

# Machine Learning for Science & Society

- Spring 2021
- Tuesdays 5:30-8:15
- Professor Sarah Brown
- CSC 592: Topics in Computer Science

In this class, we will address the challenges in applying machine learning to scientific research and in high stakes social contexts. On the science side, we will examine the role of ML in research, in particular how it works within knowledge production and how to evaluate ML in line with domain norms. On the social side, we will consider how to ensure ML-based algorithmic decision making systems uphold social values, with a focus on fairness. While these two applications are distinct, many of the challenges translate into common technical problems. Some of the common challenges include:

- missing data
- noisy or missing labels
- multiple objectives

We will look at a range of strategies for identifying and mitigating these problems including:

- robust evaluation
- model inspection
- explanations
- interpretable models

## Format

This will be a synchronous course offered via Zoom. To successfully participate in this course students will need:

- consistent internet access during class time
- to use URI SSO credentials to access readings and materials
- a microphone to participate in conversations in class, at least most sessions

The course will involve:

- reading and evaluating ML research papers
- facilitating and participating in class discussions of the papers
- producing a replication, demo, or illustration of one concept covered for a broader audience
- completing a project using ML in a scientific or social domain
- writing a CS conference style (short & concise) final paper on their project

*graduate students are encouraged to do a project related to their research*

## Prerequisites

To be successful in this class students should have:

- past experience with machine (CSC461 or equivalent)
- basic programming skills
- familiarity with concepts in probability, linear algebra, and calculus that appear in ML

varying skill in these topics is ok, but a general understanding of the basic ideas is important. If you're interested and not sure if you have the background, complete the form below

## Basic Facts

## Meetings

This class will meet on Monday and Wednesday 3-4:15pm. via Zoom (link provided to registered students via BrightSpace)

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## Tip

You can [subscribe to the Brightspace Calendar](#) to access it in your favorite calendaring tool.

## Instructor

Professor Sarah M Brown is an Assistant Professor in Computer Science. Her current research aims to answer the question, “How can machine learning produce AI systems that make fair decisions?”

## Office Hours

By appointment, link on Brightspace.

## Schedule

We will meet synchronously via Zoom: Tu 5:30-8:15

This course will proceed in three main parts: overview, deep dives, and wrap up.

## Structure

### Overview

In the first part of the course we will review ML basics, set norms for interaction and complete a survey of the topics that we will cover for the rest of the semester.

In this part of the class, Professor Brown will lead synchronous sessions. Students will be responsible for reading overviews, refreshing background material, and choosing an area for their course project. Students will start with an introductory demo or replication as a mini project.

### Deep Dives

During the middle of the course we will spend one week on each topic. There will be 1-3 papers to read each week.

Students will be responsible for presenting papers in class on a rotating basis.

During this time students will have milestones where they need to complete interim steps for their course project. The first milestone will be a proposal that includes the specific products for the remainder of the milestones based on a template.

### Conclusion

In the end of the course, we will focus on integrating ideas across multiple topics.

We will also workshop students' projects, giving substantive feedback prior to the final submissions.

Final projects will be evaluated through a presentation and paper

## Weekly topics

Class	Topic	Reading	Activities
2021-01-29	Introduction	None	introductions, expectation setting
2021-02-01	Probability Review	Model Based ML, chapter 1	reading discussion, setting
2021-02-03	ML Process & Mutual information	Scikit learn getting started, preview	live coding
2021-02-08	Missing Data: Intro strategies	<a href="#">Handling Missing Values when Applying Classification Models</a> & <a href="#">Missing data imputation using statistical and machine learning methods in a real breast cancer problem</a>	Paper discussion led by Daniel
2021-02-10	Missing data with graphical models and causal reasoning	<a href="#">Graphical Models for Inference with Missing Data</a> & <a href="#">Missing Data as a Causal and Probabilistic Problem</a>	Paper discussion led by Julian
2021-02-15	Current Challenges in Missing data	<a href="#">from Artemiss workshop</a>	Paper overview
2021-02-17	Current Challenges in Missing data	<a href="#">from Artemiss workshop</a>	Replication and testing discussion and preview of lasso and admm constraint to multiobjective reformulation'''
2021-02-22	Fairness	fairml classification chapter and friedler empirical comparison paper	Empirical setup
2021-02-24	Fairness	Reading	Activities
2021-03-01	Multi-objective & constrained opt	Reading	Activities
2021-03-03	Multi-objective & constrained opt	Reading	Activities
2021-03-08	Multi-objective & constrained opt	Reading	Activities
2021-03-10	Multi-objective & constrained opt	Reading	Activities
2021-03-15	Noisy & Missing labels	Reading	Activities
2021-03-17	Noisy & Missing labels	Reading	Activities
2021-03-22	Interpretable & Explanation	survey	Activities
2021-03-24	Interpretable	Rudin HDR, CORELS	Activities
2021-03-29	Interpretability	Science of - Kim & Doshi	Activities
2021-03-31	Interpretability	Falsifiable, survey	Activities
2021-04-05	Explanation - perturbation based	Reading	Activities
2021-04-07	Explanation	TCAV	Activities

Class	Topic	Reading	Activities
2021-04-12	Meta issues	ml & phil sci	Activities
2021-04-13	Meta issues	Roles for computing in social change	Activities
2021-04-19	Project Presentations	projects	peer feedback
2021-04-21	Project Presentations	projects	peer feedback
2021-04-26	Project Presentations	Reading	revision plans

Table 1 Schedule

## Learning Outcomes and Evaluation

This course has goals with respect to the knowledge and research skills.

Evaluation will be with respect to each of the outcomes and based on a level of mastery: general awareness, competency, or mastery.

By the end of the course students will be able to:

- Critique common ways that social or scientific applications of ML require violating ML algorithm assumptions and ways to mitigate or adapt.
- Evaluate ML Research papers for their applicability to scientific and social applications of ML.
- Communicate about ML and its limitations work to varied audiences
- Apply ML to scientific and social data responsibly

## Activities

- reading and evaluating ML research papers
- facilitating and participating in class discussions of the papers
- producing a replication, demo, or illustration of one concept covered for a broader audience
- completing a project using ML in a scientific or social domain
- writing a CS conference style (short & concise) final paper on the project

## Evaluation

The grading scheme is rooted in achieving the learning outcomes and is holistic rather than averaged over a number of activities. A more detailed rubric will be provided soon, in this space.

## Presentation and participation

Presenting papers and participating in class will contribute to demonstrating a basic awareness at each of learning objective. Active participation and presentations will be evaluated and feedback will be provided after each presentation and regularly on other participation.

## Translation mini project

For this assignment you can choose any topic other than the one your project is for and produce a short demo, illustration, or replication that makes some aspect of the the topic.

For this, you must submit a one paragraph proposal by the Friday after we cover that topic in class. Once that's approved that it will count, you have two weeks to build your demo or replication. The latest your demo may be submitted is at the same time as your final project.

## Project Timeline

Date	Milestone	Submission format
2021-02-19	Area Selection	Consultation meeting and general questions
2021-03-01	Topic Selection	Objectives and scope of work
2021-03-15	Proposal	Problem statement, lit review, method
2021-04-02	Checkin	Consultation meeting and prelim result
2021-04-13	Rough draft	Draft ready for peers to read
2021-04-19,21	Presentation	talk in class
2021-04-26	revision plan	plan for final revision, minor extensions
2021-05-07	final paper	final paper submitted for grading

## Class 1: Introductions

### Introductions & Goals

#### Course Admin

- Brightspace
- Zoom
- Google docs or markdown in the future?
- Website

### Learning outcomes

knowledge research

- identify common problems and solutions in scientific application of ML
- identify common challenges and solutions for social applications: fairness,
- implement and extend research papers

### Activities

- reading and evaluating ML research papers
- facilitating and participating in class discussions of the papers
- producing a replication, demo, or illustration of one concept covered for a broader audience
- completing a project using ML in a scientific or social domain
- reflect on methodologies used in this type of research
- writing a CS conference style (short & concise) final paper on their project

### Model Based ML and this course

<https://www.mbmlbook.com/toc.html>

- missing data
- noisy or missing labels
- multiple objectives

We will look at a range of strategies for identifying and mitigating these problems including:

- robust evaluation
- model inspection
- explanations
- interpretable models

# ML and Probability Review

## admin

- collaborative notes
- brightspace will be updated later this week
- grading details by Wed
- environment for coding demos

## More formalism

- model
- prediction algo
- cost function
- objective

## Probability

- sample distros

## Practical Application of ML & Pipelines

## Class 3: ML Pipelines

### Goals when using ML

1. Understand about the data (data science/ actual science) probability more statistics, maybe fit another examine model parameters, inspect them
2. understanding about Naive bayes fit different data varies
3. claims about the learning algorithm run multiple algorithms on the same data possibly multiple data

### Basic setup

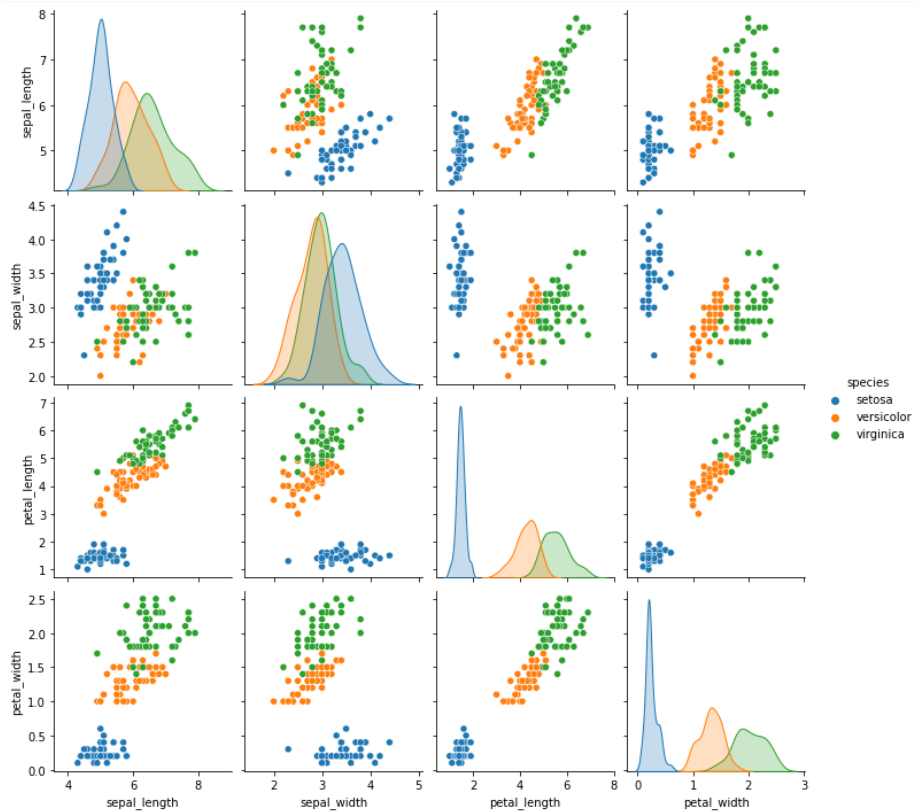
1. test train
2. training parameters
3. estimator objects
4. fit model parameters
5. metrics
6. cross validation

```
import pandas as pd
import seaborn as sns
import numpy as np
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import train_test_split
from sklearn.naive_bayes import GaussianNB
from sklearn.metrics import confusion_matrix, classification_report
from sklearn import datasets
```

```
iris_df = sns.load_dataset('iris')
```

```
sns.pairplot(iris_df, hue='species')
```

```
<seaborn.axisgrid.PairGrid at 0x7f5d7679ae50>
```



```
X,y = datasets.load_iris(return_X_y=True)
```

```
X.shape
```

```
(150, 4)
```

```
y.shape
```

```
(150,)
```

```
X_train, X_test, y_train, y_test = train_test_split(X,y,)
```

```
gnb = GaussianNB()
```

```
gnb.__dict__
```

```
{'priors': None, 'var_smoothing': 1e-09}
```

```
gnb.fit(X_train,y_train)
```

```
GaussianNB()
```

```
gnb.__dict__
```

```
{'priors': None,
 'var_smoothing': 1e-09,
 'n_features_in_': 4,
 'epsilon_': 3.115098852040817e-09,
 'classes_': array([0, 1, 2]),
 'theta_': array([[5.01025641, 3.47435897, 1.47692308, 0.25641026],
 [5.92222222, 2.75555556, 4.23333333, 1.32777778],
 [6.57297297, 3.00810811, 5.55135135, 2.04324324]]),
 'sigma_': array([[0.13374096, 0.13113741, 0.03408284, 0.0122025 ],
 [0.26839506, 0.12024692, 0.225      , 0.04645062],
 [0.32467495, 0.10128561, 0.2614171 , 0.08137327]]),
 'class_count_': array([39., 36., 37.]),
 'class_prior_': array([0.34821429, 0.32142857, 0.33035714])}
```

```
X_test[0]
```

```
array([4.8, 3. , 1.4, 0.3])
```

```
y_pred = gnb.predict(X_test)
```

```
y_pred[:5]
```

```
array([0, 2, 1, 1, 2])
```

```
y_test[:5]
```

```
array([0, 2, 1, 1, 2])
```

```
confusion_matrix(y_test, y_pred)
```

```
array([[11,  0,  0],
       [ 0, 14,  0],
       [ 0,  2, 11]])
```

```
gnb.score(X_test,y_test)
```

```
0.9473684210526315
```

```
gnb2 = GaussianNB(priors=[.5,.25,.25])
```

```
gnb2_cv_scores = cross_val_score(gnb2,X_train,y_train)
```

```
np.mean(gnb2_cv_scores)
```

```
0.9557312252964426
```

```
gnb_cv_scores = cross_val_score(gnb,X_train,y_train)
```

```
np.mean(gnb_cv_scores)
```

```
0.9557312252964426
```

```
print(classification_report(y_test,y_pred))
```

	precision	recall	f1-score	support
0	1.00	1.00	1.00	11
1	0.88	1.00	0.93	14
2	1.00	0.85	0.92	13
accuracy			0.95	38
macro avg	0.96	0.95	0.95	38
weighted avg	0.95	0.95	0.95	38



```
gnb.predict_proba(X_test)
```

```
array([[1.00000000e+000, 6.85597803e-015, 9.43917702e-026],
       [3.64835492e-164, 1.49513445e-005, 9.99985049e-001],
       [2.44895658e-117, 6.02869604e-001, 3.97130396e-001],
       [1.70611210e-085, 9.86236811e-001, 1.37631888e-002],
       [1.79831920e-118, 1.37268680e-001, 8.62731320e-001],
       [1.00000000e+000, 4.71324609e-016, 4.22602407e-026],
       [1.00000000e+000, 9.65870388e-016, 4.75782846e-026],
       [1.75153909e-109, 9.71840917e-001, 2.81590834e-002],
       [1.00000000e+000, 8.18869141e-016, 1.69694441e-026],
       [4.77969817e-237, 1.56833962e-009, 9.99999998e-001],
       [2.74916132e-178, 3.00911074e-006, 9.99996991e-001],
       [1.60432038e-081, 9.85144797e-001, 1.48552028e-002],
       [1.95823817e-153, 2.40997259e-003, 9.97590027e-001],
       [2.93923404e-163, 2.81790553e-006, 9.99997182e-001],
       [1.00000000e+000, 2.15371970e-016, 2.86010033e-026],
       [3.99624566e-193, 2.17590355e-006, 9.99997824e-001],
       [7.24588175e-064, 9.99857281e-001, 1.42719214e-004],
       [6.20829269e-134, 4.08741470e-002, 9.59125853e-001],
       [4.37909429e-095, 9.92553104e-001, 7.44689600e-003],
       [1.01670276e-067, 9.99743002e-001, 2.56998074e-004],
       [1.00000000e+000, 3.20819333e-016, 1.19111135e-026],
       [7.09041118e-079, 9.99058047e-001, 9.41953456e-004],
       [2.71522188e-087, 9.86524973e-001, 1.34750271e-002],
       [1.67874012e-091, 9.81701098e-001, 1.82989017e-002],
       [2.15058737e-062, 9.99832891e-001, 1.67109032e-004],
       [1.56024318e-098, 8.84861288e-001, 1.15138712e-001],
       [1.00000000e+000, 2.42285070e-016, 1.83810540e-026],
       [5.25044578e-192, 5.53648944e-007, 9.99999446e-001],
       [1.00000000e+000, 6.58900905e-014, 7.14786900e-026],
       [4.45922570e-238, 4.41241616e-009, 9.99999996e-001],
       [2.34864277e-058, 9.99975742e-001, 2.42578957e-005],
       [9.40024581e-073, 9.98830307e-001, 1.16969299e-003],
       [1.00000000e+000, 5.29579500e-018, 3.09021799e-028],
       [1.00000000e+000, 5.77917341e-016, 3.87039015e-026],
       [9.43114387e-031, 9.99999974e-001, 2.60000511e-008],
       [1.00000000e+000, 8.55364084e-017, 1.34338435e-027],
       [4.95952142e-061, 9.99962059e-001, 3.79414433e-005],
       [3.10578202e-193, 7.35028342e-008, 9.99999926e-001]])
```

## Class 4: Missing Data: Basic techniques

### Evaluation of missing data at training

- multiple imputation
- ML based was better than imputation which is better than dropping samples
- example datasets: 45% of patients have at least 1 missing value

### Imputation

- Mean imputation:
  - insert the mean based on the other values
- Hot deck
  - mean-like with similarity
- Multiple imputation
  - 3 diff ways

### Imputation ML

- MLP
  - fully connected
- Self organization
  - competitive learning
  - NN on modle of nodes in 2d grid,
- KNN
  - select closest complete case to impute values from
  - expensive for large datasets due to need to search everywhere for each missing value

## Testing

- Train NN based on data imputed with each technie

Conclusions:

- in general, any imputation was better than deletion
- ML based performed better

## Discussion & Questions

- interesting that even simple methods provide improvement
- SOM is sort of unclear how does that work?
- Review of MLP and [sigmoid](#)

## Handling missing values At application time

- reduced models vs imputation.
- broad approach
- 15 common datasets

## Techniques:

- Discard
- Acquire missing values
- Imputation
  - predictive value imputation
  - distribution based
  - unique values
- Reduced Feature Models
  - retrain for different feature models

Feature imputability impacts the distribution or predictive type of imputation

## More complex model

- decision tree with bagging
- again, reduced model is the best strategy

## Hybrid Models for efficient prediction

- reduced models
- a hybrid is a complete model with stored subset for most common missing features
- Reduced feature ensemble
  - N models for N features
  - each one is missing one feature
  - average these together for final prediction
  - substantial reduction in when there is a single feature is missing
  - combine with imputation for multiple features
  - relative accuracy is better than imputation

## General takeaways

- reduced models vs imputatation is a large improvement
- this is sort of an imputation

## Weaknesses

- Didn't check unique value imputation
- MCAR
- focused on

## Overall Discussion

- How might the two problems interact?
  - if missing data at both train and prediction...
  - train using missing data without imputation for training the separate models
- Questions on these ideas
- What additional things might you need to consider when choosing one?
  - feature imputability at training
- what to do with time series data
- How to check if missing CAR?
  - look at collection technique
  -
- what do to with varying data per person
  - LSTM for time series data
  - hierarchichal modeling other wise
  - [example of hierarchical with time series also](#)

## For Wednesday

1. [Graphical Models for Inference with Missing Data](#)
2. [Missing Data as a Causal and Probabilistic Problem](#)

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By Sarah M Brown

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