UVA CS CS 4501: Machine Learning

Lecture 1: Introduction

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Department of Computer Science
Welcome

• CS 4501 Machine Learning
  – TuTh 3:30pm-4:45pm,
  – Rice Hall 130

• Your UVA collab for Assignments:

• Course Website:
  – https://qiyanjun.github.io/2018sUVaCS4501003/
  – can track lecture versions @ https://github.com/qiyanjun/2018sUVaCS4501003/tree/master/Lectures
Today

- Course Logistics
- My background
- Machine Learning Basics
- Rough Plan of Course Content
- Machine Learning History
- Connecting to Artificially Intelligence
Course Staff

• Instructor: Prof. Yanjun Qi
  – QI: /ch ee/
  – You can call me “professor”, “professor Qi”;

• TA and Office Hour information @ CourseWeb

• Q0- Quiz for the minimum background test !!!!
Course Logistics

• Course email list has been setup. You will have received emails already!

• Policy, the grade will be calculated as follows:
  – Assignments (60%, Six total, each ~10%)
  – Quizzes / Exam Sample Practices (Extra 5%)
  – Midterm exam (20%)
  – Final exam (20%)
Course Logistics

• Midterm: Mar, 75mins in class
• Final: May, 75mins in class

• Six assignments (each 10%)
  – Three extension days policy (check course website)

• Quizzes / Participations (Extra 5%)
Course Logistics

• Policy,
  – Homework should be submitted electronically through UVaCollab.
  – Homework should be finished individually.
  – Due at midnight on the due date.
  – In order to pass the course, the average of your midterm and final must also be "pass".

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Late Homework Policy

• Each student has **three** extension days to be used at his or her own discretion throughout the entire course. Your grades would be discounted by 15% per day when you use these 3 late days. You could use the 3 days in whatever combination you like. For example, all 3 days on 1 assignment (for a maximum grade of 55%) or 1 each day over 3 assignments (for a maximum grade of 85% on each). After you've used all 3 days, you cannot get credit for anything turned in late.
Course Logistics

- Text books for this class is: 
  - NONE

- My slides – if it is not mentioned in my slides, it is not an official topic of the course
Course Logistics

- **Background Needed**
  - Calculus, Basic linear algebra, Basic probability and Basic Algorithm
  - Statistics is recommended.
  - Students should already have good programming skills, i.e. *python* is required for all programming assignments
  - We will review “algebra” and “probability” in class
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About Me

• Education:
  – PhD from School of Computer Science, Carnegie Mellon University (@ Pittsburgh, PA) in 2008
  – BS from Department of Computer Science, Tsinghua Univ. (@ Beijing, China)
    • My accent PATTERN : /l/, /n/, /ou/, /m/

• Research interests:
  – Machine Learning, Biomedical applications
About Me

• Five Years’ of Industry Research Lab in the past:
  – 2008 summer – 2013 summer, Research Scientist
    (Machine Learning Department @ IT industry)
  – 2013 Fall – Present, Tenure-track Assistant Professor,
    Computer Science, UVA
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OUR DATA-RICH WORLD

• Biomedicine
  – Patient records, brain imaging, MRI & CT scans, …
  – Genomic sequences, bio-structure, drug effect info, …

• Science
  – Historical documents, scanned books, databases from
    astronomy, environmental data, climate records, …

• Social media
  – Social interactions data, twitter, facebook records, online
    reviews, …

• Business
  – Stock market transactions, corporate sales, airline traffic,
BIG DATA CHALLENGES

• Data capturing (sensor, smart devices, medical instruments, et al.)
• Data transmission
• Data storage
• Data management
• High performance data processing
• Data visualization
• Data security & privacy (e.g. multiple individuals)
• ……

• Data analytics
  ○ How can we analyze this big data wealth?
  ○ E.g. Machine learning and data mining
BASICS OF MACHINE LEARNING

• “The goal of machine learning is to build computer systems that can learn and adapt from their experience.” – Tom Dietterich

• “Experience” in the form of available data examples (also called as instances, samples)

• Available examples are described with properties (data points in feature space $X$)
e.g. SUPERVISED LEARNING

• Find function to map input space $X$ to output space $Y$ 
  \[ f : X \rightarrow Y \]

• So that the difference between $y$ and $f(x)$ of each example $x$ is small.

\[
\begin{array}{|c|}
\hline
x & I believe that this book is not at all helpful since it does not explain thoroughly the material. It just provides the reader with tables and calculations that sometimes are not easily understood... \\
\hline
\end{array}
\]

\[
\begin{array}{|c|}
\hline
y & -1 \\
\hline
\end{array}
\]

Output $Y$: \{1 / Yes , -1 / No \}
e.g. Is this a positive product review?

Input $X$: e.g. a piece of English text
SUPERVISED Linear Binary Classifier

• Now let us check out a VERY SIMPLE case of

\[ f(x, w, b) = \text{sign}(w^T x + b) \]

\[ x = (x_1, x_2) \]
SUPERVISED Linear Binary Classifier

\[ f(x, w, b) = \text{sign}(w^T x + b) \]

\[ x = (x_{-1}, x_{-2}) \]

- \( w^T x + b > 0 \) denotes +1 point
- \( w^T x + b < 0 \) denotes -1 point
- \( w^T x + b = 0 \) denotes future points

"Predict Class = +1" zone
"Predict Class = -1" zone

"Predict Class = +1" zone
"Predict Class = -1" zone

Courtesy slide from Prof. Andrew Moore’s tutorial
Basic Concepts

- **Training** (i.e. learning parameters $\langle w, b \rangle$)
  - Training set includes
    - available examples $x_1, \ldots, x_L$
    - available corresponding labels $y_1, \ldots, y_L$

- Find $(w, b)$ by minimizing loss (i.e. difference between $y$ and $f(x)$ on available examples in training set)

$$(W, b) = \arg\min_{w, b} \sum_{i=1}^{L} \ell(f(x_i), y_i)$$
Basic Concepts

• **Testing** (i.e. evaluating performance on “future” points)
  - Difference between true $y$ and the predicted $f(x)$ on a set of testing examples (i.e. *testing set*)
  - Key: example $x$ not in the training set

• **Generalisation**: learn function / hypothesis from *past data* in order to “explain”, “predict”, “model” or “control” *new* data examples
Basic Concepts

• **Loss function**
  – e.g. hinge loss for binary classification task
    \[
    \sum_{i=1}^{L} \ell(f(x_i), y_i) = \sum_{i=1}^{L} \max(0, 1 - y_i f(x_i))
    \]
  – e.g. pairwise ranking loss for ranking task (i.e. ordering examples by preference)

• **Regularization**
  – E.g. additional information added on loss function to control \( f \)
    \[
    C \sum_{i=1}^{L} \ell(f(x_i), y_i) + \frac{1}{2} \|w\|^2
    \]
TYPICAL MACHINE LEARNING SYSTEM

Low-level sensing $\rightarrow$ Pre-processing $\rightarrow$ Feature Extract $\rightarrow$ Feature Select $\rightarrow$ Inference, Prediction, Recognition $\rightarrow$ Evaluation

$X \rightarrow f : X \rightarrow Y$
“Big Data” Challenges for Machine Learning

- Large size of samples
- High dimensional features

Not the focus, being covered in my advanced-level course.
Large-Scale Machine Learning: SIZE MATTERS

- One thousand data instances
- One million data instances
- One billion data instances
- One trillion data instances

Those are not different numbers, those are different mindsets !!!
The variations of both $X$ (feature, representation) and $Y$ (labels) are complex!
TYPICAL MACHINE LEARNING SYSTEM

Low-level sensing → Pre-processing → Feature Extract → Feature Select

Data Complexity of X

Data Complexity of Y

Label Collection

Inference, Prediction, Recognition

Evaluation

$f : X \rightarrow Y$
UNSUPERVISED LEARNING:
[ COMPLEXITY OF Y ]

- No labels are provided (e.g. No Y provided)
- Find patterns from unlabeled data, e.g. clustering

![Diagram showing clustering](image)

e.g. clustering => to find “natural” grouping of instances given un-labeled data
Many prediction tasks involve output labels having structured correlations or constraints among instances.

### Structured Dependency between Examples’ Y

<table>
<thead>
<tr>
<th>Input $X$</th>
<th>Sequence</th>
<th>Tree</th>
<th>Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>APAFSVSPASGACGPECA...</td>
<td>The dog chased the cat</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Output $Y$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CCEE111EEEECCCCCHHHCCC...</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Many more possible structures between $y_i$, e.g. spatial, temporal, relational...
STRUCTURAL INPUT: Kernel Methods

[ COMPLEXITY OF X ]

Vector vs. Relational data

e.g. Graphs, Sequences, 3D structures,

Original Space  Feature Space
MORE RECENT: FEATURE LEARNING

[ COMPLEXITY OF X ]

Deep Learning

Supervised Embedding

Layer-wise Pretraining
DEEP LEARNING / FEATURE LEARNING: [COMPLEXITY OF X]

Feature Engineering
☑ Most critical for accuracy
☑ Account for most of the computation for testing
☑ Most time-consuming in development cycle
☑ Often hand-craft and task dependent in practice

Feature Learning
☑ Easily adaptable to new similar tasks
☑ Layerwise representation
☑ Layer-by-layer unsupervised training
☑ Layer-by-layer supervised training
Why learn features?
Deep learning models

- End to end!
- Uses tons of data, very hands-off approach
**Deep Learning**

With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart.

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**Temporary Social Media**

Messages that quickly self-destruct could enhance the privacy of online communications and make people freer to be spontaneous.

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**Prenatal DNA Sequencing**

Reading the DNA of fetuses will be the next frontier of the genomic revolution. But do you really want to know about the genetic problems or musical aptitude of your unborn child?

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**Additive Manufacturing**

Skeptical about 3-D printing? GE, the world’s largest manufacturer, is on the verge of using the technology to make jet parts.

---

**Baxter: The Blue-Collar Robot**

Rodney Brooks's newest creation is easy to interact with, but the complex innovations behind the robot show just how hard it is to get along with people.

---

**Memory Implants**

A maverick neuroscientist believes he has deciphered the code by which the brain forms long-term memories. Next, testing a prosthetic implant for people suffering from long-term memory loss.

---

**Smart Watches**

The designers of the Pebble watch realized that a mobile phone is more useful if you don’t have to take it out of your pocket.

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**Ultra-Efficient Solar Power**

Doubling the efficiency of a solar cell would completely change the economics of renewable energy. Nanotechnology just might make it possible.

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**Big Data from Cheap Phones**

Collecting and analyzing information from simple cell phones can provide surprising insights into how people move about and behave – and even help us understand the spread of diseases.

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**Supergrids**

A new high-power circuit breaker could finally make highly efficient DC power grids practical.
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Course Content Plan ➔

Five major sections of this course

- Regression (supervised)
- Classification (supervised)
- Unsupervised models
- Learning theory
- Graphical models
Scikit-learn algorithm cheat-sheet

classification

SVC
Ensemble Classifiers

kernel approximation

KNeighbors Classifier

SGD Classifier

Naive Bayes

Text Data

Linear SVC

<100K samples

get more data

>50 samples

predicting a category

few features should be important

SGD Regressor

Lasso

ElasticNet

SVR(kernel='rbf')

RidgeRegression

SVR(kernel='linear')

clustering

Spectral Clustering

GMM

KMeans

MiniBatch KMeans

MeanShift

<10K samples

<10K categories known

number of categories known

predicting a quantity

<10K samples

just looking

<10K samples

tough luck

predicting structure

Randomized PCA

Isomap

Spectral Embedding

LLE

dimensionality reduction

scikit-learn algorithm cheat-sheet

START

Yanjun Qi / UVA CS

Scikit-learn : Regression

regression

SGD Regressor

Lasso
ElasticNet

SVR(kernel='rbf')

EnsembleRegressors

<100K samples

few features should be important

YES

NO

RidgeRegression

SVR(kernel='linear')

YES

NO

NOT WORKING
Scikit-learn : Classification

To combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator. (1) averaging / bagging (2) boosting.
Unsupervised Models

- Kmeans + GMM
- Spectral Clustering
- GMM
- KMeans
- MiniBatch KMeans
- MeanShift
- VBGMM
- number of categories known
- <10K samples
- Basic PCA
- Randomized PCA
- Isomap
- Spectral Embedding
- LLE
- kernel approximation
- <10K samples
- just looking
- NOT WORKING
- not working
- predicting structure
- tough luck
Summary

• This is not a course about how to use a toolbox

• We focus on learning fundamental principles, mathematical formulation, algorithm design and learning theory.
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What can we do with the data wealth? ➔ REAL-WORLD IMPACT

- Business efficiencies
- Scientific breakthroughs
- Improve quality-of-life:
  - healthcare,
  - energy saving / generation,
  - environmental disasters,
  - nursing home,
  - transportation,
  - ...

Transportation Data
Genomic Data
Medical Images
Brain computer interaction (BCI)
Device sensor data
When to use Machine Learning (Adapt to / learn from data)?

- **1. Extract knowledge from data**
  - Relationships and correlations can be hidden within large amounts of data
  - The amount of knowledge available about certain tasks is simply too large for explicit encoding (e.g. rules) by humans

- **2. Learn tasks that are difficult to formalise**
  - Hard to be defined well, except by examples, e.g., face recognition

- **3. Create software that improves over time**
  - New knowledge is constantly being discovered.
  - Rule or human encoding-based system is difficult to continuously re-design “by hand”.
MACHINE LEARNING IS CHANGING THE WORLD

One of 18 learned rules:
If No previous vaginal delivery, and Abnormal 2nd Trimester Ultrasound, and Malpresentation at admission
Then Probability of Emergency C-Section is 0.6

Over training data: 26/41 = 0.63,
Over test data: 12/20 = 0.60

Text analysis

Many more!
MACHINE LEARNING IN COMPUTER SCIENCE

• Machine learning is already the preferred approach for
  – Speech recognition, natural language processing
  – Computer vision
  – Medical outcome analysis
  – Robot control ...

• Why growing?
  – Improved machine learning algorithms
  – Improved CPU / GPU powers
  – Increased data capture, new sensors, networking
  – Systems/Software too complex to control manually
  – Demand to self-customization for user, environment, ...
HISTORY OF MACHINE LEARNING

• 1950s
  – Samuel’s checker player
  – Selfridge’s Pandemonium

• 1960s:
  – Neural networks: Perceptron
  – Pattern recognition
  – Learning in the limit theory
  – Minsky and Papert prove limitations of Perceptron

• 1970s:
  – Symbolic concept induction
  – Winston’s arch learner
  – Expert systems and the knowledge acquisition bottleneck
  – Quinlan’s DT ID3
  – Michalski’s AQ and soybean diagnosis
  – Scientific discovery with BACON
  – Mathematical discovery with AM

Adapted From Prof. Raymond J. Mooney’s slides
**HISTORY OF MACHINE LEARNING (CONT.)**

- **1980s:**
  - Advanced decision tree and rule learning
  - Explanation-based Learning (EBL)
  - Learning and planning and problem solving
  - Utility problem
  - Analogy
  - Cognitive architectures
  - Resurgence of neural networks (connectionism, backpropagation)
  - Valiant’s PAC Learning Theory
  - Focus on experimental methodology

- **1990s**
  - Data mining
  - Adaptive software agents and web applications
  - Text learning
  - Reinforcement learning (RL)
  - Inductive Logic Programming (ILP)
  - Ensembles: Bagging, Boosting, and Stacking
  - Bayes Net learning

Adapted From Prof. Raymond J. Mooney’s slides
HISTORY OF MACHINE LEARNING (CONT.)

• 2000s
  – Support vector machines
  – Kernel methods
  – Graphical models
  – Statistical relational learning
  – Transfer learning
  – Sequence labeling
  – Collective classification and structured outputs
  – Computer Systems Applications
    • Compilers
    • Debugging
    • Graphics
    • Security (intrusion, virus, and worm detection)
  – Email management
  – Personalized assistants that learn
  – Learning in robotics and vision

Adapted From Prof. Raymond J. Mooney’s slides
HISTORY OF MACHINE LEARNING (CONT.)

• 2010s
  – Speech translation, voice recognition (e.g. Siri)
  – Google search engine uses numerous machine learning techniques (e.g. grouping news, spelling corrector, improving search ranking, image retrieval, ...)
  – 23 and me (scan sample of person genome, predict likelihood of genetic disease, ...)
  – DeepMind, Google Brain, ...
  – IBM Watson QA system
  – Machine Learning as a service (e.g. google prediction API, bigml.com, cloud autoML.)
  – IBM healthcare analytics
  – ......
HISTORY OF MACHINE LEARNING (CONT.)
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RELATED DISCIPLINES

• Artificial Intelligence
• Data Mining
• Probability and Statistics
• Information theory
• Numerical optimization
• Computational complexity theory
• Control theory (adaptive)
• Psychology (developmental, cognitive)
• Neurobiology
• Linguistics
• Philosophy
What are the goals of AI research?

Artifacts that THINK like HUMANS

Artifacts that THINK RATIONALLY

Artifacts that ACT like HUMANS

Artifacts that ACT RATIONALLY
How can we build more intelligent computer / machine?

• Able to
  – perceive the world
  – understand the world
  – react to the world

• This needs
  – Basic speech capabilities
  – Basic vision capabilities
  – Language/semantic understanding
  – User behavior / emotion understanding
  – Able to act
  – Able to think ??
How can we build more intelligent computer / machine?

R2-D2 and C-3PO

@ Star Wars – 1977

to serve human beings, and
fluent in "over six million forms of communication"
How can we build more intelligent computer / machine?

IBM Watson

- an artificial intelligence computer system capable of answering questions posed in natural language developed in IBM's DeepQA project.

Jeopardy Game

- Requires a Broad Knowledge Base

1/21/18
How can we build more intelligent computer / machine?

Apple Siri / Amazon Echo

⇒ an intelligent personal assistant and knowledge navigator
How can we build more intelligent computer / machine? **Milestone in 2012: Image Labeling**

**ImageNet**: an image database organized according to the **WordNet**

**LSVRC**: Large Scale Visual Recognition Challenge based on ImageNet.

- 72%, 2010
- 74%, 2011
- 85%, 2012
- 89%, 2013
- 93%, 2014

Deep Convolution Neural Network (CNN) won (as Best systems) on “very large-scale” ImageNet competition 2012 / 2013 / 2014

[ training on 1.2 million images [X] vs. 1000 different word labels [Y] ]
How can we build more intelligent computer / machine? : Milestones in Recent Vision/AI Fields

- 2013, Google Acquired Deep Neural Networks Company headed by Utoronto “Deep Learning” Professor Hinton
- 2013, Facebook Built New Artificial Intelligence Lab headed by NYU “Deep Learning” Professor LeCun
- 2016, Google's DeepMind defeats legendary Go player Lee Se-dol in historic victory / 2017 Alpha Zero
Detour: three planned programming assignments about AI tasks

• HW: Semantic language understanding (sentiment classification on movie review text)

• HW: Visual object recognition (labeling images about handwritten digits)

• HW: Audio speech recognition (unsupervised learning based speech recognition task)
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ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

Next lesson: Review of linear algebra and basic calculus
References

- Prof. Andrew Moore’s tutorials
- Prof. Raymond J. Mooney’s slides
- Prof. Alexander Gray’s slides
- Prof. Eric Xing’s slides
- http://scikit-learn.org/
- Prof. M.A. Papalaskar’s slides