CSC 2515: Introduction to Machine Learning

Lecture 1: Introduction and K-Nearest Neighbours Method

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¹Credit for slides goes to many members of the ML Group at the U of T, and beyond, including (recent past): Roger Grosse, Murat Erdogdu, Richard Zemel, Juan Felipe Carrasquilla, Emad Andrews, and myself.

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How can we make an intelligent agent?

- What does it mean to have an intelligent agent?
- What do we need to create it?



Figure: An agent ...



Figure: ... observes the world \dots



Figure: ... takes an action and its states changes \dots

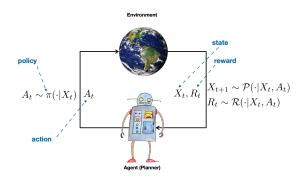


Figure: ... with the goal of achieving long-term rewards.

An AI Agent: Some Requirements

This agent has to

- predict how the world works, e.g.,
 - classify different objects
 - estimate the probability of certain events happening in the future
- plan its actions in order to achieve its long-term goals



What is learning?

"The activity or process of gaining knowledge or skill by studying, practicing, being taught, or experiencing something."

Merriam Webster dictionary

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

 $Tom\ Mitchell$

What is machine learning?

- For many problems, it is difficult to program the correct behaviour by hand
 - recognizing people and objects
 - understanding human speech
- Machine learning approach: program an algorithm to automatically learn from data, or from experience
- Why might you want to use a learning algorithm?
 - ▶ hard to code up a solution by hand (e.g. vision, speech)
 - system needs to adapt to a changing environment (e.g. spam detection)
 - \blacktriangleright want the system to perform *better* than the human programmers
 - privacy/fairness (e.g. ranking search results)

What is machine learning?

- It is similar to statistics...
 - ▶ Both fields try to uncover patterns in data
 - ▶ Both fields draw heavily on calculus, probability, and linear algebra, and share many of the same core algorithms
- But it is not statistics!
 - Stats is more concerned with helping scientists and policymakers draw good conclusions; ML is more concerned with building autonomous agents
 - ▶ Stats puts more emphasis on interpretability and mathematical rigor; ML puts more emphasis on predictive performance, scalability, and autonomy

Relations to AI

- Nowadays, "machine learning" is often brought up with "artificial intelligence" (AI)
- AI does not necessarily imply a learning-based system
 - Symbolic reasoning
 - ▶ Rule based system
 - ► Tree search
 - etc.

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Relations to human learning

- Human learning is:
 - ▶ Very data efficient
 - ► An entire multitasking system (vision, language, motor control, etc.)
 - ► Takes at least a few years :)
- For serving specific purposes, machine learning doesn't have to look like human learning in the end.
- It may borrow ideas from biological systems, e.g., neural networks.
- It may perform better or worse than humans.

What is machine learning?

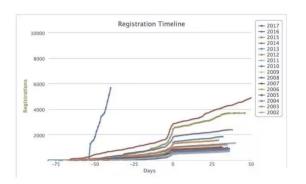
- Types of machine learning
 - Supervised learning: access to labeled examples of the correct behaviour
 - ▶ Reinforcement learning: learning system (agent) interacts with the world and learn to maximize a reward signal
 - ► Unsupervised learning: no labeled examples instead, looking for "interesting" patterns in the data

- 1957 Perceptron algorithm (implemented as a circuit!)
- 1959 Arthur Samuel wrote a learning-based checkers program that could defeat him
- 1969 Minsky and Papert's book *Perceptrons* (limitations of linear models)
- 1980s Some foundational ideas
 - Connectionist psychologists explored neural models of cognition
 - ▶ 1984 Leslie Valiant formalized the problem of learning as PAC learning
 - ▶ 1986 Backpropagation (re-)discovered by Geoffrey Hinton and colleagues
 - ▶ 1988 Judea Pearl's book *Probabilistic Reasoning in Intelligent Systems* introduced Bayesian networks

- 1990s the "AI Winter", a time of pessimism and low funding
- But looking back, the '90s were also sort of a golden age for ML research
 - ► Markov chain Monte Carlo
 - variational inference
 - kernels and support vector machines
 - boosting
 - convolutional networks
- 2000s applied AI fields (vision, NLP, etc.) adopted ML
- 2010s deep learning
 - ▶ 2010–2012 neural nets smashed previous records in speech-to-text and object recognition
 - increasing adoption by the tech industry
 - ▶ 2016 AlphaGo defeated the human Go champion

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ML conferences selling out like Beyonce tickets.



Source: medium.com/syncedreview/

ML conferences selling out like Beyonce tickets.



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Applications in Computer Vision

Object detection, semantic segmentation, pose estimation, and almost every other task is done with ML.





Instance segmentation - Link





What is there in front of the sofa?
Ground truth: table
IMG+BOW: table (0.74)
2-VIS+BLSTM: table (0.88)
LSTM: chair (0.47)



COCOQA 5078

How many leftover donuts is the red bicycle holding?

Ground truth: three IMG+BOW: two (0.51) 2-VIS+BLSTM: three (0.27) BOW: one (0.29)

Applications in Speech Recognition

Speech: Speech to text, personal assistants, speaker identification...



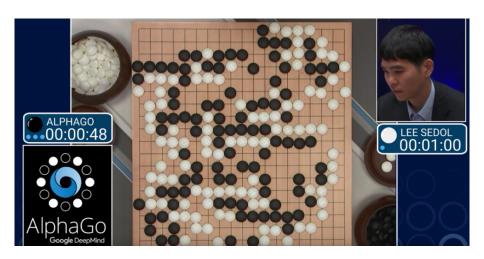
Applications in Natural Language Processing

NLP: Machine translation, sentiment analysis, topic modeling, spam filtering.

Real world example: The New York Times articles:

music band songs rock album jazz pop song singer night	book life novel story books man stories love children family	art museum show exhibition artist artists paintings painting century works	game Knicks nets points team season play games night coach	show film television movie series says life man character know
theater	clinton	stock	restaurant	budget
play	bush	market	sauce	tax
production	campaign	percent	menu	governor
show	gore	fund	food	county
stage	political	investors	dishes	mayor
street	republican	funds	street	billion
broadway	dole	companies	dining	taxes
director	presidential	stocks	dinner	plan
musical	senator	investment	chicken	legislature
directed	house	trading	served	fiscal

Applications in Playing Games



DOTA2 - Link

Applications in E-commerce & Recommender Systems : Amazon, Netflix, ...

Inspired by your shopping trends









Related to items you've viewed See more









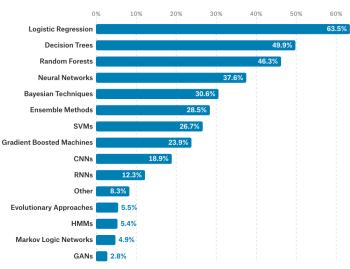
Why this class?

Why not jump straight to CSC413/2516 (Neural Networks), and learn neural nets first?

- The principles you learn in this course will be essential to really understand neural nets.
- The techniques in this course are still the first things to try for a new ML problem.
 - ► For example, you should try applying logistic regression before building a deep neural net!
- There is a whole world of probabilistic graphical models.

Why this class?

2017 Kaggle survey of data science and ML practitioners: what data science methods do you use at work?



ML Workflow

ML workflow sketch:

- 1. Should I use ML on this problem?
 - ▶ Is there a pattern to detect?
 - ► Can I solve it analytically?
 - ▶ Do I have data?
- 2. Gather and organize data.
 - ▶ Preprocessing, cleaning, visualizing.
- 3. Establishing a baseline.
- 4. Choosing a model, loss, regularization, ...
- 5. Optimization (could be simple, could be a PhD!).
- 6. Hyperparameter search.
- 7. Analyze performance and mistakes, and iterate back to step 4 (or 2).

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Implementing machine learning systems

- You will often need to derive an algorithm (with pencil and paper), and then translate the math into code.
- Array processing (NumPy)
 - vectorize computations (express them in terms of matrix/vector operations) to exploit hardware efficiency
 - ▶ This also makes your code cleaner and more readable!

```
Z = W_X + b
```

```
z = np.zeros(m)
for i in range(m):
    for j in range(n):
        z[i] += W[i, j] * x[j]
    z[i] += b[i]
z = np.dot(W, x) + b
```

Implementing machine learning systems

- Machine Learning framework: scikit-learn
- Neural net frameworks: PyTorch, TensorFlow, Theano, etc.
 - ▶ automatic differentiation
 - compiling computation graphs
 - ▶ libraries of algorithms and network primitives
 - ▶ support for graphics processing units (GPUs)
- Why take this class if these frameworks do so much for you?
 - ▶ So you know what to do if something goes wrong!
 - ▶ Debugging learning algorithms requires sophisticated detective work, which requires understanding what goes on beneath the hood.
 - ▶ That is why we derive things by hand in this class!

K-Nearest Neighbour Methods

Introduction

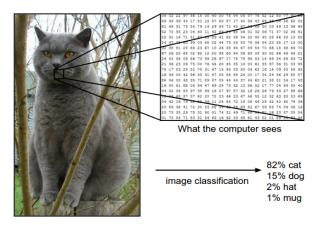
- Today (and for the next 5-6 lectures) we focus on supervised learning.
- This means we are given a training set consisting of inputs and corresponding labels (or target, output), e.g.

Task	Inputs	Labels	
object recognition	image	object category	
image captioning	image	caption	
document classification	text	document category	
speech-to-text	audio waveform	text	
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Input Vectors

What an image looks like to the computer:



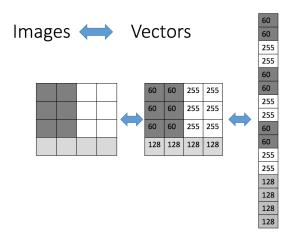
[Image credit: Andrej Karpathy]

Input Vectors

- Machine learning algorithms need to handle many different types of data: images, text, audio waveforms, credit card transactions, etc.
- Common strategy: represent the input as an input vector in \mathbb{R}^d
 - ► Representation = mapping to another space that is easy to manipulate
 - Vectors are a great representation since we can do linear algebra

Input Vectors

Can use raw pixels:



Can do much better if you compute a vector of meaningful features.

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- Mathematically, our training dataset consists of a collection of pairs of an input vector $\mathbf{x} \in \mathbb{R}^d$ and its corresponding target, or label, t
 - ightharpoonup Regression: t is a real number (e.g. stock price)
 - ▶ Classification: t is an element of a discrete set $\{1, \ldots, C\}$
 - ightharpoonup These days, t is often a highly structured object (e.g. image)
- Denote the training set $\{(\mathbf{x}^{(1)}, t^{(1)}), \dots, (\mathbf{x}^{(N)}, t^{(N)})\}$
 - ▶ Note: these superscripts have nothing to do with exponentiation!
- Question: Other examples of regression and classification problems?

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Developing our first ML algorithm

- Suppose that we are given the training set $\{(\mathbf{x}^{(1)}, t^{(1)}), \dots, (\mathbf{x}^{(N)}, t^{(N)})\}$, for a classification problem.
- Suppose we are given a novel input vector \mathbf{x} , and we are asked to classify it.
- Question: How can we do it?

Nearest Neighbours

- Suppose we are given a novel input vector \mathbf{x} we would like to classify.
- The idea: find the nearest input vector to **x** in the training set and copy its label.
- Can formalize "nearest" in terms of Euclidean distance

$$||\mathbf{x}^{(a)} - \mathbf{x}^{(b)}||_2 = \sqrt{\sum_{j=1}^d (x_j^{(a)} - x_j^{(b)})^2}$$

Algorithm:

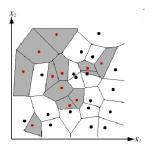
1. Find example (\mathbf{x}^*, t^*) (from the stored training set) closest to **x**. That is:

$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\operatorname{argmin}} \operatorname{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

- 2. Output $y = t^*$
- Note: we do not need to compute the square root. Why?

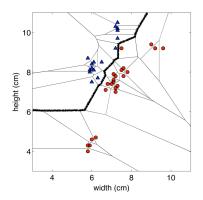
Nearest Neighbours: Decision Boundaries

We can visualize the behaviour in the classification setting using a Voronoi diagram.

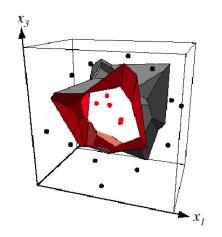


Nearest Neighbours: Decision Boundaries

Decision boundary: the boundary between regions of input space assigned to different categories.



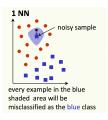
Nearest Neighbours: Decision Boundaries



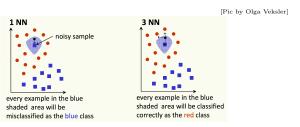
Example: 2D decision boundary

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[Pic by Olga Veksler]

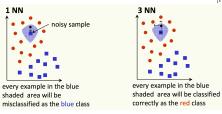


 Nearest neighbours sensitive to noise or mis-labeled data ("class noise"). Solution?



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- ullet Smooth by having k nearest neighbours vote





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- \bullet Smooth by having k nearest neighbours vote

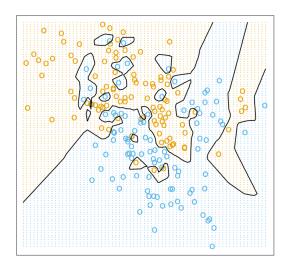
Algorithm (kNN):

- 1. Find k examples $\{\mathbf{x}^{(i)}, t^{(i)}\}$ closest to the test instance \mathbf{x}
- 2. Classification output is majority class

$$y = \operatorname*{argmax}_{t} \sum_{i=1}^{k} \mathbb{I}\{t = t^{(i)}\}$$

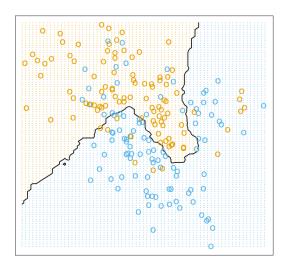
I{statement} is the identity function and is equal to one whenever the statement is true. We could also write this as $\delta(t^{(z)}, t^{(i)})$ with $\delta(a, b) = 1$ if a = b, 0 otherwise.

k = 1



[Image credit: "The Elements of Statistical Learning"]

$$k = 15$$

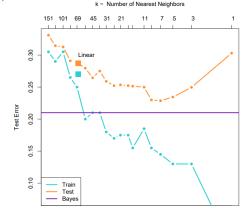


[Image credit: "The Elements of Statistical Learning"]

Tradeoffs in choosing k?

- \bullet Small k
 - Good at capturing fine-grained patterns
 - ► May overfit, i.e. be sensitive to random idiosyncrasies in the training data
- Large k
 - ▶ Makes stable predictions by averaging over lots of examples
 - ▶ May underfit, i.e. fail to capture important regularities
- Balancing k:
 - \blacktriangleright The optimal choice of k depends on the number of data points n.
 - ▶ Nice theoretical properties if $k \to \infty$ and $\frac{k}{n} \to 0$.
 - Rule of thumb: Choose $k = n^{\frac{2}{2+d}}$.
 - ightharpoonup We explain an easier way to choose k using data.

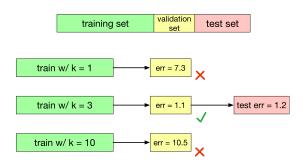
- We would like our algorithm to generalize to data it hasn't seen before.
- We can measure the generalization error (error rate on new examples) using a test set.



[Image credit: "The Elements of Statistical Learning"]

Training, Validation, and Test Sets

- The parameter k is an example of a hyperparameter, something we can't fit as part of the learning algorithm itself
- We can tune hyperparameters using a validation set:



• The test set is used only at the very end, to measure the generalization performance of the final configuration.

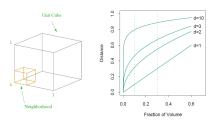
Why do we need an independent validation set?

Let us forget K-NN for a while, and focus on a much simpler problem:

- Suppose we are given real-valued random variables (r.v.) $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}$, all from the same distribution μ .
- We would like to compute the expectation of random variable $\mathbf{x} \sim \mu$ using the given data, i.e., $\mathbb{E}_{\mathbf{x} \sim \mu} [\mathbf{x}]$.
- Question: How to do it?
- Question: How to measure the quality of our estimate? (focus on N=1).

- Low-dimensional visualizations are misleading! In high dimensions, "most" points are far apart.
- If we want the nearest neighbour to be closer than ϵ , how many points do we need to guarantee it?

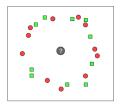
- Low-dimensional visualizations are misleading! In high dimensions, "most" points are far apart.
- If we want the nearest neighbour to be closer than ϵ , how many points do we need to guarantee it?
- The volume of a single ball of radius ϵ is $\mathcal{O}(\epsilon^d)$
- The total volume of $[0,1]^d$ is 1.
- Therefore $\mathcal{O}\left(\left(\frac{1}{\epsilon}\right)^d\right)$ balls are needed to cover the volume.



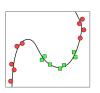
[Image credit: "The Elements of Statistical Learning"]

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• In high dimensions, "most" points are approximately the same distance. (Homework question coming up...)



• Saving grace: some datasets (e.g. images) may have low intrinsic dimension, i.e. lie on or near a low-dimensional manifold. So nearest neighbours sometimes still works in high dimensions.

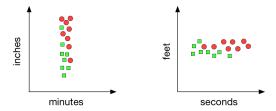






Pitfalls: Normalization

- Nearest neighbours can be sensitive to the ranges of different features.
- Often, the units are arbitrary:



• Simple fix: normalize each dimension to be zero mean and unit variance. I.e., compute the mean μ_j and standard deviation σ_j , and take

$$\tilde{x}_j = \frac{x_j - \mu_j}{\sigma_i}$$

• Caution: depending on the problem, the scale might be important!

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Pitfalls: Computational Cost

- Number of computations at training time: 0
- Number of computations at test time, per query (naïve algorithm)
 - ▶ Calculate *D*-dimensional Euclidean distances with *N* data points: $\mathcal{O}(ND)$
 - ▶ Sort the distances: $\mathcal{O}(N \log N)$
- This must be done for *each* query, which is very expensive by the standards of a learning algorithm!
- Need to store the entire dataset in memory!
- Tons of work has gone into algorithms and data structures for efficient nearest neighbours with high dimensions and/or large datasets.

Example: Digit Classification

• Decent performance when lots of data

0123456789

- Yann LeCunn MNIST Digit Recognition
 - Handwritten digits
 - 28x28 pixel images: d = 784
 - 60,000 training samples
 - 10,000 test samples
- Nearest neighbour is competitive

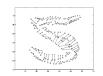
Test Error Ra	ate (%)
	(, ,
Linear classifier (1-layer NN)	12.0
K-nearest-neighbors, Euclidean	5.0
K-nearest-neighbors, Euclidean, deskewed	2.4
K-NN, Tangent Distance, 16x16	1.1
K-NN, shape context matching	0.67
1000 RBF + linear classifier	3.6
SVM deg 4 polynomial	1.1
2-layer NN, 300 hidden units	4.7
2-layer NN, 300 HU, [deskewing]	1.6
LeNet-5, [distortions]	8.0
Boosted LeNet-4, [distortions]	0.7

Example: Digit Classification

- KNN can perform a lot better with a good similarity measure.
- Example: shape contexts for object recognition. In order to achieve invariance to image transformations, they tried to warp one image to match the other image.
 - ▶ Distance measure: average distance between corresponding points on warped images
- \bullet Achieved 0.63% error on MNIST, compared with 3% for Euclidean KNN.
- Competitive with conv nets at the time, but required careful engineering.









[Belongie, Malik, and Puzicha, 2002. Shape matching and object recognition using shape contexts.]

Example: 80 Million Tiny Images

- 80 Million Tiny Images was the first extremely large image dataset. It consisted of color images scaled down to 32 × 32.
- With a large dataset, you can find much better semantic matches, and KNN can do some surprising things.
- Note: this required a carefully chosen similarity metric.



[Torralba, Fergus, and Freeman, 2007. 80 Million Tiny Images.]

Example: 80 Million Tiny Images



[Torralba, Fergus, and Freeman, 2007. 80 Million Tiny Images.]

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Conclusions

- Simple algorithm that does all its work at test time in a sense, no learning!
- Can be used for regression too, which we encounter later.
- ullet Can control the complexity by varying k
- Suffers from the Curse of Dimensionality
- Not very explainable.
- Next time: decision trees, another approach to regression and classification

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Questions?

?

Logistics

This Course

- Broad introduction to machine learning
 - ▶ Supervised learning: nearest neighbours, decision trees, ensembles, linear regression, logistic regression, SVM, neural networks
 - ▶ Unsupervised learning: PCA, K-means, mixture models
 - ▶ Reinforcement learning: Value Iteration and Q-Learning
- Coursework is aimed at advanced undergrads. We will use multivariate calculus, probability, and linear algebra.
- Do I have the appropriate background?
 - ► Linear algebra: vector/matrix manipulations, properties.
 - ► Calculus: partial derivatives/gradient.
 - ▶ Probability: common distributions; Bayes Rule.
 - Statistics: expectation, variance, covariance, median; maximum likelihood.

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- Course Website: https://amfarahmand.github.io/IntroML-Fall2021/
- Main source of information is the course webpage. Check regularly!
- We will also use Quercus for **announcements**.
- We will use Piazza for discussions.
- We will use MarkUs for assignment submission.

- This is an in-person course, but due to the risk of COVID-19's spreading within a crowded room, I intend to deliver it virtually too.
- Lectures will be delivered in-person and synchronously via Zoom. They will be recorded and shared for asynchronous viewing.

• In-person:

- ► Try to avoid coming to the classroom!
- ▶ Do not sit close to each other.
- ▶ Wear mask all the time.
- ► Get vaccinated!
- While cell phones and other electronics are not prohibited in lecture, talking, recording or taking pictures in class is strictly prohibited without the consent of your instructor. Please ask before doing!

• Virtual:

- ▶ You may download recorded lectures for your personal academic use, but you should not redistribute them.
- ▶ During lectures, please keep yourself on mute, unless you have a question.
- ▶ I encourage you to turn your videos ON. But you need to know that you may be recorded, and your videos will be publicly available.

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- Please refer to http://www.illnessverification.utoronto.ca in case of illness (you need to fill out an absence declaration form on ACORN and contact me).
- If you require additional academic accommodations, please contact UofT Accessibility Services: https://studentlife.utoronto.ca/department/accessibility-services/
- I realize that this is an unusually difficult time for all of us. I try to be as accommodating as possible.

Course Evaluation

This is tentative and may change in the next few days:

- Four (4) assignments (40%)
 - Combination of mathematical derivations, proofs, and programming exercises.
- Research Project (30%)
 - ▶ Research proposal, written report, and (possibly) class presentation.
- Take-Home Test (10%)
- Questions (10%)
- Read some seminal papers. (10%)
 - ▶ Short 1-paragraph summary and two questions on how the method(s) can be used or extended.
- Bonus (5%)
 - ▶ Finding typos in the slides, active class participation, evaluating the class, etc

Collaboration and Assignments

Collaboration:

- Collaboration on the Assignments is allowed, under certain conditions:
 - ▶ You can discuss the assignment with up to two other students (group of three).
 - ▶ You can work on the code together.
 - ▶ Each of you need to write down your homework individually. And mention the name of your collaborators clearly in the report and the source code.
- You need to form a team of 3 members to work on your projects (the exact number will be determined after finalizing the number of students enrolled).
- Collaboration on the Take-home test and Questions are not allowed.

Collaboration and Assignments

Late Submissions (assignments, proposals, reports, etc):

- Submissions should be handed in by deadline; a late penalty of 10% per day will be assessed thereafter (up to 3 days, then submission is blocked).
- Extensions will be granted only in special situations, and you will need a Student Medical Certificate or a written request approved by the course coordinator at least one week before the due date.

Related Courses and a Note on the Content

- More advanced ML courses such as CSC413/2516 (Neural Networks and Deep Learning), CSC412/2506 (Probabilistic Learning and Reasoning), and Introduction to Reinforcement Learning both build upon the material in this course.
- CSC2515 and CSC311 (previously CSC 411) have a long history at the University of Toronto. Each year, its content has been added, removed, or revised by different instructors. We liberally borrow from the previous editions.
- Credit goes to many professors, including (recent past): Roger Grosse, Murat Erdogdu, Richard Zemel, Juan Felipe Carrasquilla, Emad Andrews, etc.
- Warning: This is not a very difficult course, but it has a lot of content. To be successful, you need to work hard. For example, don't start working on your homework assignments just two days before the deadline.

Useful Resources

Recommended readings will be given for each lecture. But the following will be useful throughout the course:

- Trevor Hastie, Robert Tibshirani, and Jerome Friedman, The Elements of Statistical Learning, Second Edition, 2009.
- Christopher M. Bishop, Pattern Recognition and Machine Learning, 2006
- Richard S. Sutton and Andrew G. Barto, Reinforcement Learning: An Introduction, Second Edition, 2018.
- Amir-massoud Farahmand, Lecture Notes on Reinforcement Learning, 2021.
- Ian Goodfellow, Yoshua Bengio and Aaron Courville, Deep Learning, 2016
- Kevin Murphy, Machine Learning: A Probabilistic Perspective, 2012.
- Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani, An Introduction to Statistical Learning, 2017.
- Shai Shalev-Shwartz and Shai Ben-David, Understanding Machine Learning: From Theory to Algorithms, 2014.
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There are lots of freely available, high-quality ML resources.