Lecture I: Course introduction

CSEP 590B: Explainable Al lan Covert & Su-In Lee University of Washington

Teaching team



Su-In Lee

- Paul G. Allen Prof.
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- Office hours: course website



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 - Ph.D. student
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Participation is important

- 50 people with diverse expertise
 - Microsoft 22
 - Amazon 6
 - Boeing
 4
 - Google 3
 - Tableau 2

| FTE | Years | |
|--------|-------|--|
| Min | 2 | |
| Max | 30 | |
| Mean | 6.8 | |
| Median | 4.5 | |

- Apple, Avalara, Avnet, Best Buy, Comcast, D2K Technologies, Doctor.com, Facebook, Hulu, Petrin Technology Consulting LLC, Provoke Solutions, Salesforce, SAP Qualtrics, Twitter 1
- This course is a unique opportunity to share ideas about using XAI in industry
- Please do not hesitate to contact us with comments or feedback

Today

- Section 1
 - Motivation & aims



- Course logistics
- Examples in the healthcare space
- Section 2
 - Discussion: "Statistical Modeling: The Two Cultures"
- Section 3
 - Example scenario and ML review

Traditional algorithms

Find customers for rewards program

```
gold = []
platinum = []
for customer in customers:
    if customer.savings > amount1:
        platinum.append(customer)
    elif customer.savings > amount2:
        gold.append(customer)
    return gold, platinum
```

Program based on simple rules, written by people

Machine learning algorithms

Decide if customer should be given a loan

```
default_risk = risk_prob(customer)
```

if default_risk < thresh:</pre>

return **True**

else:

return False

Based on many inputs (savings, age, income, job, homeownership...)

No simple rules → **learned from data**

ML now used for many problems

- Credit risk
- Medical diagnosis
- Biomedical discoveries
- Recidivism prediction
- Job candidate screening
- Content recommendation
- Ad targeting
- Search engines
- Text summarization



Models

Technology has improved





Learning ML models from data: supervised learning

ML ingredients

- Function class f(x) to describe y based on x
- Training data with n samples of features x and labels y



ML today: black-box models



State-of-the-art accuracy

Performance tied to revenue, user experience, customer retention, etc.



However, lack of transparency!

- Identify key factors in underlying process
- Generate scientific hypotheses

Accurately predicting clinical outcomes is important, but the key question is *why*



Accurately modeling biological phenotypes is important, but the key question is *why*



Explainable AI for biology and health







- **Explainability** can be as important as accuracy
 - Which features contributed to a certain prediction and how?
 - How to learn or select features that are most interpretable or informative?
 - How to make biological or clinical sense of a blackbox model?

ML today: black-box models



State-of-the-art accuracy

Performance tied to revenue, user experience, customer retention, etc.



Transparency goals

- Identify key factors in underlying process
- Generate scientific hypotheses
- Diagnose model failures
- Audit for unwanted dependencies
- Enable regulation
- Improve dataset
- Build user, organizational trust
- Inform users of recourse options
- Pinpoint shortcuts, spurious signals

Transparency for any model

Explainable AI (XAI) ingredients

- Model: predictive model, possibly black-box (such as DNN, GBM, etc.)
- **Data:** individual data sample, or entire dataset
- **Question:** what do you need to understand?

Design algorithms to answer specific questions about ML models

Feature importance



ML model



Feature importance



ML model



Concept



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Feature importance



Important concepts



Concept



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Feature importance



Data (instance) importance



Important concepts



How much does each sample contribute to model training?



Course goals

What to expect

- Broad overview: learn about many areas of XAI, an emerging area of ML research
- Preparation for learning: the field is fast-moving, and we'll cover principles that help learn new techniques on your own
- Usage experience: get experience working with several popular tools and libraries (e.g., shap)

Prerequisites

- Background in calculus, probability, linear algebra
- ≥1 previous ML courses (ugrad or grad level)
 - Most PMP students with a B.S. in Computer Science should fulfill the prerequisites. If you're unsure, please contact us

Course overview

- Course introduction (1 lecture)
- Feature importance explanations (3 lectures)
 - Removal-based explanations
 - Shapley values
 - Propagation-based explanations
- Evaluating explanations (1 lecture)
- Inherently interpretable models (1 lecture)
- Other approaches (2 lectures)
 - Concept-based explanations, neuron interpretation
 - Counterfactual explanations, instance explanations
- Enhancing human-Al collaboration (1 lecture)
- XAI in industry, model improvement (1 lecture)





Concept



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Lecture format

Before: read a research paper, write discussion post

During (2 hrs 50 mins):

- Discussion (50 mins) followed by 10 min break
- Lecture part 1 (50 mins) followed by 10 min break
- Lecture part 2 (50 mins)

Textbooks

- The field is young and rapidly changing
 - No single textbook covers all relevant content
 - Christoph Molnar's <u>e-book</u> is pretty good
- Instead, we'll read and discuss recent papers
 - Active vs. passive learning
 - Keep up with new content, practice reading papers
 - Student-led discussions

Grading basis

- 50% Homework
- 40% Paper discussions
 - Discussion board posts and in-class discussion
 - Bonus: leading the discussion
- 10% In-class participation

Homework assignments

- HW 0 (30 points, due next Monday 11:59 pm)
 - Refresher on probability, calculus, ML models
- HW 1, 2, 3 (100 points each)
 - Several problems, including math and programming
 - You'll have several weeks for each assignment, but start early

Homework policies

Collaboration:

- Students must submit their own answers and their own code for programming problems
- Limited collaboration is allowed, but you must indicate on the homework with whom you collaborated

Late policy:

- Homeworks must be submitted online on Canvas by the posted due date
- The penalty for late work is 20 points per day, and each student gets 3 free late days for the quarter

Homework tools

- Submitted electronically on Canvas, PDF format
 - Preference: Latex > Word > handwritten
- Programming in Python only
- We'll use open-source software:
 - numpy, pandas, matplotlib
 - sklearn, Pytorch/Tensorflow
 - shap, lime

Discussion posts

- Read the paper prior to class
- Discussion post due the night before
 - What is the paper about?
 - How does the method work?
 - What questions does it answer about a model?
 - How does it differ from other methods we've discussed?
 - Does it seem technically sound? What concerns do you have?
 - Could you use it in your job? How?
- Graded on 0-2 scale

In-class discussion

- Led by two student volunteers
 - Prepare slides, a short summary of the paper
 - Suggest topics to discuss about the method, its evaluation, etc.
 - Beyond the paper: broader questions, utility in business or scientific research, relationship with other methods

We need volunteers!

- Bonus points towards final grade
- We'll email a link to schedule spreadsheet

Course information

- Course website (<u>link</u>)
 - Required readings, course information
- Ed discussion board (link)
 - Discussion post submission, HW questions, etc.
- Canvas (<u>link</u>)
 - Lecture slides, HW submission
- Mailing list: <u>csep590b_sp22@cs.washington.edu</u>

Course schedule

| Student-led | | | 1 | |
|----------------------|----|------|--------------------------------|--------------------------|
| discussions begin | 1 | 3/29 | | |
| | 2 | 4/5 | 4/4 (Mon) | HW0: Warm-up (30 points) |
| | 3 | 4/12 | | |
| | 4 | 4/19 | | |
| | 5 | 4/26 | 4/25 (Mon) | HW1: Feature importance |
| | 6 | 5/3 | | (100 points) |
| | 7 | 5/10 | | |
| | 8 | 5/17 | 5/16 (Mon) | HW2: TBD (100 points) |
| | 9 | 5/24 | | |
| | 10 | 5/31 | 5/30 (Mon) | HW3: TBD (100 points) |

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Accurately predicting clinical outcomes is important, but the key question is *why*



Scott Lundberg, [...], and Su-In Lee. Explainable AI for Trees: From Local Explanations to Global Understanding. Nature Machine Intelligence (2020) – Cover article

Our solution: a technique that can explain any prediction

- Accuracy vs. interpretability
 - Simple models often lead to worse performance
 - Complex models are often considered to be a black box



Scott Lundberg and Su-In Lee. A Unified Approach to Interpreting Model Predictions. NeurIPS (2017) – Oral presentation NeurIPS workshop on Interpretable ML (2016) – Best paper award

Accurately predicting clinical outcomes is important, but the key question is *why*



Scott Lundberg, et al. Explainable AI for Trees: From Local Explanations to Global Understanding. Nature Machine Intelligence (2020) – Cover article

Identifying expression markers for phenotypes is important, but the key question is the *mechanistic explanation*



Nicasia Beebe-Wang, [...], Sara Mostafavi* and Su-In Lee.* Unified AI framework to uncover deep interrelationships between gene expression and Alzheimer's disease neuropathologies. *Nature Communications* (2021)

Identifying genes that are important to neuropathological phenotypes

• XAI methods can uncover each gene's contribution to the output variables





 Previously unknown sex-specific associations between immune response genes and AD neuropathological phenotypes

Nicasia Beebe-Wang, [...], Sara Mostafavi* and Su-In Lee.* **Unified AI framework to uncover deep interrelationships between gene** expression and Alzheimer's disease neuropathologies. *Nature Communications (2021)*

Providing *explainable predictions* improves healthcare provider's ability to predict clinical outcomes



Our *Prescience* method predicts hypoxemia in the next 5 minutes, provides explanations in real time

Our approach, SHAP

For a particular prediction





Scott M. Lundberg, [...], and Su-In Lee. Explainable machine-learning predictions for the prevention of hypoxaemia during surgery. Nature Biomedical Engineering 2, 749–760 (2018) – Cover article

Explainable AI enables model auditing and cost-aware AI

- We revealed that many published AI systems to detect COVID-19 rely on "shortcuts" rather than genuine pathology
- CoAl enables drastic reduction in feature acquisition cost (e.g., time) to help emergency medicine or ICU patients





Alex DeGrave*, Joe Janizek*, and Su-In Lee. Al for radiographic COVID-19 detection selects shortcuts over signal. Nature Machine Intelligence (2021) Gabe Erion, Joe Janizek [...] Nathan White*, and Su-In Lee* CoAI: Cost-Aware Artificial Intelligence for Health Care. In Press Nature Biomedical Engineering

Explainable prediction of drug synergy in AML (EXPRESS)



Joseph Janizek, [...], Kamila Naxeriva*, and Su-n Lee*. Uncovering expression signatures of synergistic drug response using an ensemble of explainable AI models. In Revision *Nature Biomedical Engineering*

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 - 10 min break: <u>office hours poll</u> (see your email)
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