# xHour Mini Tutorial on Python Programming for Machine Learning

COSC74/174: Machine Learning and Statistical Data Analysis | Winter 2019 | Dartmouth

# **Outline**

In this mini tutorial session, you will learn:

- Python installation and programming interfaces
- Basic python
- The *NumPy* module for mathematical operations
- Scikit-learn (sklearn) for machine learning

Along the way, we will show examples and/or resources for:

- (Optional) pandas and scipy modules
- (Optional) Data visualization using matplotlib
- (Optional) Writing documents with math expressions using LaTex (Overleaf) & Markdown

# **Python Versions and Dependencies**

(Credit: E. Yao'19, J. Wei'20, D. Chen GR)

Why Python at all?

- Fast to code. Syntax is very easy, many built-in functionalities with the language (sum(), max(), min(), etc.)
- Flexible. If you really want performance, it's pretty easy to write C extensions to code to make things run faster. In fact, the NumPy library is written in C.
- Forgiving. Unless you're working in a large codebase or mission-critical code, why would you ever want static typing?
- Popularity in machine learning, deep learning and data science community

Python3 is recommended. Most of data-science frameworks, particularly more recent ones, are adapted to, or developed in, Python3. It's OK if you prefer to use Python2, just keep in mind some commands may be different.

# **Programming Interfaces for Python**

### **Jupyter Notebook (recommended)**

#### **Pros**

- Free and open source
- Supports both code and Markdown chunks that can be assembled into a professionally looking document
- Compatible with most libraries and standard installation approach

#### **Cons**

 Takes time to get used to, particularly if you are used to IDE-based programming (e.g. RStudio)

#### For COSC74/174 Canvas submission

- Execute all code chunks (Kernel -> Restart and Run All), and save the notebook. Submit the .ipynb file
- (Optional) HTML or PDF report of your .ipynb notebook
- Submit any required output files (e.g. CSV results, written description/report)
   wherever appropriate

### Integrated Developer Environment (IDE)

You are free to try out and choose an IDE that works for you.

Examples: PyCharm (IDEA), Spyder (via Anaconda)

#### **Pros**

- Pretty, customizable programming interface
- *PyCharm*, for example, has similar layout as other products by IDEA (e.g. IntelliJ for Java, Rider for C#)
- Custom programming environment

#### Cons

- Might not be free or open source (or free with reduced functionality)
- Module installation can be tricky

#### For COSC74/174 Canvas submission

- Submit .py script containing all functions
- Submit any required output files (e.g. CSV results, written description/report) wherever appropriate

### Command line (not recommended for beginners)

- Use of your favorite text editor (e.g. Atom, Eclipse, VS Code, TextWrangler)
- In a terminal/command line, execute python script via python3 <script-name>

The following structure is commonly used:

Same Canvas submission procedure as the previous slide

# **Anaconda Python Distribution**

(Credit: E. Yao'19, J. Wei'20, D. Chen)

A distributor of python that bundles many useful components for data science and machine learning!

#### **Pros:**

- Choice between Python 2 and Python 3 (e.g. Kernel -> Change Kernel)
- Many libraries are preinstalled (numpy, scipy, django, jupyter, beautifulsoup, etc.)
- Also has a package manager like pip! (conda install <module-name>)
- Easy to install Windows and Mac installers are the 'clicky kind'. You can probably get by without opening a Terminal.

#### Cons:

• Still "semi-global" - you can screw up dependencies in anaconda, but at least you don't have to delete python from your system!

#### Anaconda installation/usage instructions:

- 1. Download Anaconda from <a href="https://www.anaconda.com/download/#macos">https://www.anaconda.com/download/#macos</a> (<a href="https://www.anaconda.com/download/#macos">https://www.anaconda.com/download/#macos</a>)
- 2. Run jupyter notebook in Terminal to open up jupyter notebook.
- 3. To create an environment, put in terminal: conda create -n <your-env-name> python=x.x anaconda
- 4. To activate the environment, source activate <your-env-name>
- 5. To install libraries, run pip3 install sklearn

# (Optional) Installation via Virtual Environment (venv)

(Credit: E. Yao'19)

#### virtualenv installation/usage instructions

- 1. Install *virtualenv* using pip/pip3 for an existing python distribution (do this only once) (pip install virtualenv, pip3 install virtualenv should work for most people)
- 2. Create a virtualenv for an example project inside the folder (do this once per project) (cd to/project/folder && virtualenv .env (NOTE: .env can be any folder you prefer). virtualenv will install a python interpreter and depedencies to the folder you just created
- 3. Start the *virtualenv* (need to do this every time before you start working on the project). Assuming you installed to ./.env, run source .env/bin/activate or .env/bin/activate
- 4. Once you are done with everything, be sure to run deactivate to quit virtualenv

If the above works, you should see some informations in parenthesis before the BASH/shell prompt.

Now, whenever you pip install something, it will be installed to the subfolder .env and you will only be able to use it when you have the virtualenv activated. While venv is activated, your global python installation won't be touched.

To remove a venv, you can simply delete the .env folder.

# **Basic Python Tutorial**

These are tutorials that you can learn and practice at your own times.

- Variables
- Lists (arrays)
- Dictionaries
- Control structure
- Functions

# Variables, Types, and Basic Math

# **Special operators**

### Lists

- Creation
- Concatenation
- Access elements within lists
- List comprehension

### List creation

```
In [5]: zero_list = [0] * 3
    string_list = ['hello'] * 3
    empty_list = list()
    # empty_list = [] #alternative

    print(zero_list)
    print(string_list)
    print(empty_list)

[0, 0, 0]
['hello', 'hello', 'hello']
[]
```

#### List concatenation and access

```
In [6]: ## Create new list:
    new_list = zero_list + string_list
    print(new_list)

[0, 0, 0, 'hello', 'hello']

In [7]: ## Access elements in a list (i.e. indexing):
    print(new_list[0])
    print(new_list[0:2])
    print(new_list[-1])

0
    [0, 0]
    hello
```

### List comprehension

List comprehension is not found in other programming languages, but very common and effective in python.

I Love Machine Learning

Check out some more details with hands-on example in this <u>DataCamp blogpost</u> (https://www.datacamp.com/community/tutorials/python-list-comprehension).

#### **Dictionaries**

Important: Unlike lists that are ordered, dictionaries aren't.

```
In [10]: empty_dict = dict()
    # empty_dict = {} #alternative

    ## Key-value pair:
    ## Integer keys:
    num_key_dict = {3: 'Hello', 4:'World!'}

print(num_key_dict)

{3: 'Hello', 4: 'World!'}

In [11]: ## String keys:
    string_key_dict = {'Hello':3, 'World!':4}
    print(string_key_dict)

{'World!': 4, 'Hello': 3}
```

# **Control Structure**

- if-elif-else statements
- for loops
- while loops

### if-elif-else statement

```
if x < 0:
    x = 0
    print('x is negative but now changed to zero!')
elif x == 0:
    print('Zero')
elif x == 1:
    print('One')
else:
    print('Something else')</pre>
```

Something else

### For loops

Control structure that allows iterative operations (e.g. through a range of values)

Note for programmers in C#, PHP: for loops in python syntax can accomplish tasks done by foreach loop

# While loops

Note: You may use the break statement to exit loops including a while loop

# **Functions in Python**

### Functions using def keyword

The def keyword is used for "defining" a function in python.

**Note:** Key components of your machine learning algorithm implementation are required to be formatted in function format.

### (Advanced) Functions using lambda keyword

lambda is another reserved word in python for more succinctly creating a function.

- lambda-based function definition is good for short, simple functions, but less suitable for longer and more complex functions
- A common use of lambda is when passing the given function as argument into another function

```
In [16]: addition_via_lambda = lambda a,b: a+b
print(addition_via_lambda(3,4))
```

7

# The *NumPy* Module

NumPy is one of the most commonly used libraries in python. In a nutshell, NumPy supports:

- Basic mathematical operations
- Matrix computations
- Statistical methods (e.g. t, Wilcoxon, Kolgomorov-Simirnov tests)
- Data object manipulation (e.g. reshaping)
- Compatibility with operations within built-in python methods and other modules (e.g. pandas)

There are numerous free tutorials for *Numpy*, including

- Official documentation (https://docs.scipy.org/doc/numpy/user/quickstart.html)
- <u>DataCamp's Intro to Python for DataScience (https://www.datacamp.com/courses/intro-to-python-for-data-science)</u>
- <u>Udacity's Intro to Data Analysis (https://www.udacity.com/course/intro-to-data-analysis--ud170)</u>
- Harvard EdX's Using Python for Research (https://www.edx.org/course/usingpython-for-research)

### Array-based operation in NumPy

```
In [17]: import numpy as np

## Create arrays:
    x = np.array([[1,2,3],[4,5,6]], dtype=np.float64)
    y = np.array([[7,8,9],[10,11,12]], dtype=np.float64)

print(x)
print(y)

[[ 1.    2.    3.]
    [ 4.    5.   6.]]
    [[ 7.    8.   9.]
    [ 10.   11.   12.]]
```

```
In [18]: ## Element-wise addition:
    print(x + y)
# print(np.add(x, y)) #equivalent

[[ 8. 10. 12.]
    [ 14. 16. 18.]]

In [19]: ## Element-wise subtraction:
    print(x - y)
# print(np.subtract(x, y)) #equivalent

[[-6. -6. -6.]
    [-6. -6. -6.]]
```

```
In [20]: ## Element-wise multiplication:
         print(x * y)
         # print(np.multiply(x, y)) #equivalent
         [[ 7. 16. 27.]
          [ 40. 55. 72.]]
In [21]: ## Element-wise division:
         print(x / y)
         # print(np.divide(x, y)) #equivalent
         [[ 0.14285714 0.25
                                   0.333333331
          [ 0.4
                        0.45454545 0.5
                                             11
In [22]: ## Element-wise square root:
         print(np.sqrt(x))
         # print(x ** (1/2)) #equivalent
                       1.41421356 1.73205081]
         [[ 1.
          [ 2.
                       2.23606798 2.44948974]]
```

#### Summarize data in matrix format

```
In [23]: | ## Calculate mean along rows:
         print("Average (arithmetic mean) of rows:")
         np.mean(x, axis=0)
         Average (arithmetic mean) of rows:
Out[23]: array([ 2.5, 3.5, 4.5])
In [24]: ## Calculate mean along the columns:
         print("Average (arithmetic mean) of columns:")
         np.mean(x, axis=1)
         Average (arithmetic mean) of columns:
Out[24]: array([ 2., 5.])
In [25]: ## Calculate matrix mean:
         print("Average (arithmetic mean) of entire matrix x:")
         np.mean(x, axis=None)
         Average (arithmetic mean) of entire matrix x:
Out[25]: 3.5
```

### Basic commands to manipulate arrays

```
In [26]: ## Transposing arrays:
         print("Original:")
         print(x)
         print("\n Transposed:")
         print(np.transpose(x))
         # print(x.T) #equivalent
         Original:
         [[ 1. 2. 3.]
          [ 4. 5. 6.]]
          Transposed:
         [[ 1. 4.]
          [ 2. 5.]
          [ 3. 6.]]
In [27]: ## Reshaping arrays:
         print("\n Reshaped:")
         print(np.reshape(x, (3,2)))
          Reshaped:
         [[ 1. 2.]
          [ 3. 4.]
          [ 5. 6.]]
```

### **Commands for Matrix Algebra**

Please see the <u>numpy linear algebra documentation (https://docs.scipy.org/doc/numpy/reference/routines.linalg.html)</u> for full list of functionality. These commands are very useful especially if you are working with deep learning applications. Below are a few very basic examples.

#### **Dot Product**

#### **Cross Product (aka vector product)**

#### **Matrix Multiplication**

- Be sure to apply the <u>"row-column" (https://en.wikipedia.org</u> /wiki/Matrix (mathematics)) rule for dimensions. Otherwise you'll see error!
- Remember, order of the two matrices matter!

```
In [30]: print("Dimension of matrix x:" + str(x.shape))
print("Dimension of matrix y:" + str(y.shape))

Dimension of matrix x:(2, 3)
Dimension of matrix y:(2, 3)
```

The resultant matrix of  $XY^{\top}$  is therefore:

Likewise, in this example you can also calculate  $\mathbf{X}^{\mathsf{T}}\mathbf{Y}$ :

# (Optional) pandas module

pandas is an open-source library for efficient data-frame object manipulation in python.

To install pandas with Anaconda, run the following in the command line / terminal:

```
conda install pandas

or with pip:

python3 -m pip install --upgrade pandas
```

There are several good tutorials for *pandas*, including:

- Official documentation (https://pandas.pydata.org/pandas-docs/stable /10min.html)
- Free course on Udacity (https://www.udacity.com/course/intro-to-data-analysis--ud170)
- YouTube tutorial by J James (https://www.youtube.com/watch?v=e60ItwlZTKM)

# (Optional) SciPy and statsmodel Modules

<u>SciPy (https://docs.scipy.org/doc/scipy/reference/stats.html)</u> and <u>statsmodel</u> (<u>https://www.statsmodels.org/stable/index.html</u>) provides many useful functions related to scientific computing, particularly *statistics*.

Both modules are compatible with NumPy and pandas.

You may use these already-implemented functions for this course, and perhaps for your own research and studies as well.

# Scikit-learn for Supervised and Unsupervised Learning

You are highly encouraged to review the tutorials in the <u>official documentation</u> (<u>http://scikit-learn.org/stable/tutorial/index.html</u>).

#### **Dataset**

We will use the build-in Iris data set as an example. Othere toy data sets could be explored (<a href="sklearn.datasets">sklearn.datasets</a> (<a href="http://scikit-learn.org/stable/datasets">http://scikit-learn.org/stable/datasets</a>) for more detail).

#### **Approaches**

- Logistic regression (supervised learning)
- *K*-means (unsupervised learning)

# Supervised Learning: a Simple Example

```
In [33]: import sklearn
    from sklearn.datasets import load_iris #built-in data
    import matplotlib.pyplot as plt #data visualization

Iris = load_iris()
    X = Iris.data[:,[1,3]] #select 2 features for demo
    y = (Iris.target == 2) #create a binary DV

print("Dimension of feature space: " + str(X.shape))
    print("Dimension of class label (should be a column vector): " + str(y.shape))

Dimension of feature space: (150, 2)
```

Dimension of class label (should be a column vector): (150,)

[ 3.6 0.2]]

0.333333333333

[False False False]

sklearn offers a convenient function, train\_test\_split, to divide you data into a training set and a held-out validation set.

Training-test split is typically done at a ratio, which could be 80:20,70:30, or even 60:40. There is no steadfast rule on this.

```
In [35]: from sklearn.model_selection import train_test_split

TEST_SIZE = 0.30 #adjust as desired
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=TEST_SIZE, ran dom_state=42)
```

```
In [36]: from sklearn.linear_model import LogisticRegression

## Initialize the logistic regression classifier
clf = LogisticRegression()

## Fit the training set to the initialized classifier
clf.fit(X_train, y_train)
```

Out[36]: LogisticRegression(C=1.0, class\_weight=None, dual=False, fit\_intercept=True, intercept\_scaling=1, max\_iter=100, multi\_class='ovr', n\_jobs=1, penalty='12', random\_state=None, solver='liblinear', tol=0.0001, verbose=0, warm\_start=False)

```
In [37]: ## Apply the model to held-out test set:
    ## Class labels:
    test_class = clf.predict(X_test)
    print(test_class)

## Probability scores for being in Class 1/True
    ## Required for computing area under the curve (AUC)
    test_score = clf.predict_proba(X_test)
    print(test_score[:,1])
```

[False False True False False False True True False True False False False False True False True False True False False True True False False False False False False True False False False True False False False False [ 2.03482773e-01 2.54386105e-03 9.38921527e-01 3.82473836e-01 3.37543332e-01 6.52019113e-03 2.36951279e-01 8.78953518e-01 6.38984628e-01 2.28876780e-01 6.89320643e-01 4.22750324e-03 2.82415139e-03 3.64077876e-03 2.54386105e-03 3.24346027e-01 8.56602972e-01 2.20997742e-01 2.65131755e-01 8.89668882e-01 4.42209336e-03 6.00259153e-01 6.52019113e-03 8.50961252e-01 4.74254570e-01 8.94027831e-01 7.60707099e-01 8.62065746e-01 8.39656062e-03 5.13408067e-03 2.43171893e-03 1.46221422e-03 2.45220050e-01 3.27970665e-03 4.42209336e-03 8.17837295e-01 2.83113387e-01 2.82415139e-03 2.43171893e-03 8.14647298e-04 7.68837219e-01 2.92375811e-01 3.14520960e-01 3.09050622e-03 2.09370278e-031

### **Model Evaluation**

The confusion matrix is useful in calculating metrics, including

- TPR
- TNR
- FPR
- FNR
- Sensitivity
- Specificity
- Precision
- Recall

See <a href="mailto:this://en.wikipedia.org/wiki/Confusion\_matrix">this page (https://en.wikipedia.org/wiki/Confusion\_matrix</a>) for detail.

The F1 Score (https://en.wikipedia.org/wiki/F1 score) and Area under the receiveroperation curve (AUROC, or ROC) (https://developers.google.com/machine-learning/crashcourse/classification/roc-and-auc) are common metrics for evaluate classifiers, and are superior to the "crude" accuracy defined as:

$$accuracy = \frac{TP + TN}{TP + FP + FN + TN}$$

Details are to be covered in the course.

```
In [39]: from sklearn.metrics import fl_score, roc_auc_score, roc_curve

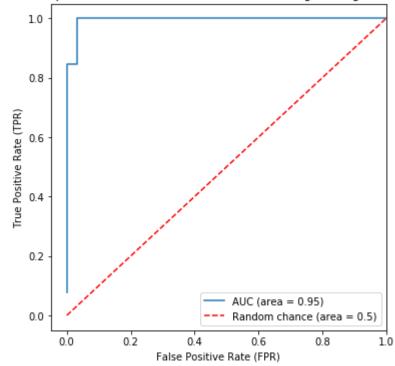
## F1 scores on test set:
f1 = f1_score(y_test, test_class, average="binary", sample_weight=None)
print("F1 score:" + str(f1))

## AUC on test set:
logit_roc_auc = roc_auc_score(y_test, clf.predict(X_test))
print("AUC score:" + str(logit_roc_auc))
```

F1 score: 0.923076923077 AUC score: 0.945913461538

```
In [40]: ## Sketch ROC curve and show AUC:
    fpr, tpr, thresholds = roc_curve(y_test, clf.predict_proba(X_test)[:,1])
    plt.figure(2, figsize=(6,6))
    plt.plot(fpr, tpr, label='AUC (area = %0.2f)' % logit_roc_auc)
    plt.plot([0, 1], [0, 1], 'r--', label="Random chance (area = 0.5)")
    plt.xlim([-0.05, 1.0])
    plt.ylim([-0.05, 1.05])
    plt.ylabel('False Positive Rate (FPR)')
    plt.ylabel('True Positive Rate (TPR)')
    plt.title('Receiver operation characteristic (ROC) curve for logistic regression m odel')
    plt.legend(loc="lower right")
    plt.show()
```

#### Receiver operation characteristic (ROC) curve for logistic regression model



# Summary of *sklearn* Supervised Learning

- *sklearn* offers many already written and extensively tested machine-learning algorithms
- Aside of machine learning, *sklearn* offers useful functionalities
- Learning to search and learn from documentation is a critical skill of a good programmer!

# Notes on Programming Component of Homework Assignments

• For every machine-learning algorithm, you are required to include the following components as *functions* (though you are free to name your functions differently from below):

```
    train_model(...)
    apply_model(...) or predict
    evaluate_model(...) (optional, doesn't have to be in functional form)
```

- You may have additional functions (e.g. cross\_validate(...)), if necessary. Likewise, you may write your own helper functions/methods.
- Good programming etiquette, which includes writing clean, well-documented and reasonably commented code, is highly encouraged. Poor organization, messy code shows lack of care and may be penalized.
- While optional, you are encouraged to explore the data before implementing machine learning, visualize the data as well as your results after building the model. These optional procedures do not have to be implemented as functions.

(Continued on the next page)

## Example: train\_model function

You could wrap the code shown in the previous several slides as follows.

Documentation (doc string) is encouraged but not required.

#### To use this function:

```
myLogisticModel = train model(myFeatures, myLabels)
```

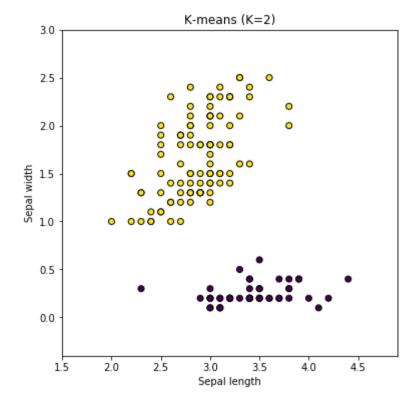
# **Unsupervised Learning: a Simple Example**

In unsupervised learning, there is no ground truth, and we determine *clusters* based on some *distance metrics* (more details are to be covered in lecture).

We will use K-means clustering as a demo for unsupervised learning, where K indicates the number of clusters, each of which has a centroid.

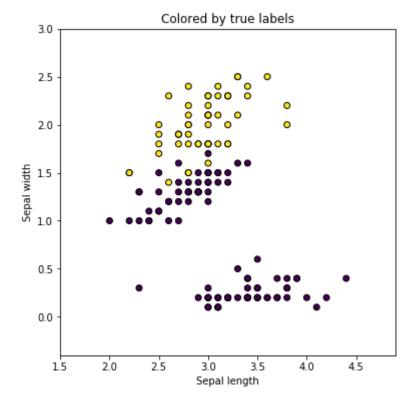
```
In [42]: ## Color by K-means centroids:
    x_min,x_max = X[:,0].min()-0.5, X[:, 0].max()+0.5
    y_min,y_max = X[:,1].min()-0.5, X[:, 1].max()+0.5
    plt.figure(figsize=(6,6))
    plt.clf()
    plt.scatter(X[:, 0], X[:, 1], c=cluster_labels, edgecolor='k')
    plt.xlabel('Sepal length')
    plt.ylabel('Sepal width')
    plt.xlim(x_min, x_max)
    plt.ylim(y_min, y_max)
    plt.title('K-means (K=2)')
```

Out[42]: Text(0.5,1,u'K-means (K=2)')



```
In [43]: ## Color by true labels:
    plt.figure(figsize=(6,6))
    plt.clf()
    plt.scatter(X[:, 0], X[:, 1], c=y, edgecolor='k')
    plt.xlabel('Sepal length')
    plt.ylabel('Sepal width')
    plt.xlim(x_min, x_max)
    plt.ylim(y_min, y_max)
    plt.title('Colored by true labels')
```

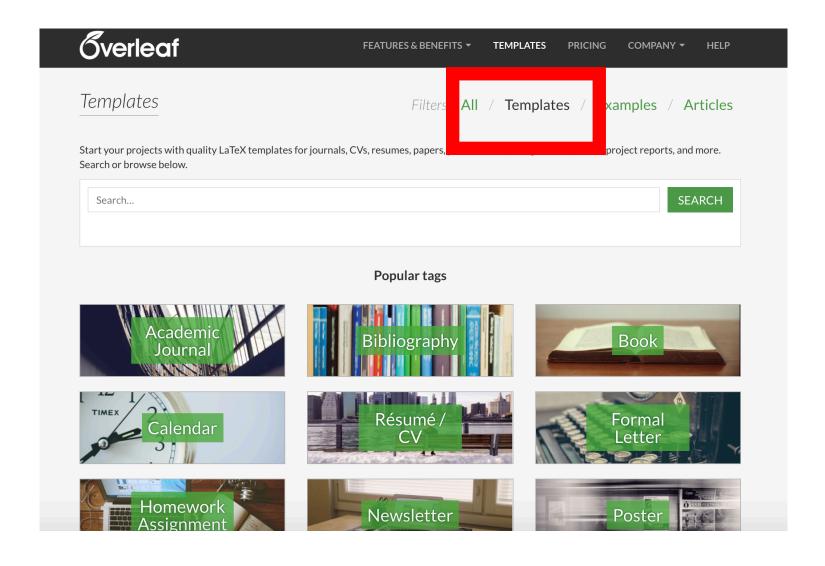
Out[43]: Text(0.5,1,u'Colored by true labels')



# Resources on LaTex/Markdown Language for Writing Report Consisting of Math/Scientific Expressions

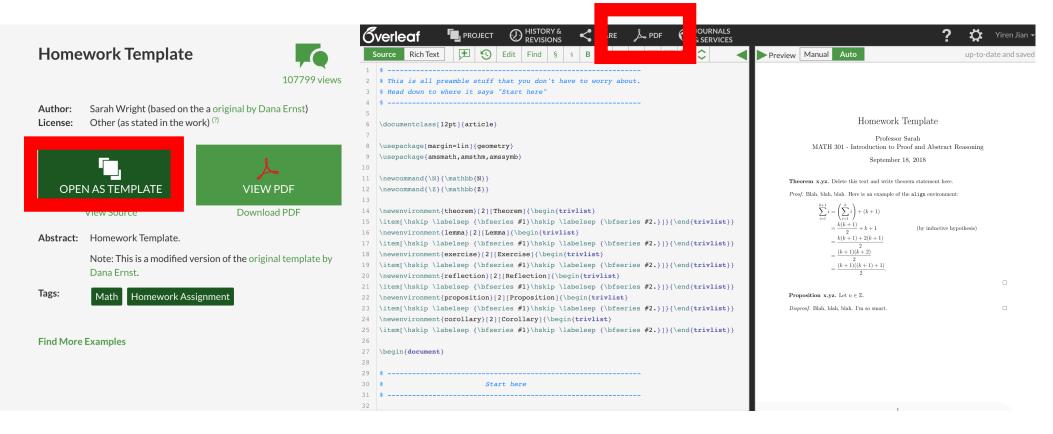
- For non-programming, theoretical homework problems, you are highly encouraged to use LaTex to produce a professional-looking document, instead of having them handwritten and scanned/photographed
- In fact, in the programming portion of the presentation, you already saw the use of Markdown/LaTex language.
- If you are using Jupyter Notebook, the "Markdown" option for any given chunk supports LaTex syntax.
- Take a look at this <u>LaTex tutorial (https://www.latex-tutorial.com/quick-start/)</u>
- There are also numerous good YouTube tutorials, such as <a href="mailto:this.one-by-L.Smith">this one by L. Smith</a> (<a href="https://www.youtube.com/watch?v=mfRmmZ-84Mw">https://www.youtube.com/watch?v=mfRmmZ-84Mw</a>).
- LaTex can be operated in many editors (e.g. MikTex, TexStudio), which will require installation. Overleaf is an online editor that does not require installation.

Overleaf is a free online Latex platform. You can use it without installing any software and packages. It also provides you with a lot of templates, not only for your homework, but also thesis paper, CV...



After you register your account, choose a template from homework assignment.

You can download the PDF file once you finish.



You edit your text here and it will automatically render the PDF file for you.

### http://physics.clarku.edu/sip/tutorials/TeX/intro.html

This is a good example showing how to make equation, tables, lists, figures and special symbols. And you can always ask help from Google.