Artificial Intelligence: an introduction

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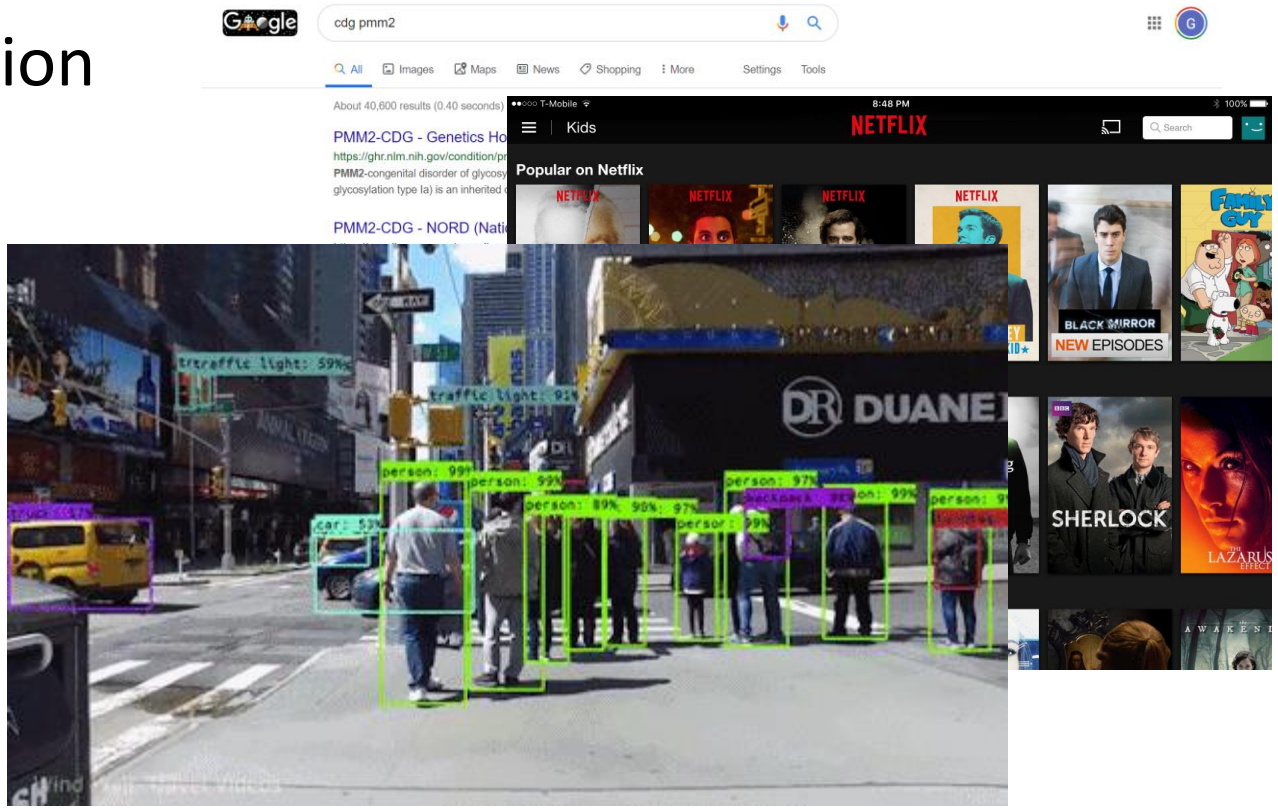
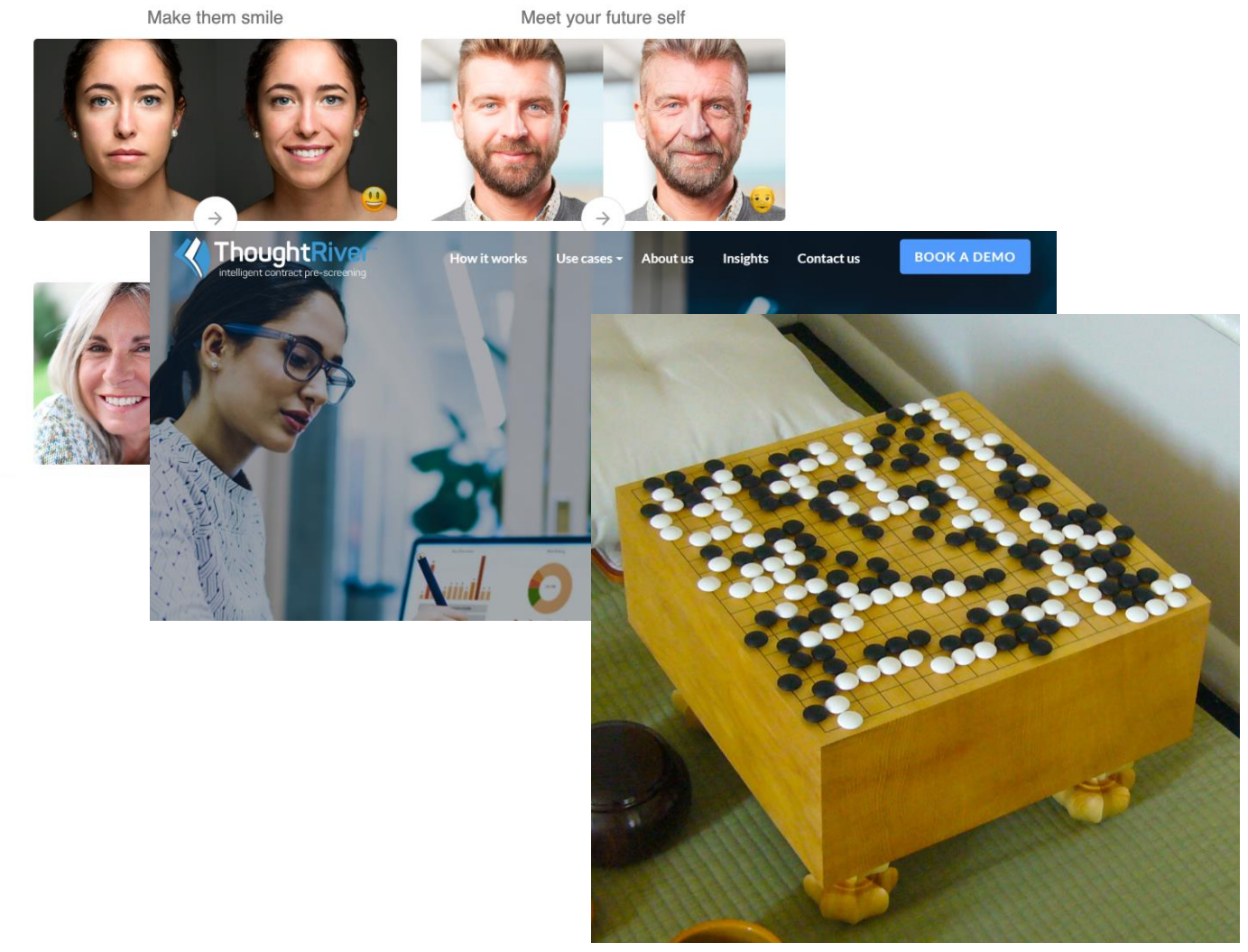
Artificial Intelligence is Everywhere

- Search
- Content Recommendation
- Image Analysis



Artificial Intelligence is Everywhere

- Image Synthesis
- Legal Services
- *Solving* Games



The Aim of Artificial Intelligence?

To design, understand and apply computer programs that learn from experience (*i.e.*, data) for the purpose of modeling, prediction, or control. (Source: Lecture 1 from 6.86x, MIT)

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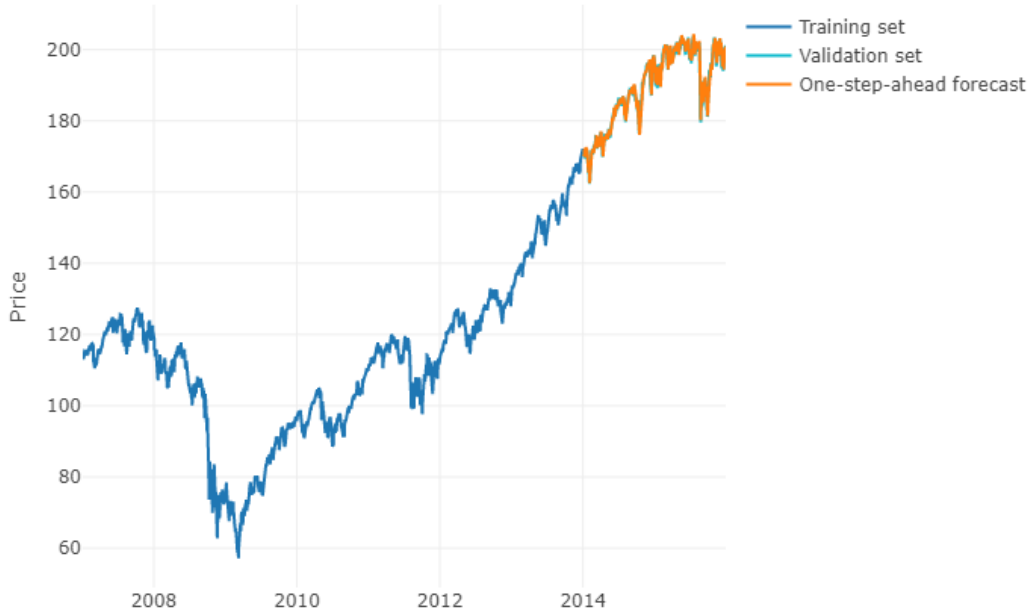
Prediction Problems

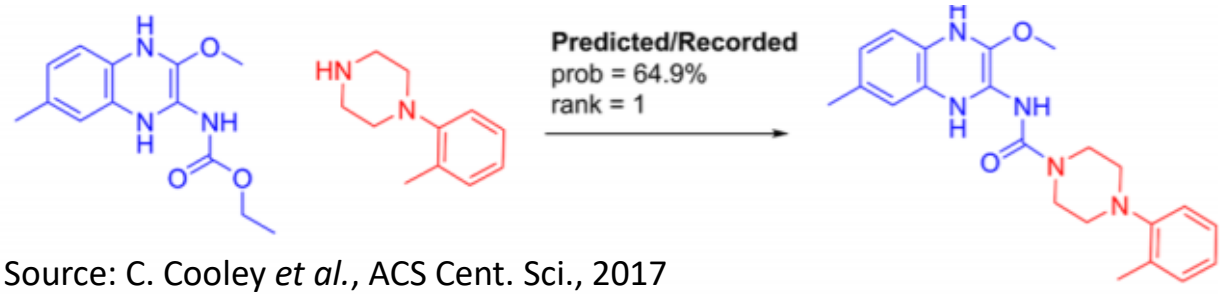
- About the future



Prediction Problems

- About Properties

What is in this image?



Source: C. Cooley *et al.*, ACS Cent. Sci., 2017

What will be the outcome of this organic reaction?

Prediction Problems

- Can you recognize this animal?

Several dog breeds

Source: The Oxford-IIIT Pet Dataset

How?

$$f(x) = y$$

- Conventional programming: given an input x we write a computer program f that given x produces y.

$$f(\text{  }) = \text{“dog”}$$

How?

$$f(x) = y$$

- Artificial intelligence: a computer program that learns the best program *f* from examples.

f() = “dog”

f() = “dog”

f() = “not a dog”

⋮

How?

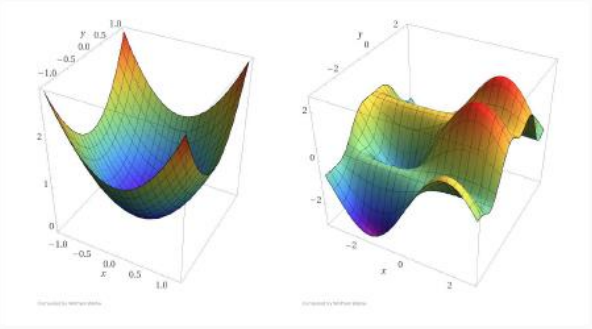
- Each input represented as a mathematical entity.

- The problem of learning the program *f* is posed as a minimization problem.

Objective:

$$\hat{\Theta} = \underset{\Theta}{\operatorname{argmin}}\Big(\overbrace{\frac{1}{n}\sum_{i=1}^{n} L(f(x_i;\Theta), y_i)}^{loss} + \overbrace{\lambda R(\Theta)}^{regularization}\Big)$$

with $f(x_i;\Theta) = \tilde{y}_i$.



AI and Rare Diseases

- Rare means hard for big companies to get interested.
- Artificial Intelligence can help:
  - Cutting time and costs
  - Seing what we cannot see
  - In diagnostics
  - In therapeutics

Example: AI assisted review of literature

- Goal: write a review of literature article on quality of life in rare diseases (CDG & Allies—PPAIN research group, Lisbon).
- Problem: a keywords based search of scientific articles produced more than 16000 results. Many are not relevant, we just don’t know which, *a priori*.
- Proposed solution: learn a classifier that is able to make a preliminary screening of the articles based on title and abstract only.

Diagnostics: examples.

- Face2Gene app (diagnostics namely by face image analysis). FDNA

  Y. Gourovich *et al.*, PNAS, 2019.

- Electronic Health Records: big data to the rescue.

  R. Colbaugh *et al.*, AMIA Annu. Symp. Proc., 2018.

- VarCoPP and Orval (IB2, Bruxelles).

  S. Papadimitriou *et al.*, PNAS, 2019.

Therapeutics: Computational Drug Repurposing

	Description	Examples of preclinical successes
Molecular	Compare drug gene expression signatures pre-and postdrug treatment with disease gene expression signatures in order to predict drugs that may reverse disease gene signatures.	• Parbendazole for osteoporosis [23] • Cimetidine for lung adenocarcinoma [20] • Citalopram for metastatic colon cancer [24] • Topiramate for inflammatory bowel disease [25]
Clinical	Leverage large-scale health data such as EMRs and patient medication histories to identify drugs effective for indications other than the primary use.	• Statin therapy for AD [54,55] • Terbutaline sulfate for ALS [56] • Glitazone for PD [83]
Biophysical	Leverage the biochemical properties of drugs such as binding affinity or biophysical properties such as 3D conformation to achieve drug-target predictions.	• Droperidol for AD [107]

Source: M. Paranjpe *et al.,* TIPS, 2019.

Challenges for AI in Rare Diseases

- Develop further methods able to fuse all of the available data modalities.
- Create and develop more data and datasets, *e.g.*, anonymized Electronic Health Records type.
- More research on few shot learning.

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