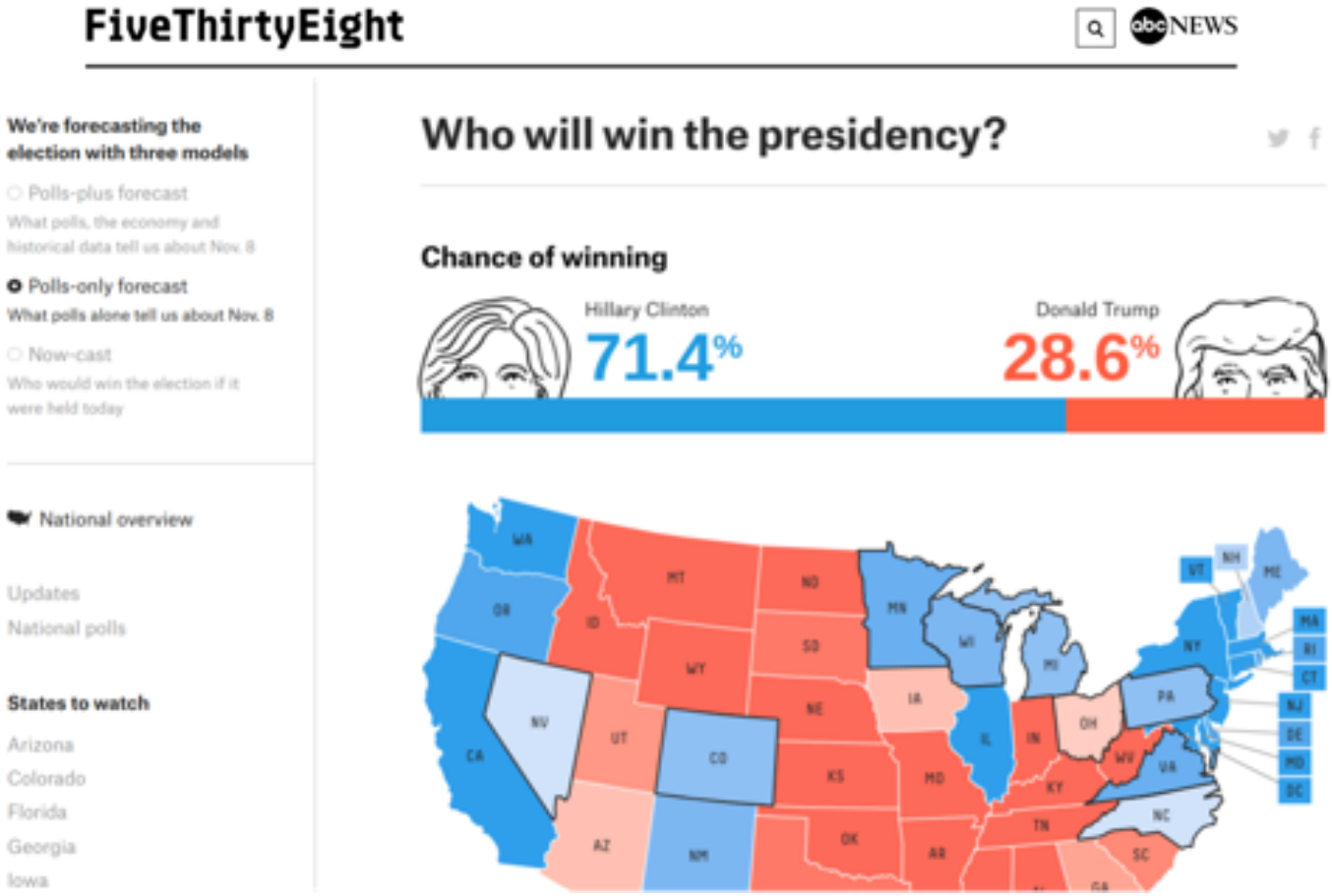
Today's Polls and Final Election Projection: Obama 349, McCain 189

By Nate Silver

It's Tuesday, November 4th, 2008, Election Day in America. The last polls have straggled in, and show little sign of mercy for John McCain. Barack Obama appears poised for a decisive electoral victory.

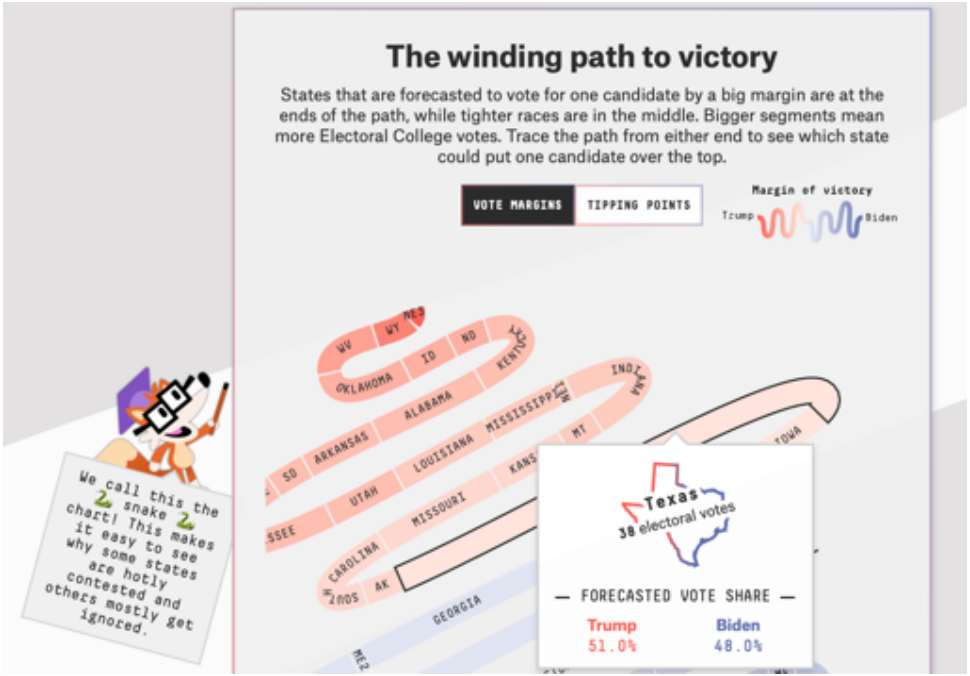
Our model projects that Obama will win all states won by John Kerry in 2004, in addition to Iowa, New Mexico, Colorado, Ohio, Virginia, Nevada, Florida and North Carolina, while narrowly losing Missouri

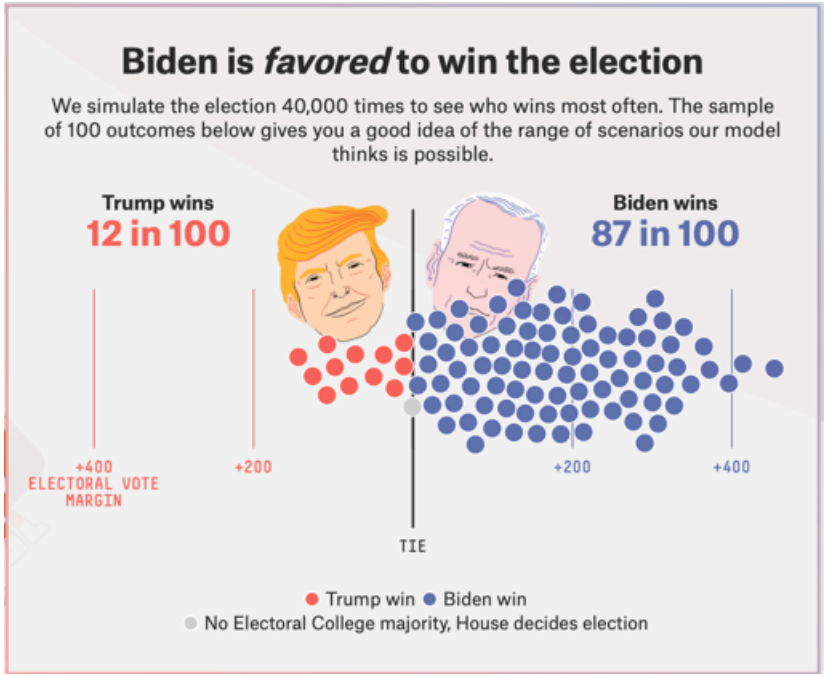
https://fivethirtyeight.com/features/todays-polls-and-final-election/



https://projects.fivethirtyeight.com/2016-election-forecast/

Data Science in Politics



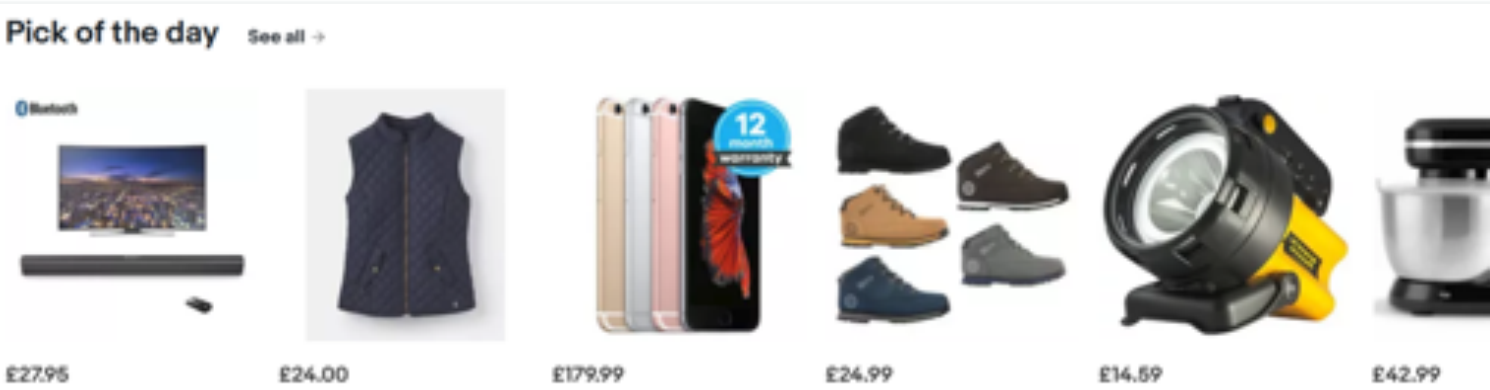


https://projects.fivethirtyeight.com/2020-election-forecast/

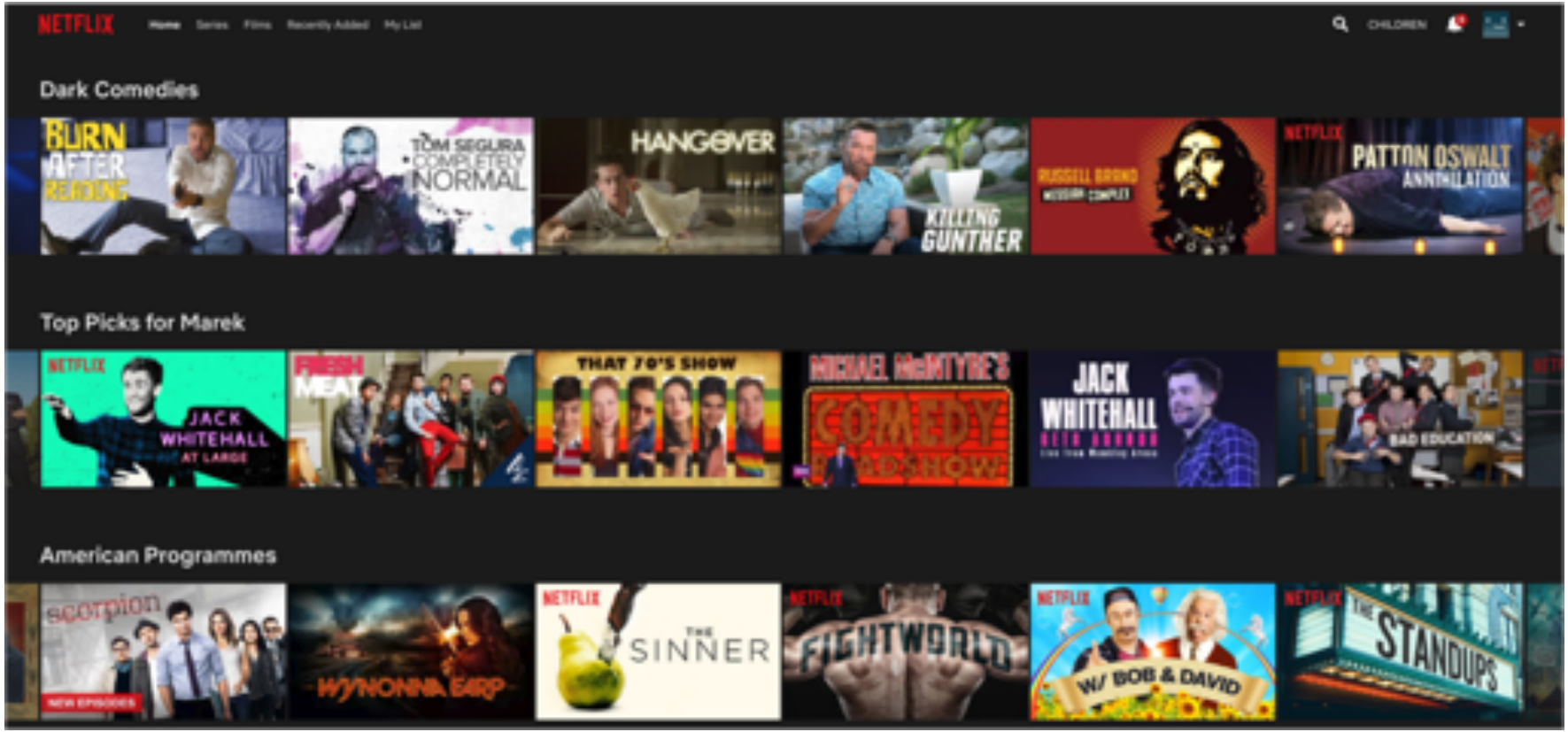
Data Science in Commerce

amazon

ebay



Data Science in Commerce



Netflix Challenge

In 2006, Netflix offered 1 million dollars for an improved movie recommendation algorithm.

Provided 100M movie ratings for training.

The goal: Improve over Netflix's own algorithm by 10% to get the prize.

Several teams joined up and claimed the prize on in 2009.

movie	user	date	score
1	56	2004-02-14	5
1	25363	2004-03-01	3
2	855321	2004-07-29	3
2	44562	2004-07-30	4
3	42357	2004-12-10	1
3	1345	2005-01-08	2

Data Science in Climate Control

How Data Science can help solve Climate Change

Data-driven solutions will lead the Transition to Clean Energy

Marco Pasini Follow

Aug 21 · 6 min read ★

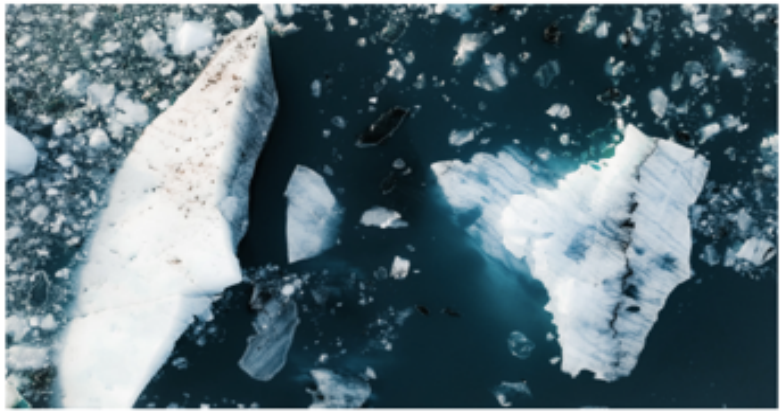
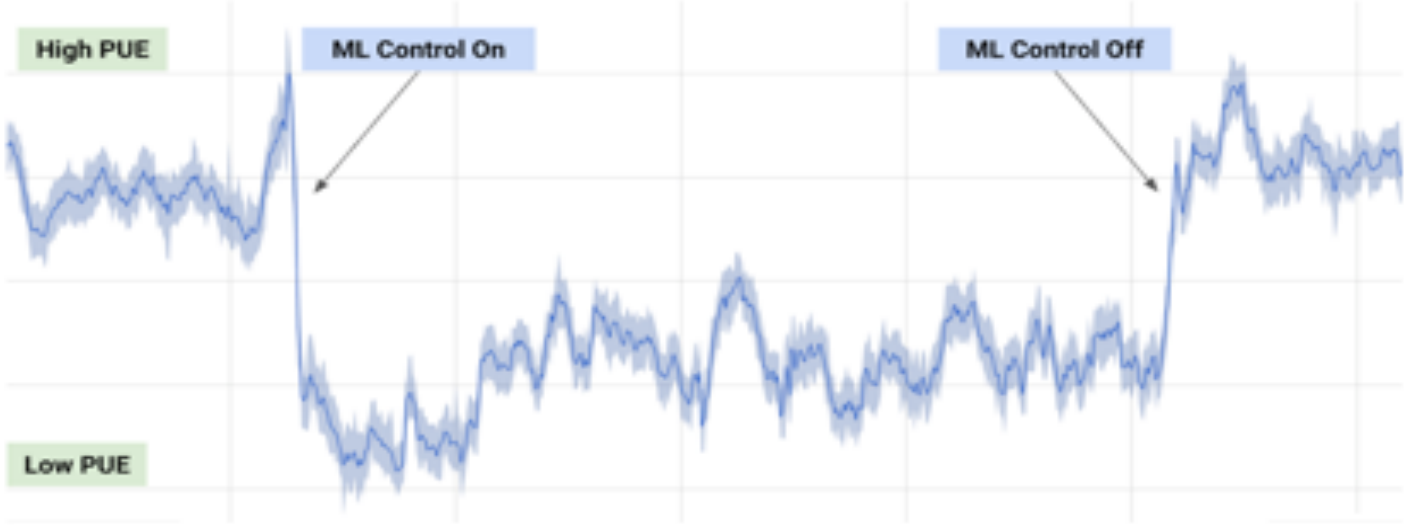


Photo by Bogdan Pasca on Unsplash

https://towardsdatascience.com/how-data-science-can-help-solve-climate-change-12b28768e77b

Data Science in Climate Control



Our machine learning system was able to consistently achieve a 40 percent reduction in the amount of energy used for cooling, which equates to a 15 percent reduction in overall PUE overhead after accounting for electrical losses and other non-cooling inefficiencies. It also produced the lowest PUE the site had ever seen.

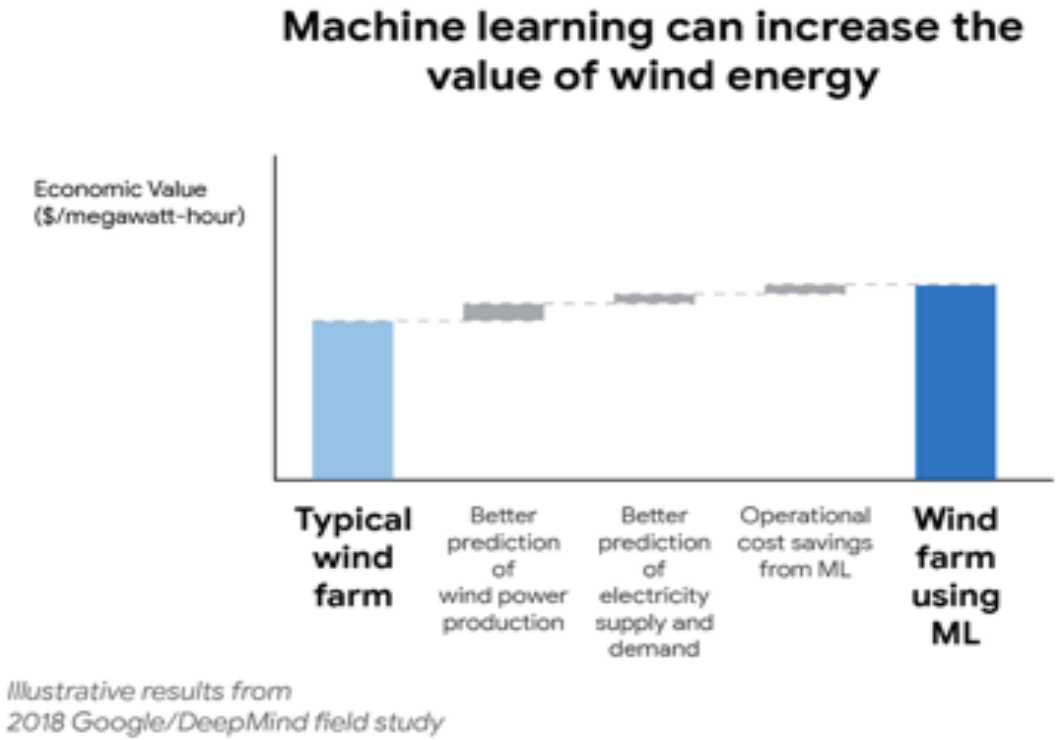
https://deepmind.com/blog/article/deepmind-ai-reduces-google-data-centre-cooling-bill-40

Data Science in Climate Control

A number of **recent studies** propose Reinforcement Learning (RL, a branch of machine learning in which an **agent** interacts with an **environment**, becoming progressively better at a specified **goal** defined by a reward function) as the solution: applying this kind of algorithm to increase efficiency of different buildings shows incredible and **promising results**, with **up to 70% (!!!) reduction** in HVAC energy usage (source).

https://ywang393.expressions.syr.edu/wp-content/uploads/2016/07/Deep-reinforcement-learning-for-HVAC-control-in-smart-buildings.pdf

Data Science in Climate Control



https://deepmind.com/blog/article/machine-learning-can-boost-value-wind-energy

Getting Practical

Using Python. Why Python?

Fast to write and modify

Great for working with datasets

Portable

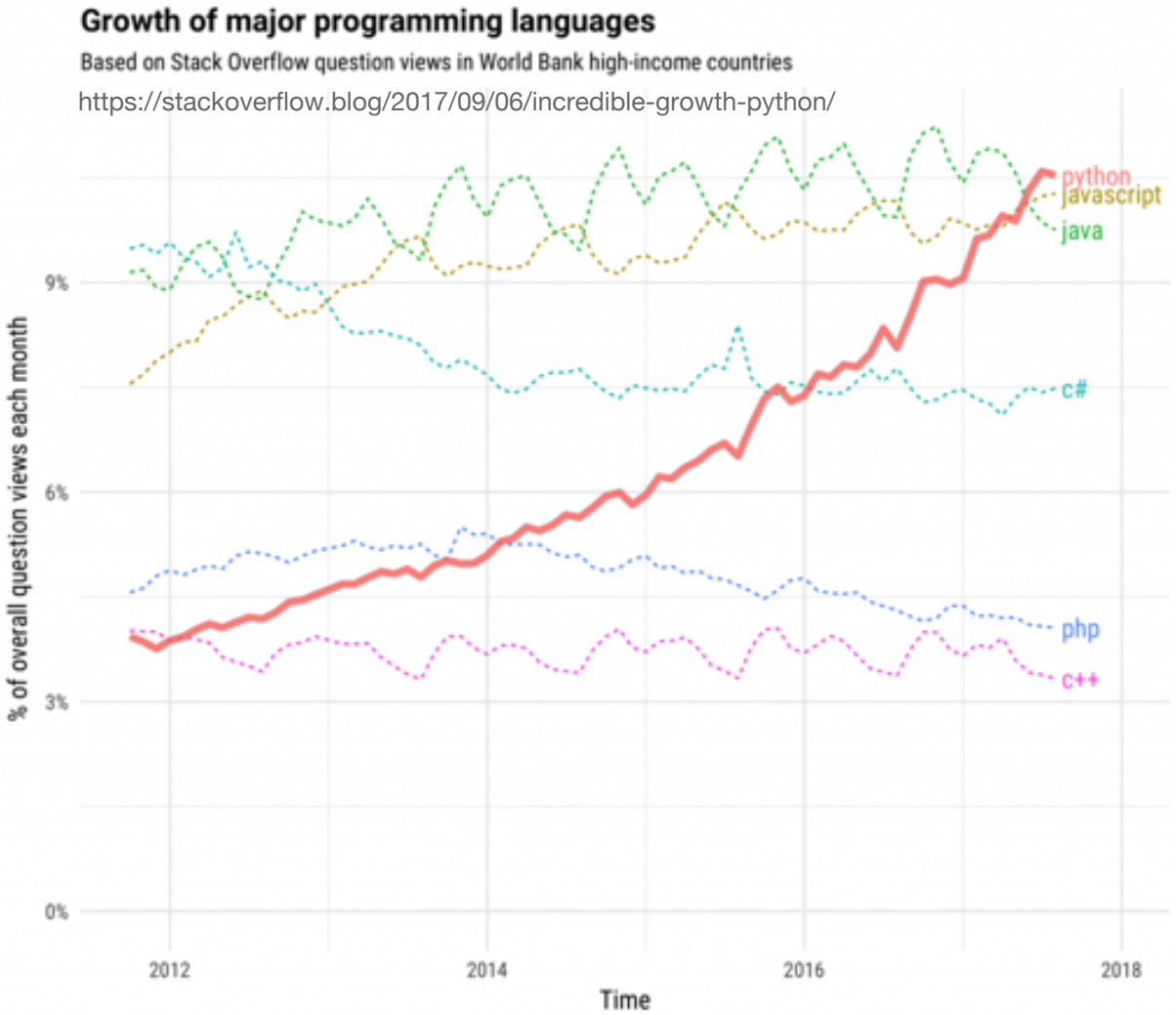
Most machine learning research happens in python

Actually useful for other things besides data science

Dynamically typed (can cause run-time errors)

Not as fast as lower-level languages (sometimes)

Not good for unusual platforms


Growth of major programming languages
Based on Stack Overflow question views in World Bank high-income countries
https://stackoverflow.blog/2017/09/06/incredible-growth-python/
python
javascript
java
c#
php
c++
9%
6%
3%
0%
% of overall question views each month
2012
2014
2016
2018
Time

Using Jupyter Notebooks

- Easy to use and update
- Provides interactive environment
- Portable
- Allows you to combine code with text, images, visualizations, etc.
- Allows you to share your results with others

Installation:

- https://jupyter.org
- https://www.anaconda.com/products/individual

Dataset: Country Statistics

World Bank data about 161 countries

- Country Name
- GDP per Capita (PPP USD)
- Population Density (persons per sq km)
- Population Growth Rate (%)
- Urban Population (%)
- Life Expectancy at Birth (avg years)
- Fertility Rate (births per woman)
- Infant Mortality (deaths per 1000 births)
- Enrolment Rate, Tertiary (%)
- Unemployment, Total (%)
- Estimated Control of Corruption (scale -2.5 to 2.5)
- Estimated Government Effectiveness (scale -2.5 to 2.5)
- Internet Users (%)

Dataset: Country Statistics

```
Country Name,GDP per Capita (PPP USD),Population Density (persons per sq km),Population Growth Rate (%),Urban
Population (%),Life Expectancy at Birth (avg years),Fertility Rate (births per woman),Infant Mortality (deaths
per 1000 births),"Enrolment Rate, Tertiary (%)","Unemployment, Total (%)",Estimated Control of Corruption (scale
-2.5 to 2.5),Estimated Government Effectiveness (scale -2.5 to 2.5),Internet Users (%)
Afghanistan,1560.67,44.62,2.44,23.86,60.07,5.39,71,3.33,8.5,-1.41,-1.4,5.45
Albania,9403.43,115.11,0.26,54.45,77.16,1.75,15,54.85,14.2,-0.72,-0.28,54.66
Algeria,8515.35,15.86,1.89,73.71,70.75,2.83,25.6,31.46,10,-0.54,-0.55,15.23
Antigua and Barbuda,19640.35,200.35,1.03,29.87,75.5,2.12,9.2,14.37,8.4,1.29,0.48,83.79
Argentina,12016.2,14.88,0.88,92.64,75.84,2.2,12.7,74.83,7.2,-0.49,-0.25,55.8
Armenia,8416.82,104.08,0.17,64.16,74.33,1.74,14.7,48.94,18.4,-0.62,-0.04,39.16
Australia,44597.83,2.91,1.6,89.34,81.85,1.87,4.1,83.24,5.2,2,1.61,82.35
Austria,43661.15,102.22,0.46,67.88,81.03,1.42,3.3,71,4.3,1.35,1.66,81
Azerbaijan,10125.23,110.98,1.35,53.89,70.55,1.92,38.5,19.65,5.2,-1.13,-0.79,54.2
Bahrain,24590.49,1701.01,1.92,88.76,76.4,2.12,8.2,33.46,1.1,0.39,0.65,88
Bangladesh,1883.05,1174.33,1.19,28.89,69.89,2.24,33.1,13.15,5,-0.87,-0.83,6.3
Barbados,26487.77,655.36,0.5,44.91,74.97,1.84,16.9,60.84,11.6,1.66,1.45,73.33
Belgium,39751.48,364.85,0.85,97.51,80.49,1.84,3.4,69.26,7.5,1.55,1.59,82
Belize,7936.84,13.87,2.43,44.59,73.49,2.74,15.7,21.37,8.2,0.01,-0.18,25
Benin,1557.16,86.73,2.73,45.56,58.94,5.21,58.5,12.37,0.7,-0.92,-0.53,3.8
Bhutan,6590.69,19,1.68,36.34,67.28,2.32,35.7,8.74,2.1,0.82,0.48,25.43
Bolivia,5195.58,9.53,1.65,67.22,66.63,3.31,39.3,37.69,3.4,-0.7,-0.37,34.19
Bosnia and Herzegovina,9392.47,75.28,-0.14,48.81,75.96,1.25,6.7,37.74,28.1,-0.3,-0.47,65.36
Brazil,11715.7,23.28,0.87,84.87,73.35,1.81,12.9,25.63,6.7,-0.07,-0.12,49.85
Brunei,52482.33,77.14,1.4,76.32,78.07,2.03,6.7,24.34,4.7,0.64,0.83,60.27
Bulgaria,15932.63,67.69,-0.6,73.64,74.16,1.51,10.5,59.63,11.2,-0.24,0.14,55.15
Burkina Faso,1512.97,58.46,2.86,27.35,55.44,5.78,65.8,4.56,3.3,-0.52,-0.63,3.73
Burundi,551.27,371.51,3.19,11.21,53.14,6.21,66.9,3.17,0.5,-1.12,-1.33,1.22
Cambodia,2494.39,82.74,1.76,20.19,62.98,2.93,33.9,14.5,0.2,-1.04,-0.83,4.94
```

Common File Formats

CSV - comma-separated values

```
Bahrain,24590.49,1701.01,1.92,88.76,76.4,2.12,8.2,33.46,1.1,0.39,0.65,88
Bangladesh,1883.05,1174.33,1.19,28.89,69.89,2.24,33.1,13.15,5,-0.87,-0.83,6.3
Barbados,26487.77,655.36,0.5,44.91,74.97,1.84,16.9,60.84,11.6,1.66,1.45,73.33
Belgium,39751.48,364.85,0.85,97.51,80.49,1.84,3.4,69.26,7.5,1.55,1.59,82
```

TSV - tab-separated values

```
Bahrain    24590.49    1701.01    1.92    88.76    76.4    2.12    8.2    33.46
Bangladesh    1883.05    1174.33    1.19    28.89    69.89    2.24    33.1    13.15
Barbados    26487.77    655.36    0.5    44.91    74.97    1.84    16.9    60.84
Belgium    39751.48    364.85    0.85    97.51    80.49    1.84    3.4    69.26
```

Worked Example

Open lecture1.ipynb[1]

[1] Available on https://github.com/ekochmar/cl-datasci-pnp-2021

Python Refresher

In [1]:
```
import random

my_list = ["camel", "elephant", "crocodile"]
for word in my_list:
    print(word + " " + str(random.random()))
```

```
camel 0.5333896529549417
elephant 0.8289440919886492
crocodile 0.5635699354595317
```

Python tutorial: https://www.tutorialspoint.com/python/index.htm

Loading CSV files

In [2]:
```
import pandas as pd

data = pd.read_csv('data/country-stats.csv')
data.head()
```

Out[2]:

	Country Name	GDP per Capita (PPP USD)	Population Density (persons per sq km)	Population Growth Rate (%)	Urban Population (%)	Life Expectancy at Birth (avg years)	Fertility Rate (births per woman)	Infant Mortality (deaths per 1000 births)
0	Afghanistan	1560.67	44.62	2.44	23.86	60.07	5.39	71.0
1	Albania	9403.43	115.11	0.26	54.45	77.16	1.75	15.0
2	Algeria	8515.35	15.86	1.89	73.71	70.75	2.83	25.6
3	Antigua and Barbuda	19640.35	200.35	1.03	29.87	75.50	2.12	9.2
4	Argentina	12016.20	14.88	0.88	92.64	75.84	2.20	12.7

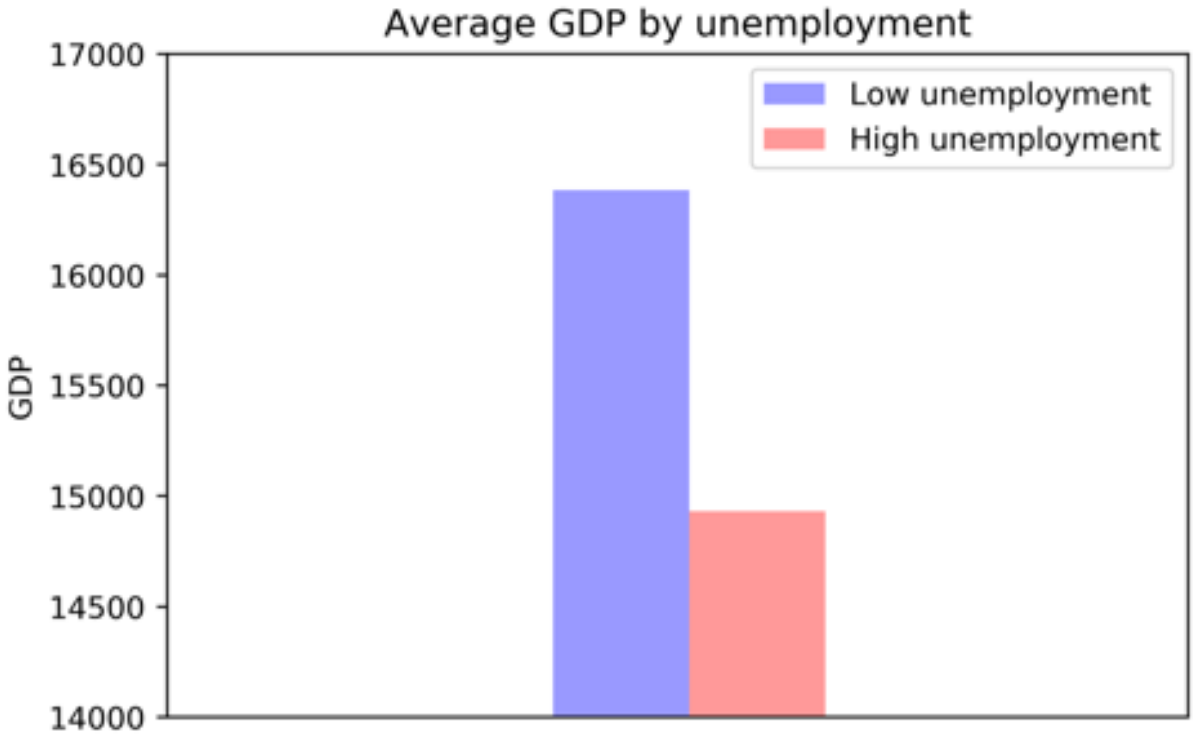
Calculating Statistics over the Data

```
In [3]: data["GDP per Capita (PPP USD)"].mean()
Out[3]: 15616.289378881998
```

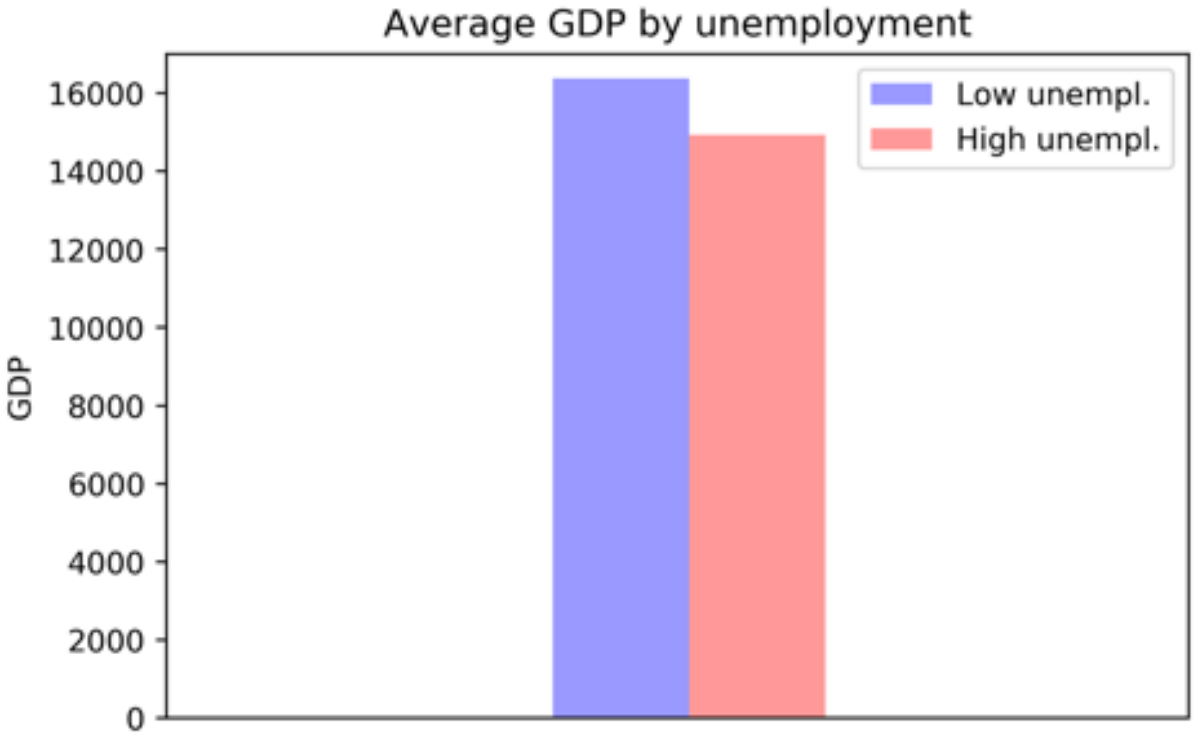
```
In [4]: low_unemployment_countries = data[data["Unemployment, Total (%)"] < 7]
        low_unemployment_countries["GDP per Capita (PPP USD)"].mean()
Out[4]: 16383.713421052627
```

```
In [5]: high_unemployment_countries = data[data["Unemployment, Total (%)"] >= 7]
        high_unemployment_countries["GDP per Capita (PPP USD)"].mean()
Out[5]: 14930.121999999996
```

Calculating Statistics over the Data



Calculating Statistics over the Data



Calculating Statistics over the Data

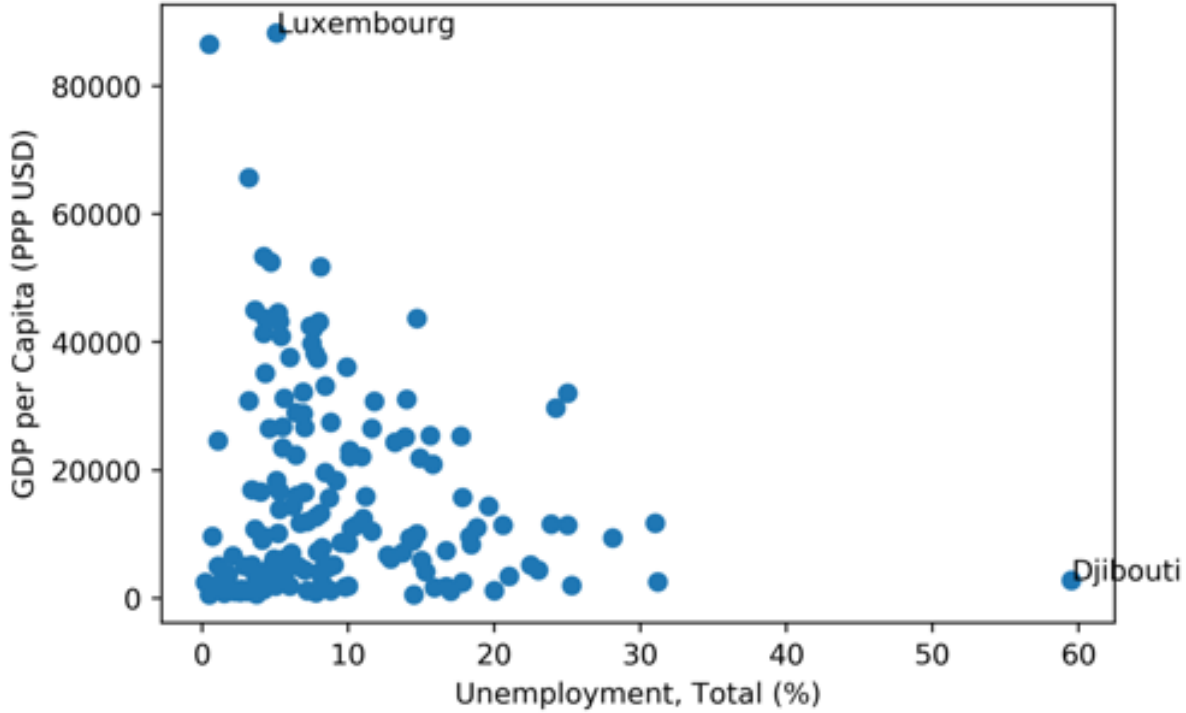
In [9]:
```
low_unemployment_countries = data[data["Unemployment, Total (%)"] < 7]
low_unemployment_countries["GDP per Capita (PPP USD)"].std()
```

Out[9]:
```
19752.912647780504
```

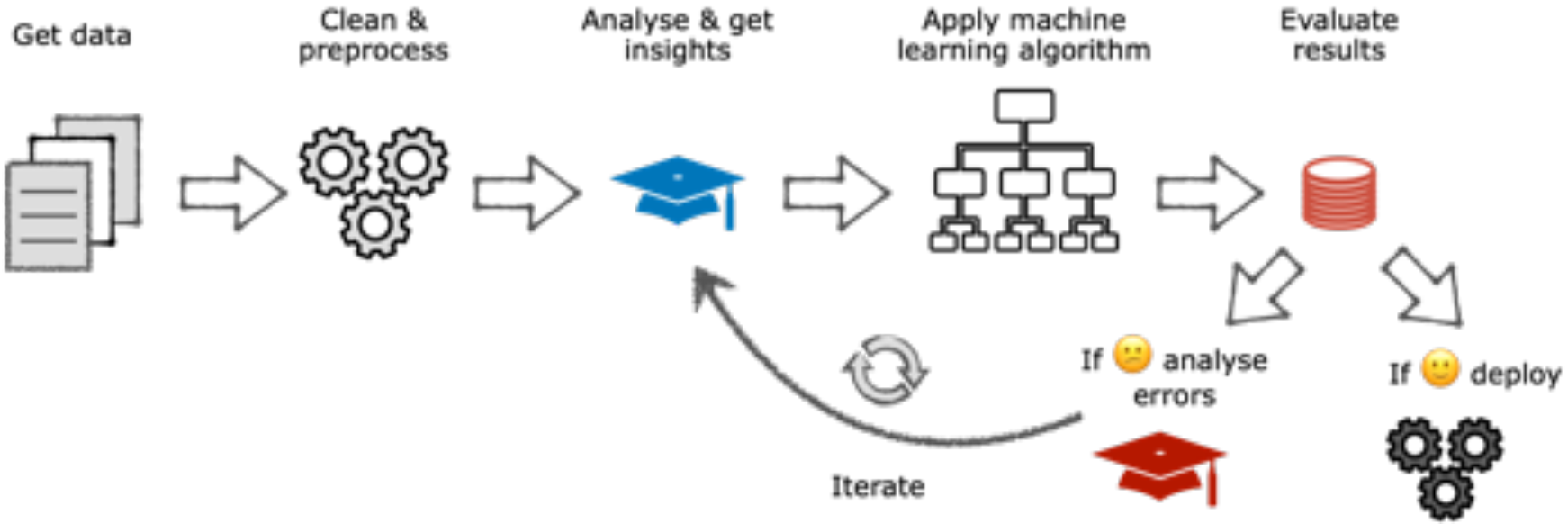
In [10]:
```
high_unemployment_countries = data[data["Unemployment, Total (%)"] >= 7]
high_unemployment_countries["GDP per Capita (PPP USD)"].std()
```

Out[10]:
```
12781.059320722152
```

Calculating Statistics over the Data



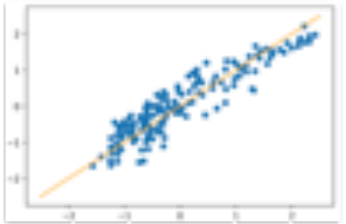
Structuring your DS Project



Machine Learning Overview

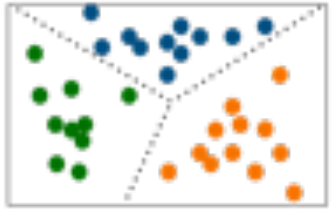
Supervised Learning

- You have access to training data with desired labels
- Learn a function to map observations to labels



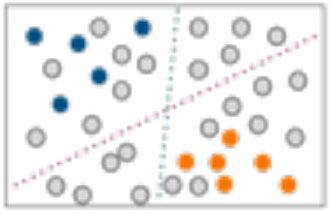
Unsupervised Learning

- Your training data is unlabelled
- Discover structure in data, (ir)regularities, groups of similar instances, etc.



Semi-supervised Learning

- You have a small amount of labelled data and a lot of unlabelled data
- Combine the strengths of both supervised and unsupervised approaches



Reinforcement Learning

- A learning system (*agent*) observes the environment, selects and performs actions, and gets *rewards* / *penalties* in return
- Learns the best strategy (*policy*) by itself

This course will focus on supervised and unsupervised techniques

Course Logistics

Course Objectives

Focusing on the practical aspects of data science

After this course you should be able to

1. Understand the principles of data science
2. Use the necessary software tools for data processing, statistics and machine learning
3. Visualize data, both for exploration and presentation
4. Rigorously analyze your data using a variety of approaches

Course Format

10 lectures

6 practicals

Assessment

- 20% from practicals (pass/fail)
- 80% from take-home assignment

Final assignment

- Practical end-to-end project
- Given out after Lecture 8
- Submit a report
- The report will be marked by two assessors

Course Syllabus

1. Introduction	Friday, 6 November
2. Linear Regression	Monday, 9 November
3. **Practical1:** Linear Regression	Tuesday, 10 November
4. Classification I	Wednesday, 11 November
5. **Practical2:** Classification I	Thursday, 12 November
6. Classification II	Monday, 16 November
7. **Practical3:** Classification II	Tuesday, 17 November
8. Deep Learning Basics	Wednesday, 18 November

Course Syllabus

9. Deep Learning with TensorFlow	Monday, 23 November
10. **Practical4:** DL with TensorFlow	Tuesday, 24 November
11. Deep Learning Architectures	Wednesday, 25 November
12. **Practical5:** DL Architectures	Thursday, 26 November
13. Visualization I	Friday, 27 November
14. Visualization II	Monday, 30 November
15. **Practical6:** Visualization	Tuesday, 1 December
16. Challenges in Data Science	Wednesday, 2 December

Course Pages

Course homepage: https://www.cl.cam.ac.uk/teaching/2021/DataSciII/

Github: https://github.com/ekochmar/cl-datasci-pnp-2021