Navigating an ML project

CEMS
Chemical Engineering
& Materials Science

Problem statement:

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- What would this enable?
- How do you define success?

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- How will you assess IID and OOD performance?

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- Local or global explanations?
- Understanding model or generalization?

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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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Where to go next

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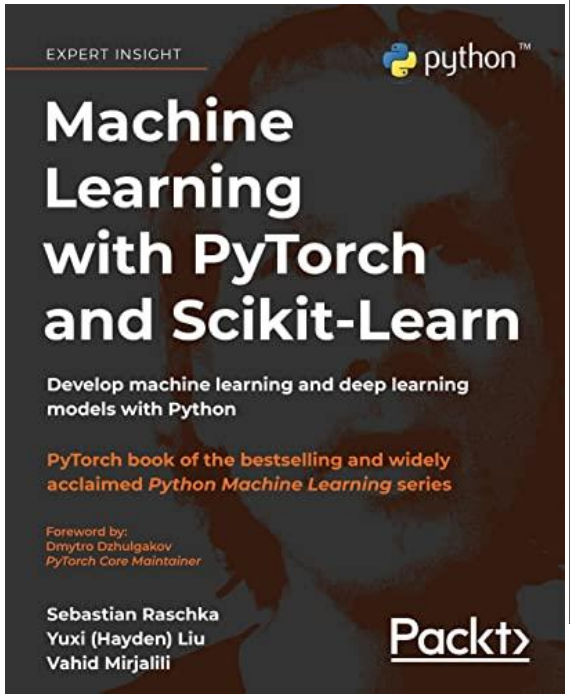
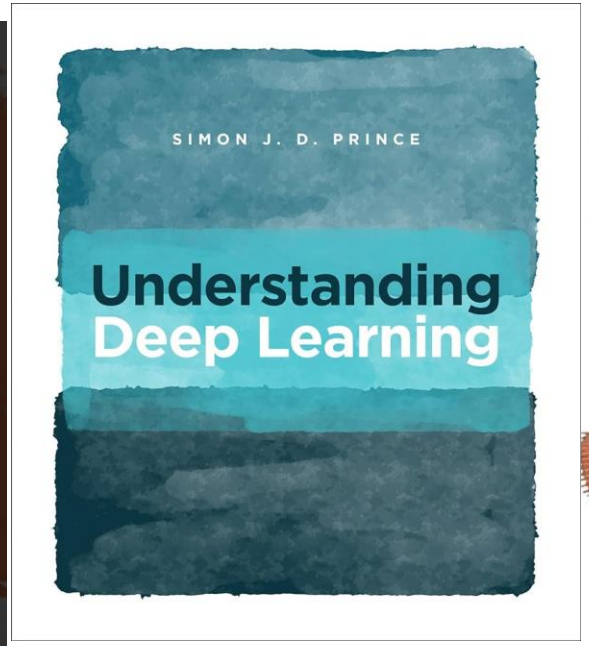
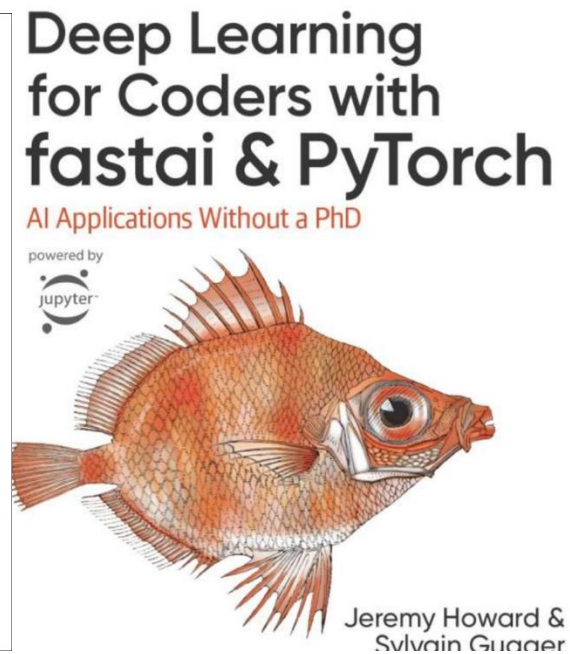
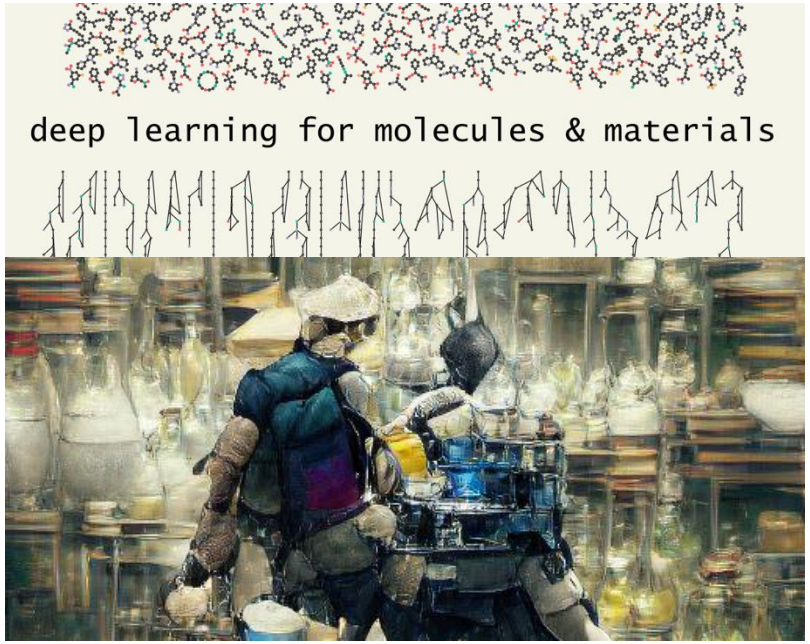




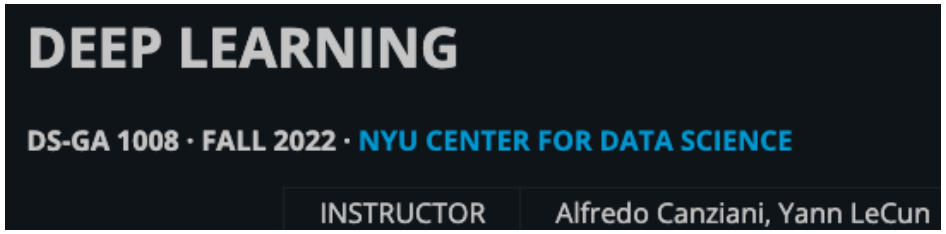




CS231n: Deep Learning for Computer Vision

YouTube

Stanford - Spring 2023



Some quick advice on coding

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- Use .py instead of .ipynb files

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- **Use an IDE (e.g., VSCode+CoPilot)**

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

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

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2) **You are (probably) not going to invent a new ML method from scratch**

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2) You are (probably) not going to invent a new ML method from scratch

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

Most important things to think about

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2) Do I understand the problem well enough to propose good features?

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

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2) Do I understand the problem well enough to propose good features?

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

4) Do my results pass a sanity check?!