Case Studies: AI for Drug Discovery

ter.ps/389iweek8

Last week, we discussed:

- Discovery of new therapeutics

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- Timeline from lab research → clinical trials → approval

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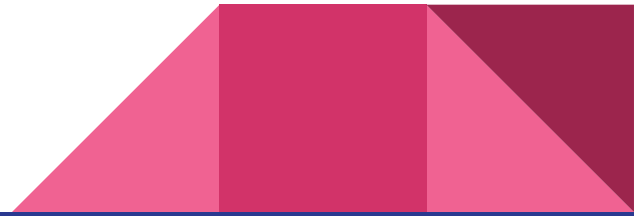
- Discovery of new therapeutics
- Timeline from lab research → clinical trials → approval
- How AI can intervene & accelerate the process

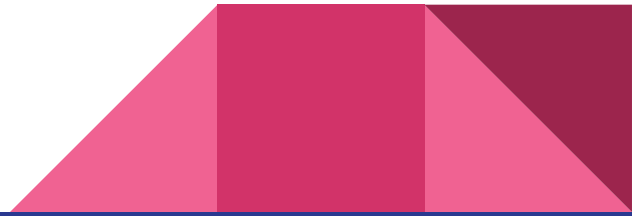
This week

- Exploring examples of current industry initiatives



This week

- Exploring examples of current industry initiatives
- Motivation:



This week

- Exploring examples of current industry initiatives

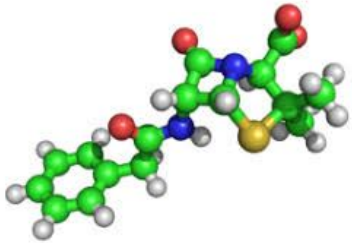
- Motivation:

*Finding **cures** for **diseases** that are lacking!*


FUTURE OF
PHARMA

Compound Libraries for Drug Discovery

- Features describe content, chemistry, and molecular topology
- Encoded by feature vector
  - Number of carbon & nitrogen atoms
  - Hydrogen-bonding donors and acceptors
  - Charges
  - Polar and nonpolar atoms
  - Functional groups (ketone, carboxylic acid, etc.)
  - Which atoms are bonded to which other atoms



https://towardsdatascience.com/predicting-molecular-activity-using-deep-l g-in-tensorf
5b6f8457f9

Many companies are in this space

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


abbvie


AMGEN

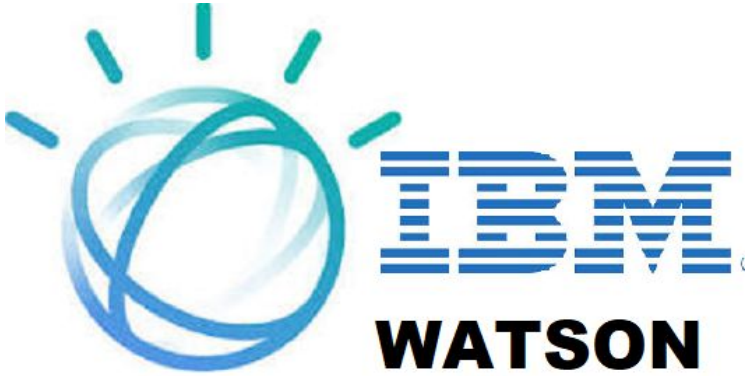

AstraZeneca


Celgene

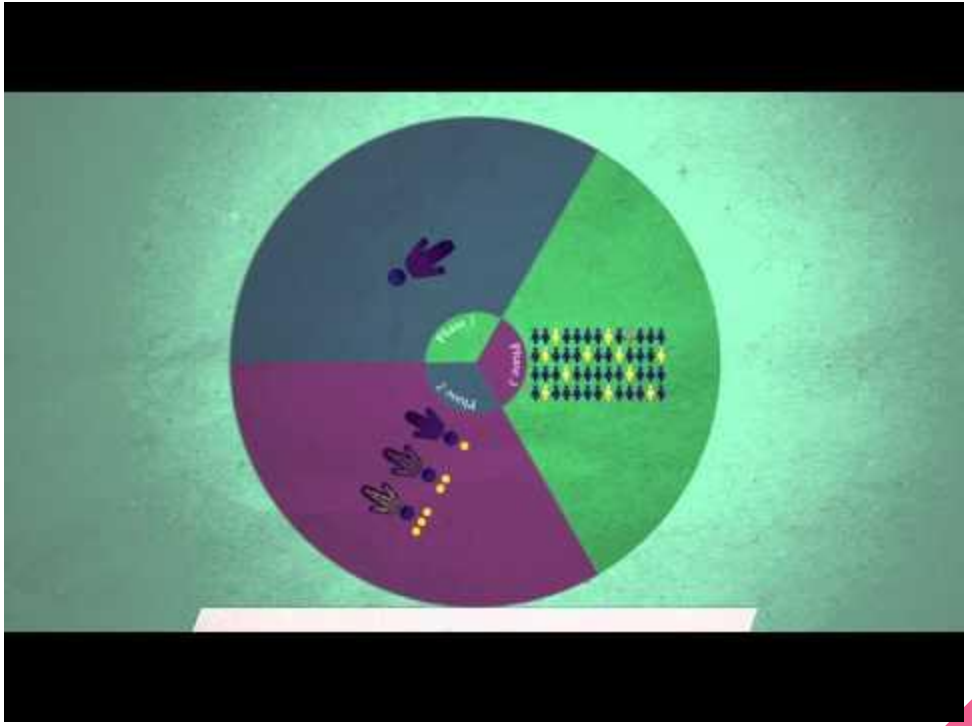

Genentech

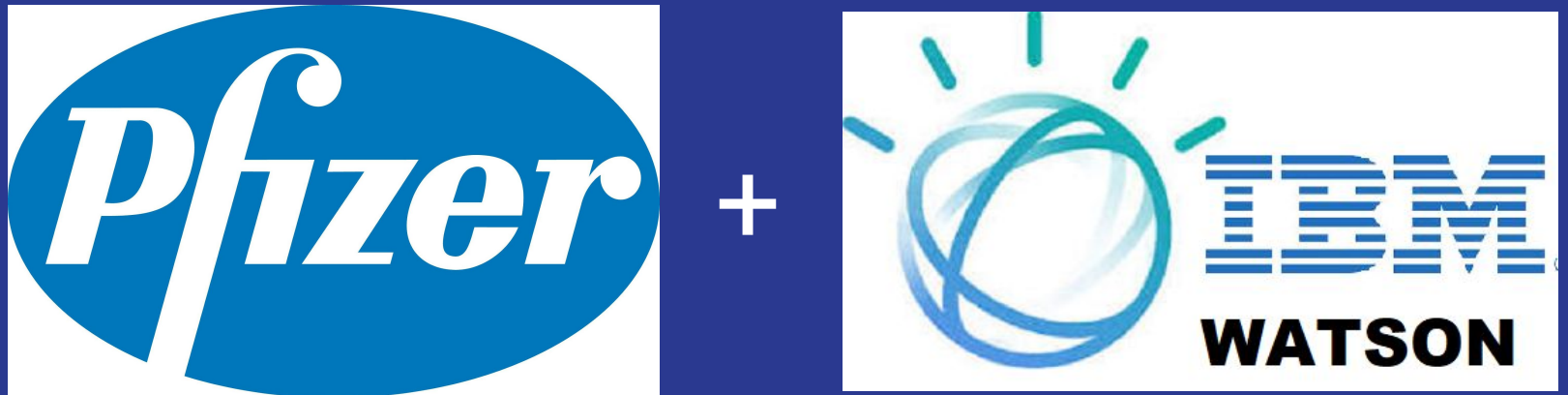

Pfizer


Roche


IBM
WATSON

Industry giants are partnering with smaller startups


Phase 1
Phase 2
Phase 3


Pfizer
+
IBM
WATSON

Pfizer implements IBM Watson

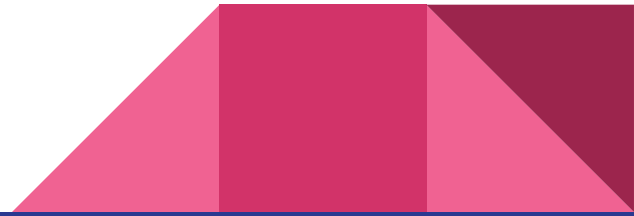
- 2016

- immuno-oncology
  - using immune system to fight cancer

Pfizer implements IBM Watson

Pfizer implements IBM Watson

- Avg. human researcher reads 200-300 science papers/year



Pfizer implements IBM Watson

- Avg. human researcher reads 200-300 science papers/year

- Watson has analyzed
  - 25 million Medline abstracts
  - > 1 million full-text medical journal articles
  - 4 million patents

Combination medicines

Drugs working together > single drugs working alone

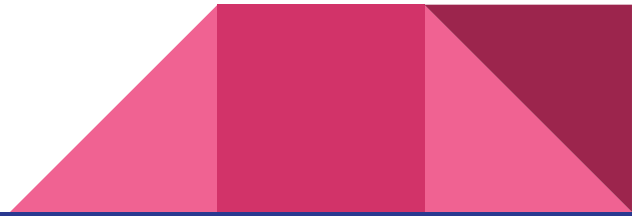
- Synergy
- Target multiple pathways
- Beat drug resistance

Combination medicines: Pfizer

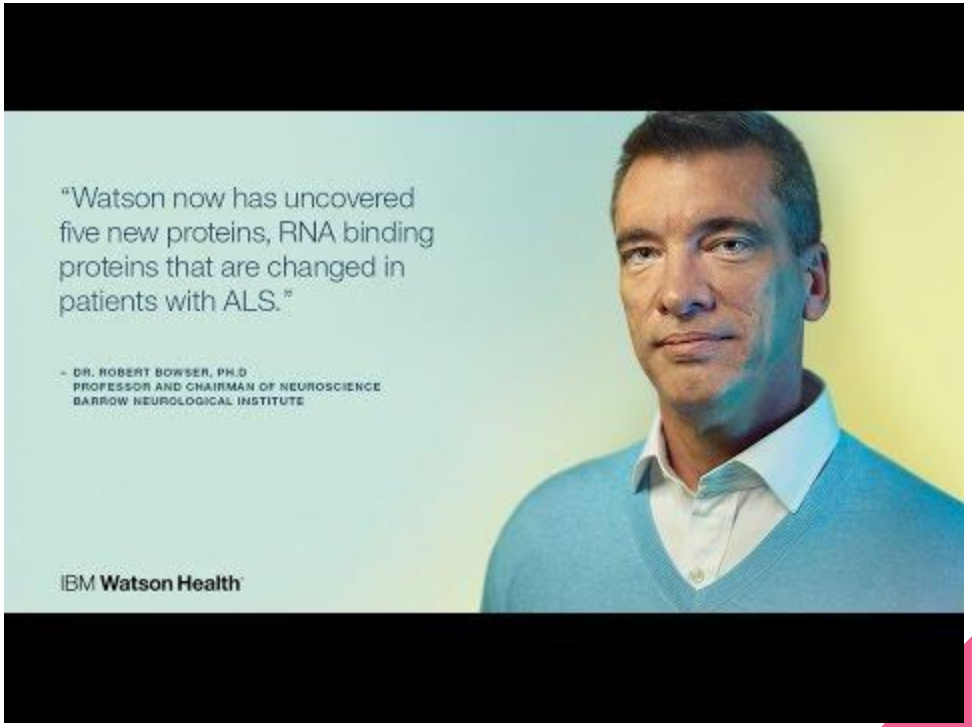
- Best way to fight tumor:

  Combination of drugs to kill tumor via the immune system

- M*any* combinations exist
- IBM Watson → narrow combinations
- Prediction



IBM Watson: ALS



However...IBM Watson in Hot Water

- IBM Watson still has to prove itself!
  - not a generalizable framework

- MD Anderson breakup
  - $62 million, 4 years, no output
  - https://www.technologyreview.com/s/607965/a-reality-check-for-ibms-ai-ambitions/
  - https://thomaswdinsmore.com/2018/02/21/notes-on-a-watson-fail/

Recursion Pharmaceuticals

The latest news from Google AI

Automating Drug Discoveries Using Computer Vision

Thursday, July 12, 2018

Vincent Vanhoucke, Principal Scientist, Google Brain Team

Protein Crystal Identification

“Every time you miss a protein crystal, because they are so rare, you risk missing on an important biomedical discovery.”

- Patrick Charbonneau, Duke University Dept. of Chemistry and Lead Researcher, MARCO initiative.

Neural networks ⟶ >94% accuracy on protein crystal identification

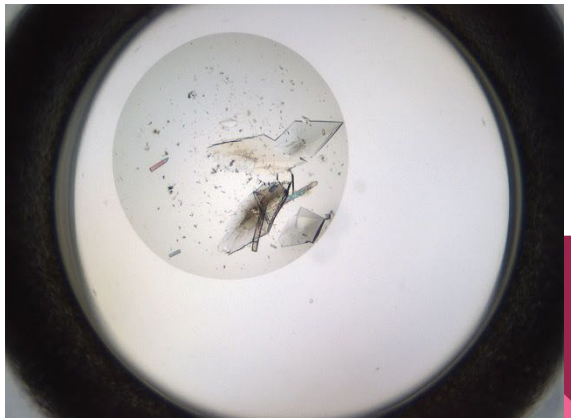


Image of protein crystal, courtesy of the MARCO repository (CC-BY-4.0 license)

How AI Can Speed Up Drug Discovery

https://medium.com/syncedreview/how-ai-can-speed-up-drug-discovery-3c7f01654625

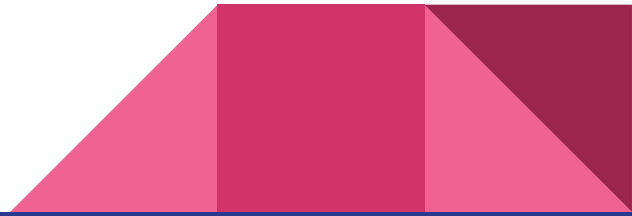
Challenges

Challenges

- Forbes survey:
  “Nearly Half Of All Scientists Are Unfamiliar With AI For Drug Discovery”
- 41% of drug discovery scientists are unfamiliar with AI
- Skepticism

Challenges cont’d

- Even with AI, most drug candidates will still fail
- The goal is to make them fail *less*
  - *proving that the failure rate is slightly smaller requires large datasets*
- Trade secrets



The Promise

- Creating new compounds
- Finding combination medicines
- Discovering new uses of existing medicines
- Personalized medicine

Datasets

- https://www.kaggle.com/uciml/bioassay-datasets
- https://www.kaggle.com/c/MerckActivity/data
- https://www.kaggle.com/c/toxic-molecule-prediction/data

In-Class Activity

Pick ONE to read

https://www.nature.com/articles/nbt0717-604

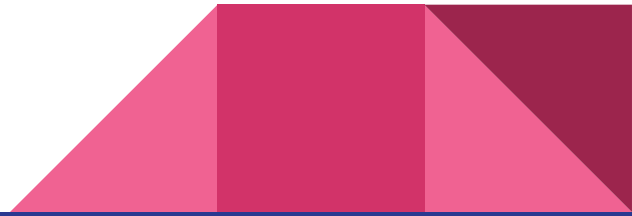
https://www.nature.com/articles/d41586-018-05267-x

Get in groups of 3-4 & discuss

Write down 3 things you learned

Next Week

- Mental health
- Codelab - questions?



Readings

https://www.techemergence.com/machine-learning-drug-discovery-applications-pfizer-roche-gsk/

https://www.forbes.com/sites/forbestechcouncil/2018/02/02/the-top-barrier-to-ai-in-drug-discovery-may-surprise-you/#7af9100d4fd1

https://www.nature.com/articles/d41586-018-05267-x

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https://www.forbes.com/sites/forbestechcouncil/2018/02/02/the-top-barrier-to-ai-in-drug-discovery-may-surprise-you/#7af9100d4fd1