Selected Techniques in Machine Learning

Chi-kwan "CK" Chan, PHYS 305, 2025-02-27

Goals

- Overview ullet
- Know where to look
- Terminology ullet
- How to ask/answer the "right" questions
- The value of data
- Opportunities (in astronomy) ullet
- Challenges ullet
- How to answer questions with data?
- How to use data to come up with good questions?

Historical Context

- Data science is NOT NEW! ullet
- Data-intensive/driven science: ullet
 - Science that we do based on data, e.g., astronomy
- Data science: ightarrow
 - Emergent discipline motivated by data-intensive/driven science.
 - The science of how to: collect, handle, clean, store, visualize, and model with data.

Tycho Brahe

- 1546–1601
- Collected rich data set of motion of planets
- Noticed inconsistencies of model at the time with what he observed
- Realized as a teenager to collect data to make a science of data
- Had a "science island" between Copenhagen and Sweden
- Knew the value of his data, didn't let other people (Kepler) have full access!

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Johannes Kepler

- 1571–1630
- An assistant to the Tycho Brahe
- Discovered three (geometrical) laws of planetary motion:
 - Planets move in elliptical orbits with the Sun as a focus
 - A planet covers the same area of space in the same amount of time no matter where it is in its orbit
 - A planet's orbital period is proportional to the size of its orbit

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Sir Isaac Newton

- 1642–1726
- Formulated the laws of motion and universal gravitation
- Derived Kepler's laws of planetary motion
- Explained "why"
- Generalizable; enabled us to put people on the moon
- "Higher order" theory
- In data-driven science, in astrophysics, maybe an ultimate goal is push from Kepler to Newton







The FOURTH PARADIGM

DATA-INTENSIVE SCIENTIFIC DISCOVERY

EDITED BY TONY HEY, STEWART TANSLEY, AND KRISTIN TOLLE

Experiments/ Observations

Data Science

Science

Theory

Computational Science



Computational Science

- "Traditional" simulation
- Forward problem:
 - model -> solution
- Equations is (relatively) simple
- Algorithms are well understood, often designed to preserve equation properties
- Complexity is in the many DoF and nonlinearity
- Codes are usually developed by a small team in University or national labs

Data Science

- "Cool" machine learning
- Inverse problem:
 - data -> model
- Data is usually messy
- The most powerful algorithms are less well understood, as long as "they work"
- Complexity is in the coefficients learned from the data
- Codes are developed by large communities, many support by big tech (Tensorflow, PyTorch, JAX)

n



Machine Learning



Data Science

Big Data Deep Learning

Artificial Intelligence

Advancement of Machine Learning

- Some of the most exciting applications of deep learning
 - DQN Breakout
 - <u>AlphaGo</u> (core algorithm <u>mctx</u>, <u>documentary</u>)
 - <u>AlphaZero</u>
 - <u>AlphaFold3</u>
 - DALL-E3
 - <u>ChatGPT</u>
 - <u>Segmenting Anything 2</u>
 - <u>AlphaGeometry</u>
 - GraphCast
- What will the "ChatGPT moment" be like in astronomy?



THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE

nainre

At last – a computer program that can beat a champion Go player PAGE 484

ALL SYSTEMS GO

À LA CARTE illegal harvest of millions of Mediterranean birds PAGE 452

PAGE 452

A LA CARTI

TRANSPARENCY Don't let openness backfire on individuals PAGE 450

PAGE 459

GOT 'SELFISH Dawkins's calling

card 40 years on PAGE 462

PAGE 452



Machine Learning

- Building useful models from data
- Models hopefully improve with increase volume of data ightarrow
- Misconcept 1: ML is magic
- Reality: built on foundational advances in math and computer science in decades: ightarrow
 - optimization & regression
- Most useful background fields: linear algebra, optimization, statistics ullet
- Misconcept 2: ML is just Neural Network (Deep Learning)
- Reality: outside NN/DL, there are many ML techniques that are: ullet
 - effective, efficient, and very often understandable/interpretable

Machine Learning Goals

- Model be "useful" in the future
- Accurate
- Fast
- Generalizable (f = ma)
- Interpretable/explainable •
- Certify/guarantee •

Cross-Validation

- Past: training data ullet
- Future: testing data ullet
- Split available to 80% for training and 20% for "testing"
- K-fold validation for increase statistics
- Never trust/publish any ML results without cross-validation!!!

Supervised

- With labels
- Classification (discrete): classify type I and II supernovae
 - SVM
 - neural network
 - decision tree
- Regression (continue): light curve of AGNs
 - linear,
 - generalized linear,
 - Gaussian process
- Optimization and control

Semi-supervised

- Some feedbacks
- Generative models (selfsupervised)
 - Generative adversarial networks (GAN)
- Reinforcement learning
 - Deep reinforcement learning

Unsupervised

- No labels, "data mining"
- Cluster (discrete)
 - k-means
 - k nearest neighbor
 - spectral clustering
- Embedding, dimensionality ulletreduction, pattern extraction
 - PCA
 - autoencoder
 - diffusion maps







Resources

- Scikit-learn: <u>https://scikit-learn.org</u>
- Keras: <u>https://keras.io</u>
- AstroML: <u>https://www.astroml.org</u>