Welcome to Machine Learning!

COMP 4630 | Winter 2025

Charlotte Curtis

What is this course about?

- Continuing the supervised/unsupervised learning algorithms from COMP 3652, with a focus on **Neural Networks**
- First half: the history, theory, and math behind neural networks
- Second half: applications of NNs in computer vision, natural language processing, and more

> *This is not (just) a course on building models using libraries like TensorFlow or PyTorch, it is a course on understanding the theory*

How did I get involved with ML?

1

UNIVERSITY of GUELPH

Biomedical Engineering

Signal processing

2

UNIVERSITY OF CALGARY

MSc: Image registration
PhD: Radar image reconstruction

Time/frequency transforms

3

Statistical modelling
simple CNNs

Baker Hughes

Pipeline inspection algorithms research → data science

4

MOUNT ROYAL UNIVERSITY 1910

Vector graphics manipulation for sewing patterns

Open source software,
mostly heuristics

What do you want to learn about ML?

Grade Assessment

Component	Weight
Assignments	3 x 10%
Midterm (theory) exam	20%
Journal club	15%
Final project	35%

Bonus marks may be awarded for *substantial* corrections to materials, submitted as pull requests

Course materials repo: https://github.com/mru-comp4630/w25

Textbooks and other readings

Primary Textbook:

- Hands on Machine Learning with Scikit-Learn and Tensorflow
- Associated GitHub repo

More mathy details:

- Deep Learning

Journal club list:

- MRU Library Reading List

Machine Learning Project Checklist

Appendix A of the hands-on textbook

1. **Frame the problem** and look at the big picture.
2. **Get the data.**
3. **Explore the data** to gain insights.
4. **Prepare the data** to better expose the underlying data patterns to Machine Learning algorithms.
5. Explore many different models and short-list the best ones.
6. Fine-tune your models and combine them into a great solution.
7. Present your solution.
8. Launch, monitor, and maintain your system.

Bold stuff is what we'll discuss in this topic

1. Look at the big picture

Example Dataset: California housing prices (1990)

❓ Discussion questions:

- How does the company expect to use and benefit from this model?
- What is the current solution?
- What kind of ML task is this?
- What kind of performance measure should we use?

2. Get the data

For this class, we'll use readily available datasets. Some sources are:

- UCI Machine Learning Repository
- Kaggle
- Google Dataset Search
- Various Government open data portals (e.g. Calgary, Alberta, Canada)

After fetching the data, set aside a test set and **don't look at it**.

> ***"Get the data"*** *can often be a huge task in itself!*

2a. Set aside a test set

❓ Discussion questions:

- Why do we need an independent test set?
  - Avoid data snooping bias
  - Relevant XKCD
- Why would we use a random seed?
- What is naive about simply selecting a random sample?
- What else could we do?
- What is stratified sampling?

Side tangent: Sampling bias

- Simple example: assume 80% of population likes cilantro
- Goal: ensure our sample is representative of the population, $\pm 5\%$

The binomial distribution can be used to model the probability of choosing k people who like cilantro from n total participants:

$$P(X = k) = \binom{n}{k} p^k (1 - p)^{n-k}, \text{where} \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

Side tangent: Sampling bias continued

$P(X = k)$ is the probability mass function, and the corresponding cumulative distribution function is just the sum up to k:

$$P(X \leq k) = \sum_{i=0}^{k} \binom{n}{i} p^i (1-p)^{n-i}$$

By adding together $P(X \leq 0.8 - 0.05)$ and $P(X \geq 0.8 + 0.05)$, we get the probability of sampling bias (by the $\pm 5\%$ definition).

> *This is also my excuse to review some probability theory and notation*

3. Explore the data

? Discussion questions:

- What do you notice about the data?
- Do the values make sense for the labels?
- Is the scale of the features comparable? Does this matter?
- What possible biases might be present in the data?

3a. Look for correlations

The Pearson correlation coefficient is a measure of the linear correlation between two variables X and Y (commonly denoted as r):

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

where $\bar{x}$ and $\bar{y}$ are the sample means of X and Y, respectively.

- What do correlations of 0, 1, and -1 mean?
- What are some limitations of Pearson correlation?

4. Prepare the data

General goals:

- Handle missing data, and maybe outliers
- Drop irrelevant features
- Combine features using domain knowledge
- Apply various transformations (e.g. scaling, encoding)
- Apply scaling when necessary

4a. Handling missing data

In the book 3 options are listed to handle the NaN values:

```
housing.dropna(subset=["total_bedrooms"], inplace=True) # option 1
housing.drop("total_bedrooms", axis=1)                   # option 2
median = housing["total_bedrooms"].median()              # option 3
housing["total_bedrooms"].fillna(median, inplace=True)
```

❓ Discussion questions:

- What is each option doing?
- What are the pros and cons of each option?
- Which one should we choose?

4b. Handling non-numeric data

Most of the math in ML algorithms is based on numbers, so we need to convert text and categorical attributes to numbers. This is called **encoding**.

❓ Discussion questions:

- Which columns of our data are categorical?
- What methods could we use to convert them to numbers?
- What are the assumptions about the various encoding methods?

4c. Scaling the data

Many ML algorithms don't like features with vastly different scales. Common scaling methods are **min-max scaling** and **standardization**.

> *Important: scaling is **computed** on the training set and **applied** to the validation and test sets - they are not scaled independently!*

❓ Discussions questions:

- What are the bounds of each method?
- Which method is more affected by outliers?
- How would you decide which method to use?

4e. Standardization details

A general Gaussian distribution is given by:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

where μ is the mean and σ is the standard deviation. The standard normal distribution is a special case where $\mu = 0$ and $\sigma = 1$, reducing the equation to:

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

4f. Other transformations

- **Log transformation**: useful for data that is heavily skewed
- Also **square root, squaring, etc.**: try to remove heavy tails
- **Feature engineering**: combining features to create new ones
- **Binning**: turning continuous data into discrete categories
    - Possibly using K-means clustering
    - Relies on domain knowledge
- Best to create a **transformation pipeline** and apply it to the data rather than saving the transformed data