Navigating an ML project

Problem statement:

- What do you want to predict or learn?
- What would this enable?
- How do you define success?

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Chemical Engineering
& Materials Science

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- How will you assess IID and OOD performance?

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Prediction:
- How should this model be used?
- What are the limitations?
- Where is the model/data/code?

Shallow vs deep learning

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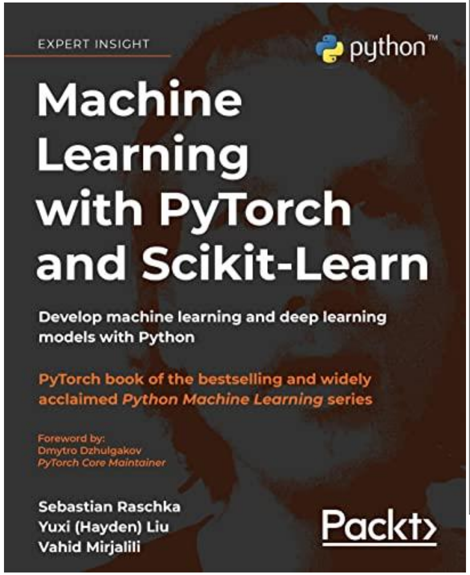
Shallow ML ⇒ we know the features (structured)

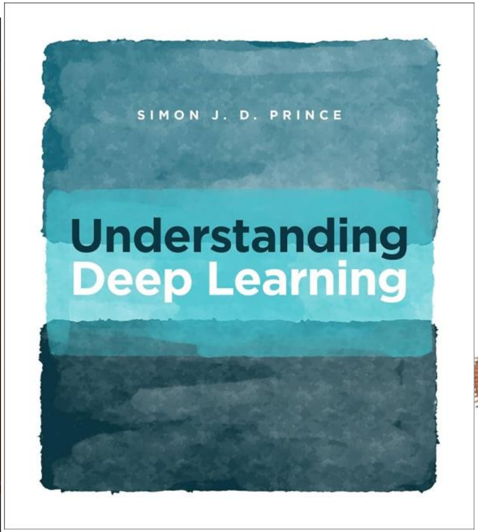
Deep ML ⇒ we learn the features (unstructured)
↳ requires a lot of data
(10^4+)
↳ transfer learning can help.

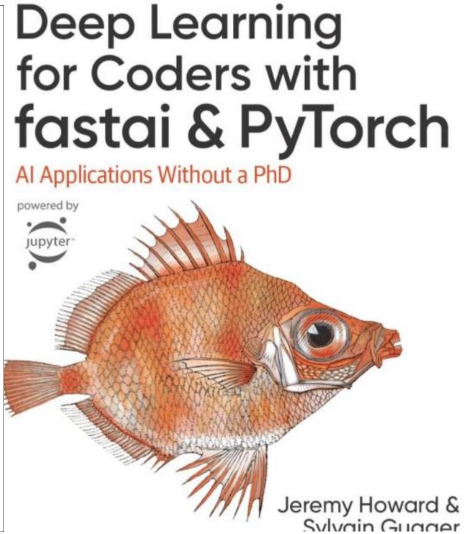
Similar concepts apply
↳ validation
↳ defining success
↳ understanding features/representation

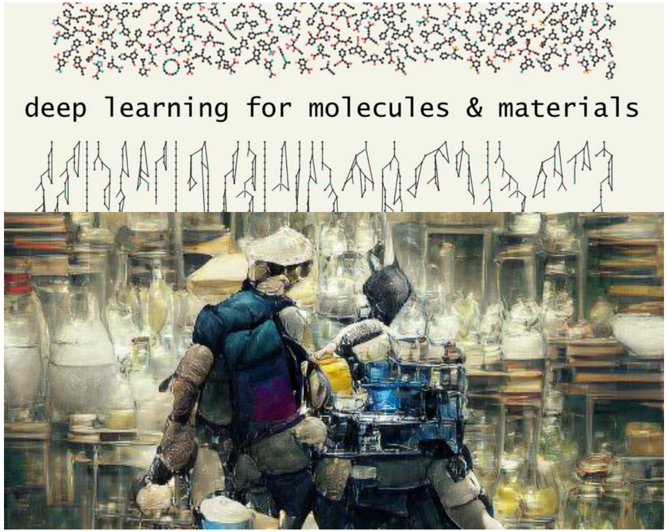
New challenge ⇒ training takes a long time
($10^6 - 10^{12}$ weights)

Where to go next









CS231n: Deep Learning for Computer Vision

YouTube

Stanford - Spring 2023

DEEP LEARNING

DS-GA 1008 · FALL 2022 · NYU CENTER FOR DATA SCIENCE

INSTRUCTOR Alfredo Canziani, Yann LeCun

Some quick advice on coding

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- Use .py instead of .ipynb files
- Everything should be in a function
- Build classes to collect related functions/properties
- Use an IDE + AI assistant (e.g., VSCode+CoPilot)
- **Make sure your work is reproducible (track experiments, build python packages, use environments)**

Using ML for your research

1) Let your fundamental research questions drive the use of ML

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3) **Still, your domain knowledge can lead to creative data-driven solutions and solve your problems!**

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3) **Does my validation/testing scheme align with how the model will be used in practice?**

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4) **Do my results pass a sanity check?!**