Technology Lab: Using AI Frameworks in Jupyter Notebook

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11/29/2022

High Performance Research Computing
DIVISION OF RESEARCH

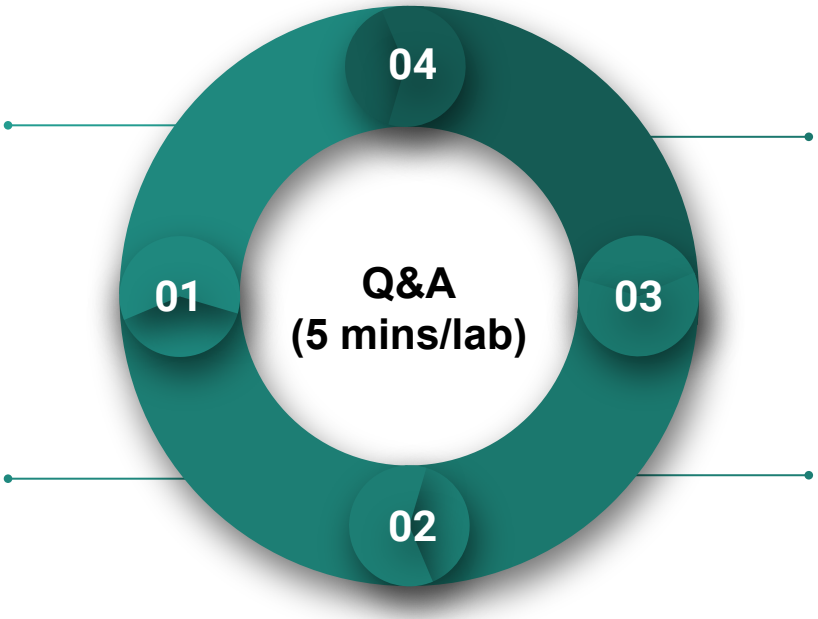
AI Tech Labs

Lab I. JupyterLab (30 mins)

We will load required modules with Jupyter Lmode extension and run JupyterLab.

Lab II. Data Exploration (30 mins)

We will go through some examples with two popular Python libraries: Pandas and Matplotlib for data exploration.



Lab IV. Deep Learning (30 minutes)

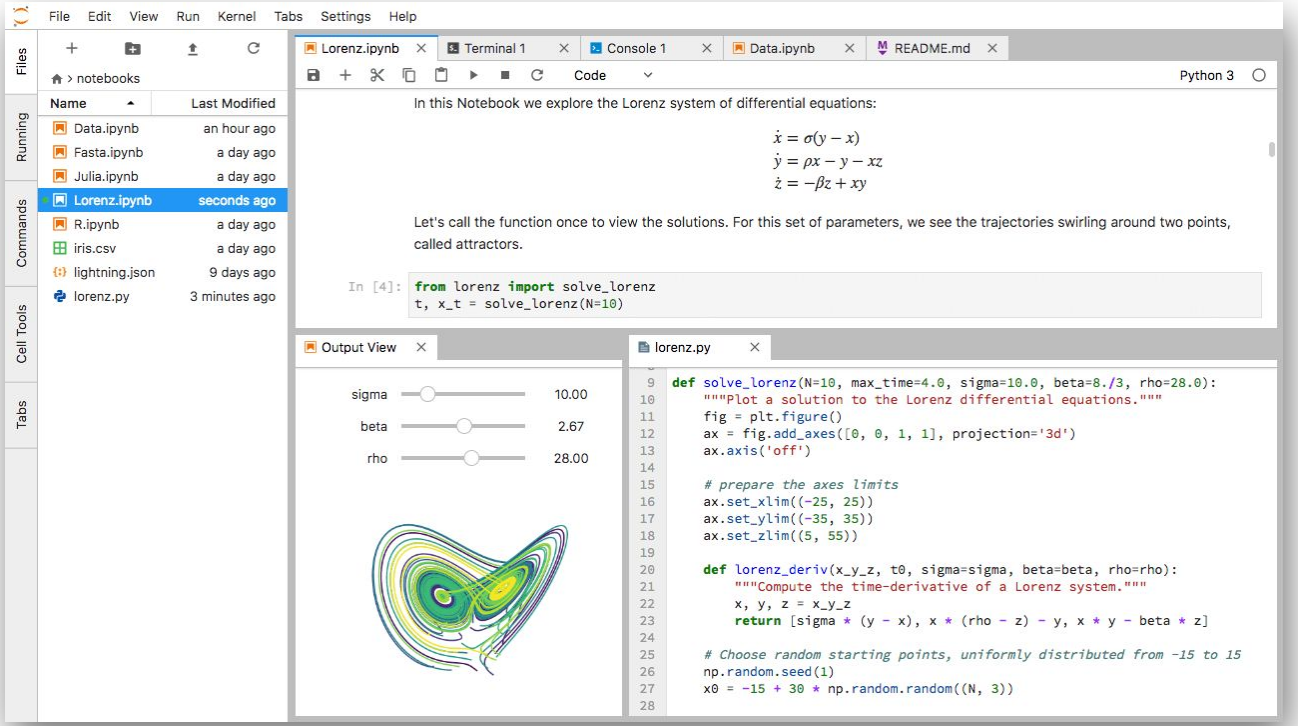
We will learn how to use Keras to build and train a simple image classification model with deep neural network (DNN).

Lab III Machine Learning (30 minutes)

We will learn to use scikit-learn library for linear regression and classification applications.

Figure 1. Structure of the Technology Lab.

Lab I. JupyterLab



L1 - Resources

- Texas A&M High Performance Research Computing (HPRC)
- FASTER Quick Start Guide
- ACES Phase I Guide
- ACCESS Documentation
- FASTER Portal
- HPRC YouTube Channel
- help@hprc.tamu.edu

Getting Started with FASTER and ACES

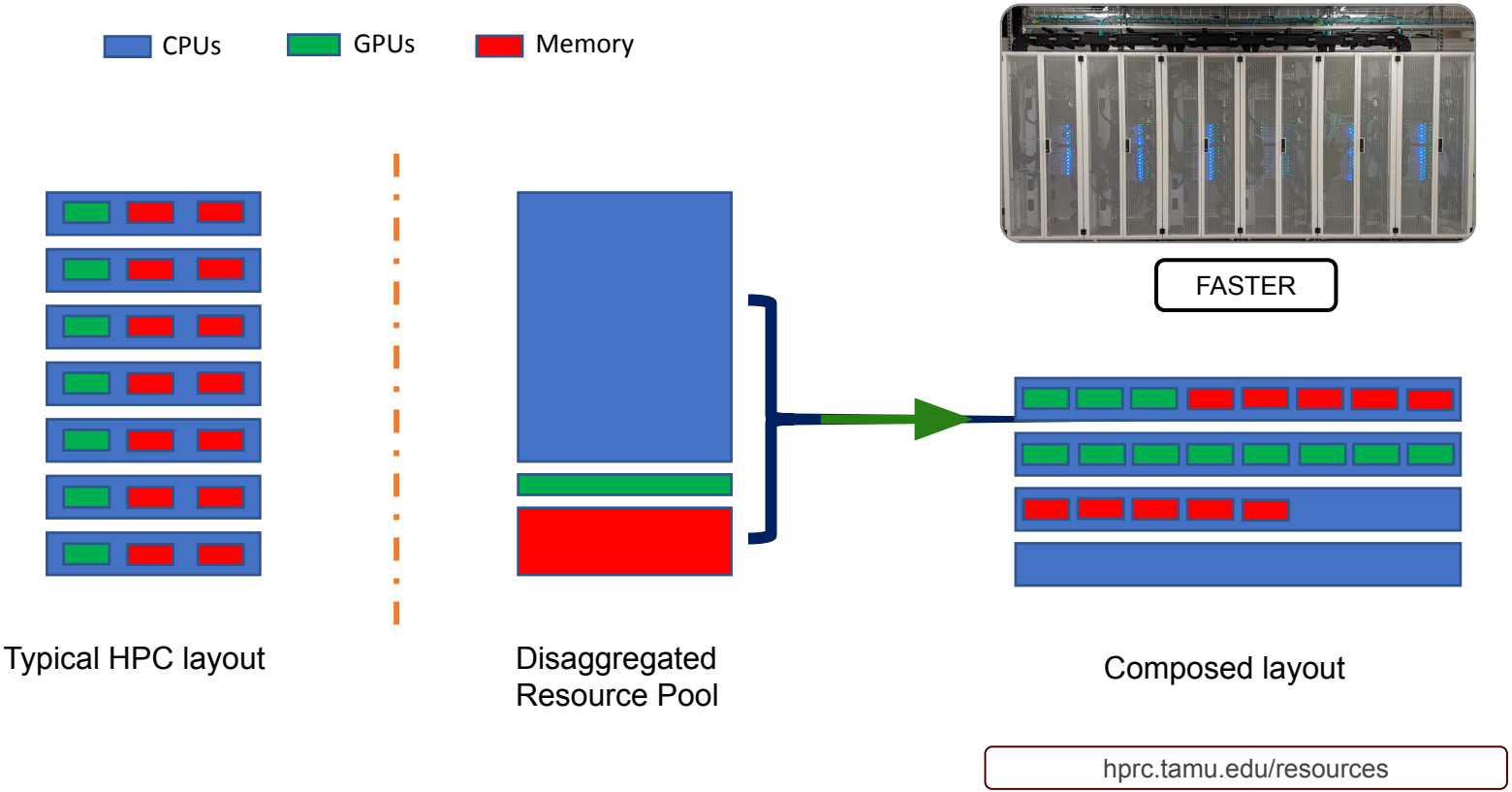
FASTER Cluster

hprc.tamu.edu/wiki/FASTER:Intro

Node Type	Quantity
64-core login nodes	4 (3 for TAMU, 1 for ACCESS)
64-core compute nodes (256GB RAM each)	180 (11,520 cores)
Composable GPUs	200 T4 16GB 40 A100 40GB 10 A10 24GB 4 A30 24GB 8 A40 48GB
Interconnect	Mellanox HDR100 InfiniBand (MPI and storage) Liqid PCIe Gen4 (GPU composability)
Global Disk	5PB DDN Lustre appliances

FASTER (Fostering Accelerated Sciences Transformation Education and Research) is a 180-node Intel cluster from Dell featuring the Intel Ice Lake processor.

Composability at the Hardware Level

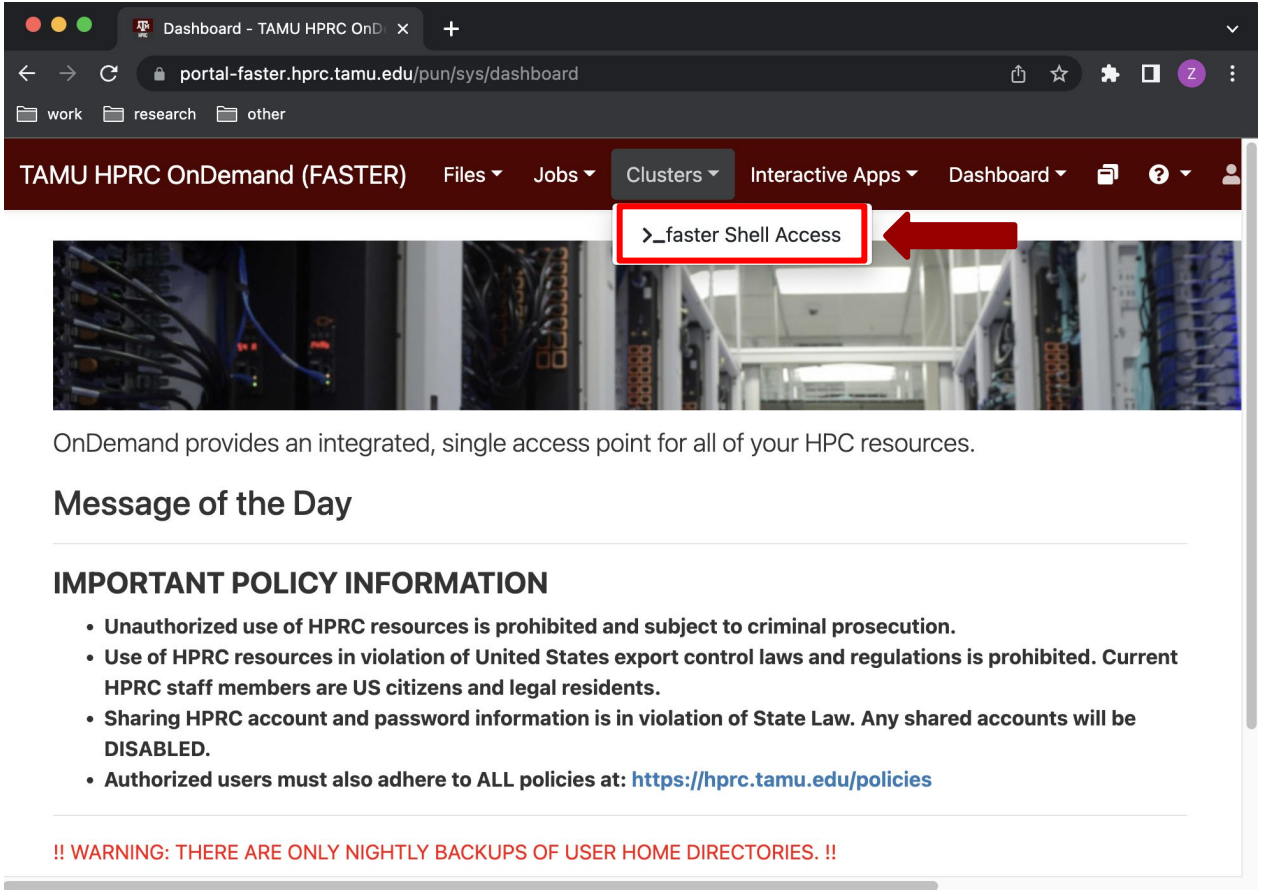


ACES - Accelerating Computing for Emerging Sciences (Phase I)

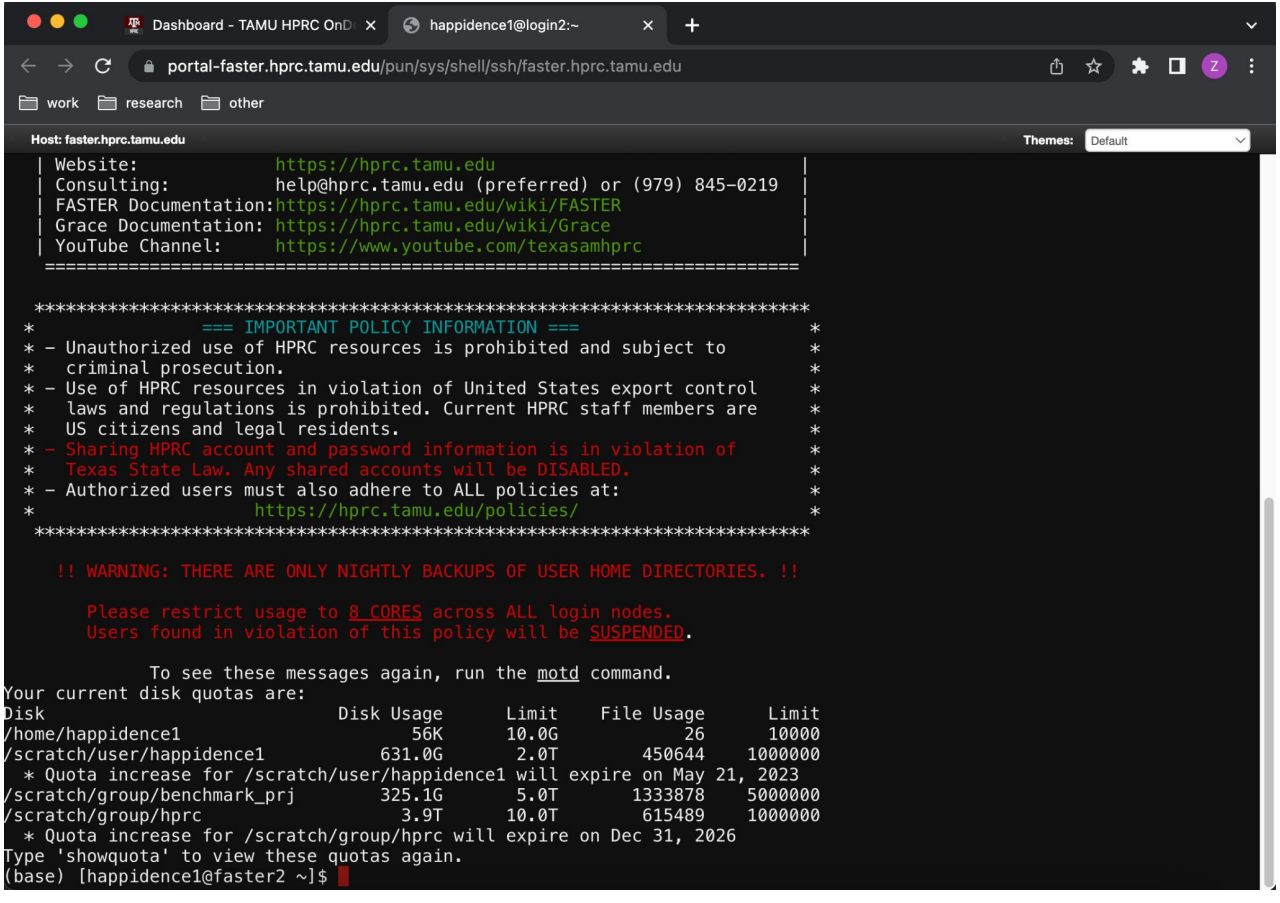
Component	Quantity	Description
Graphcore IPU	16	16 Colossus GC200 IPUs and dual AMD Rome CPU server on a 100 GbE RoCE fabric
Intel FPGA PAC D5005	2	FPGA SOC with Intel Stratix 10 SX FPGAs, 64 bit quad-core Arm Cortex-A53 processors, and 32GB DDR4
Intel Optane SSDs	8	3 TB of Intel Optane SSDs addressable as memory using MemVerge Memory Machine.

ACES Phase I components are available through FASTER

Shell Access - I



Shell Access - II



Commands to copy the materials

- Navigate to your personal scratch directory

  ```
  $ cd $SCRATCH
  ```

- Files for this course are located at

  ```
  /scratch/training/ai_tech_labs
  ```

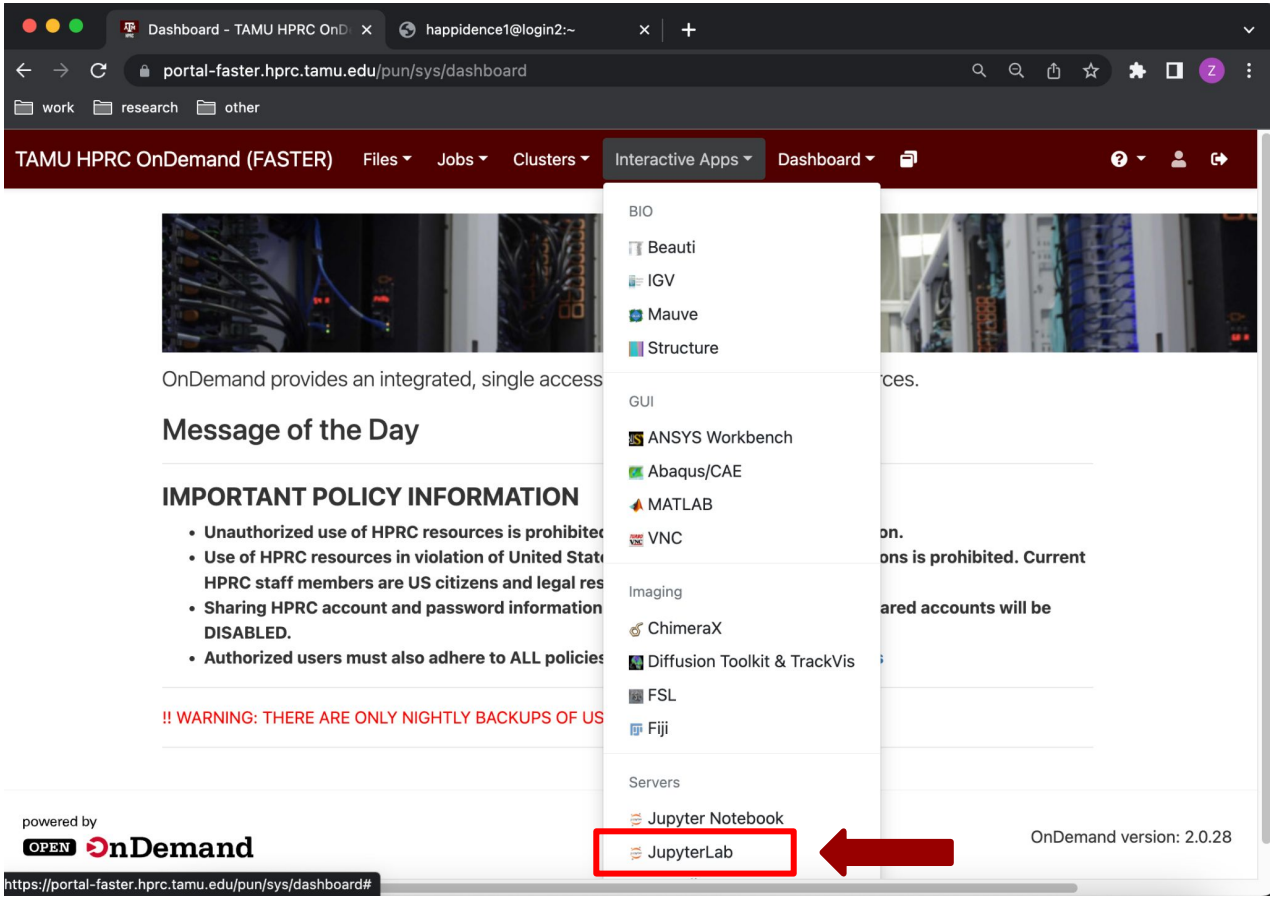
  Make a copy in your personal scratch directory

  ```
  $ cp -r /scratch/training/ai_tech_labs $SCRATCH
  ```

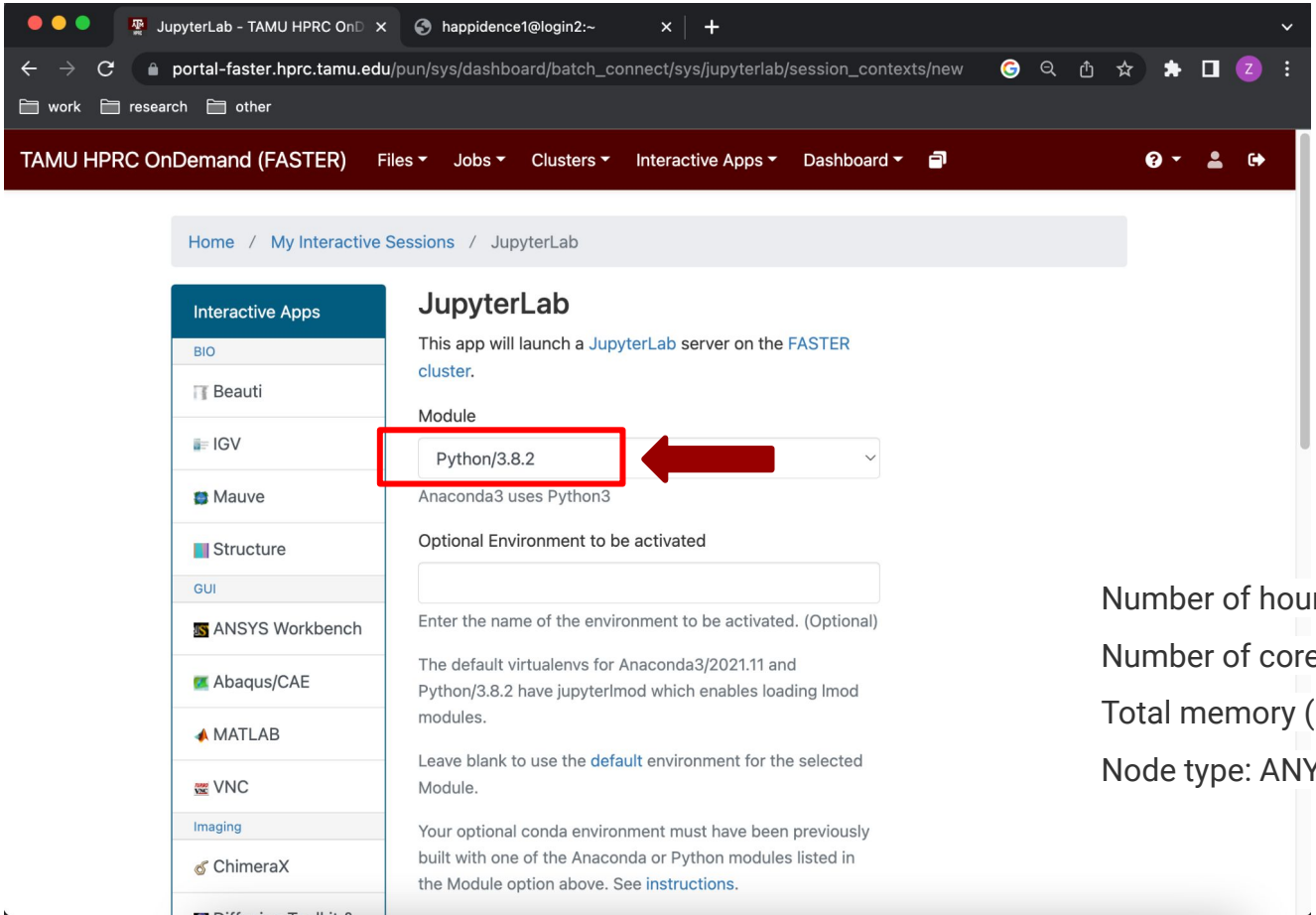
- Enter this directory (your local copy)

  ```
  $ cd ai_tech_labs
  ```

Go to JupyterLab Page



JupyterLab Page



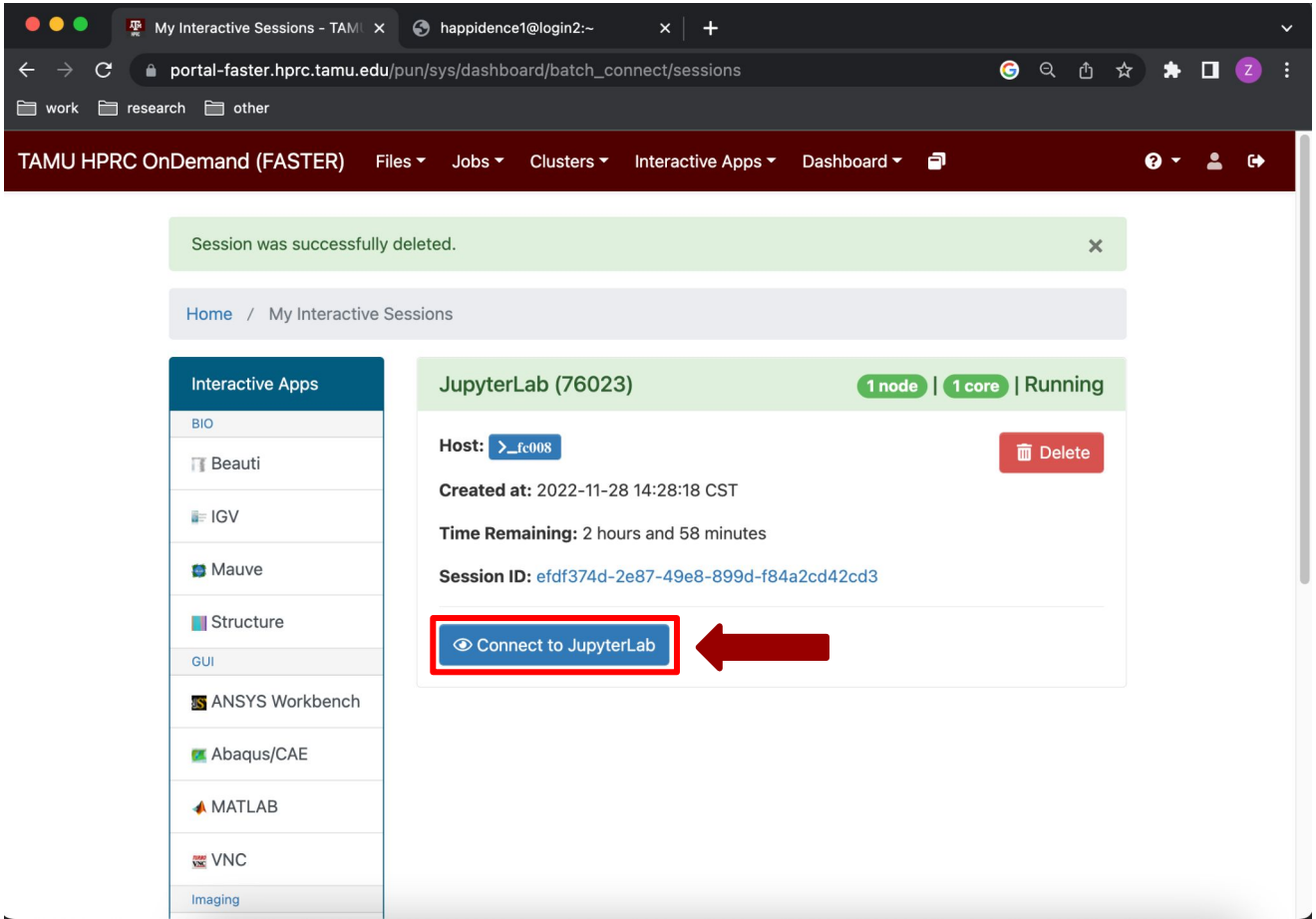
Number of hours: 3

Number of cores: 1

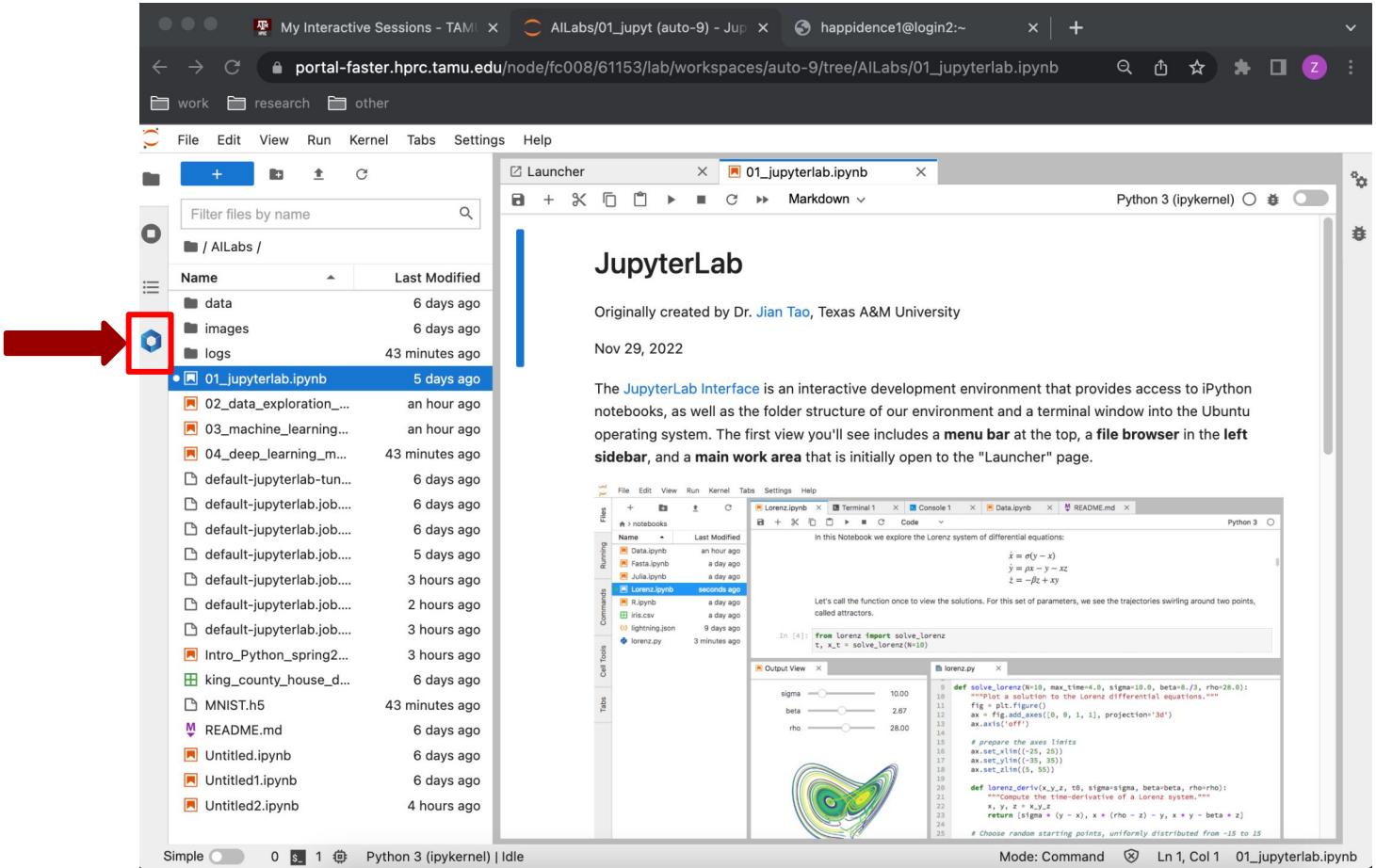
Total memory (GB): 2

Node type: ANY

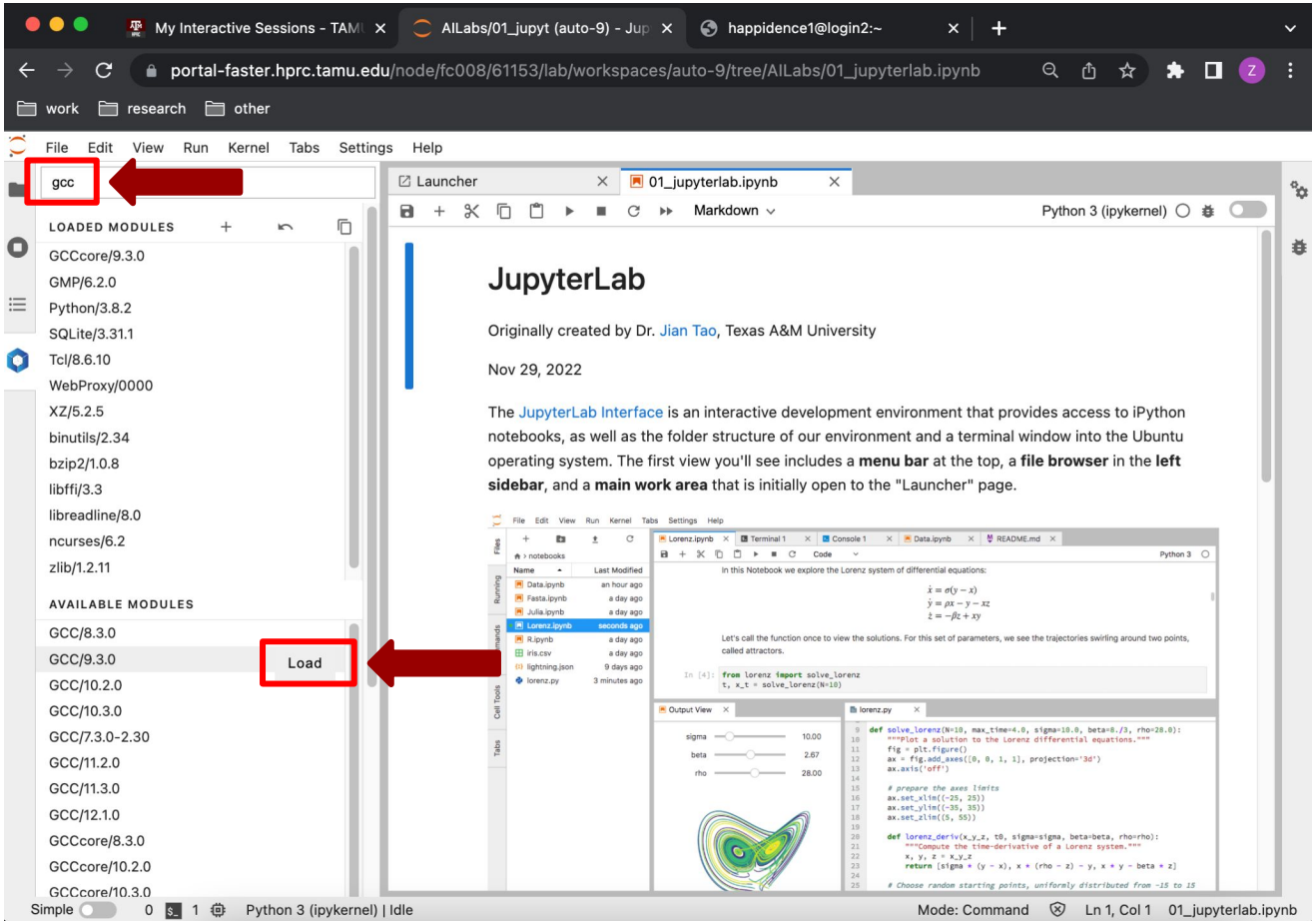
Connect to JupyterLab



JupyterLab Lmod Extension



JupyterLab Lmod Extension

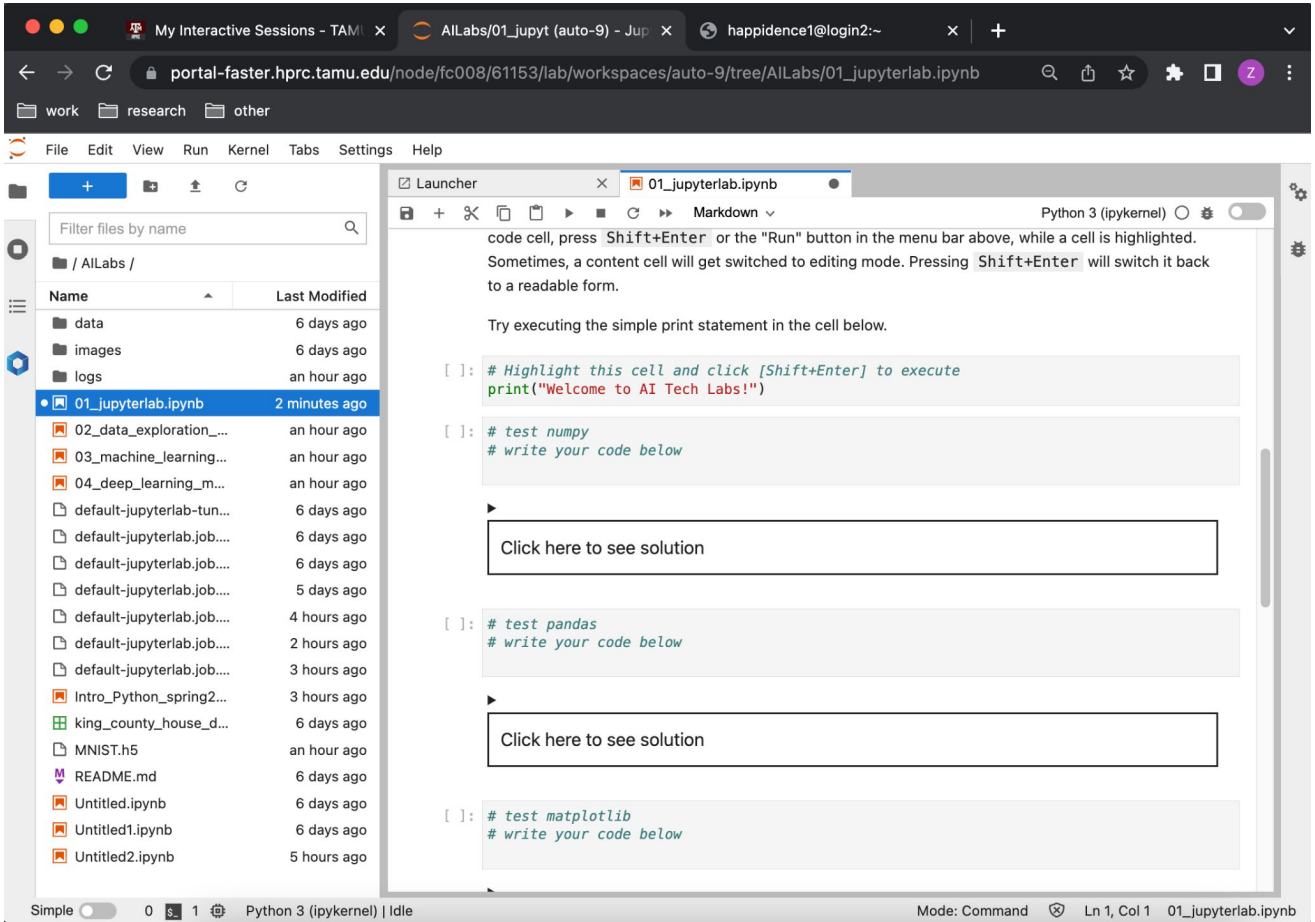


Exercise: Load Required Modules

- GCC/9.3.0
- OpenMPI/4.0.3
- scikit-learn/0.23.1-Python-3.8.2
- TensorFlow/2.3.1-Python-3.8.2

Note: numpy and matplotlib have already been in the Scipy-bundle/2020.03-Python-3.8.2 module.

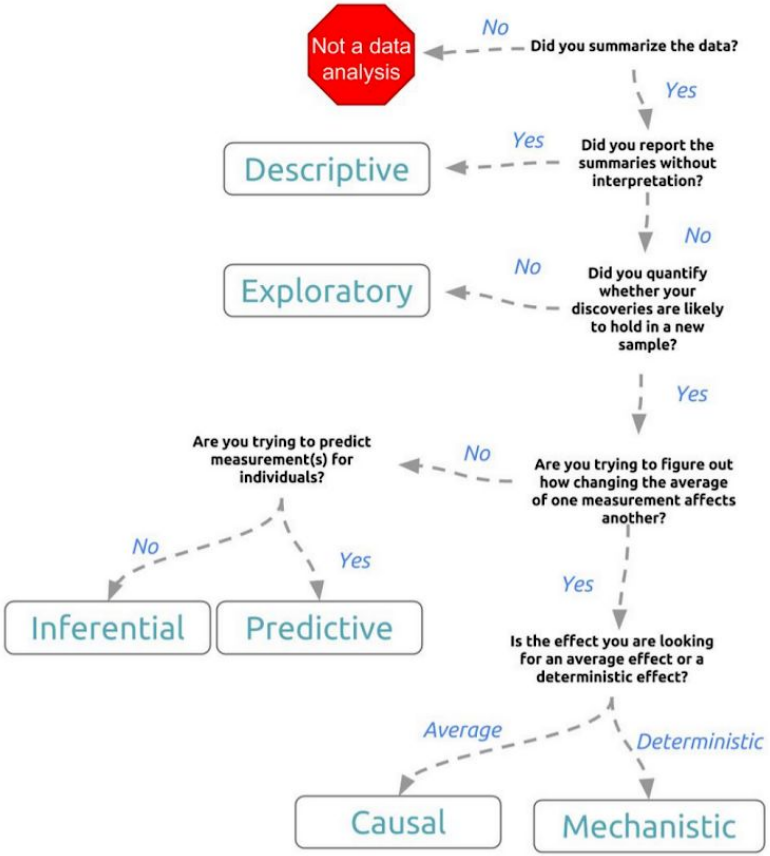
Test loaded modules



Lab II. Data Exploration

Types of Data Science Problems

- **Descriptive** (summaries, e.g., census)
- **Exploratory** (search for unknowns, e.g., four-planet solar system)
- **Inferential** (find correlations, e.g., many social studies)
- **Predictive** (make predictions, e.g., Face ID, Echo, Siri)
- **Causal** (explore causation, e.g., smoking versus lung cancer)
- **Mechanistic** (determine governing principles, e.g., experimental science)



Credit: Jeff Leek - The Elements of Data Analytic Style

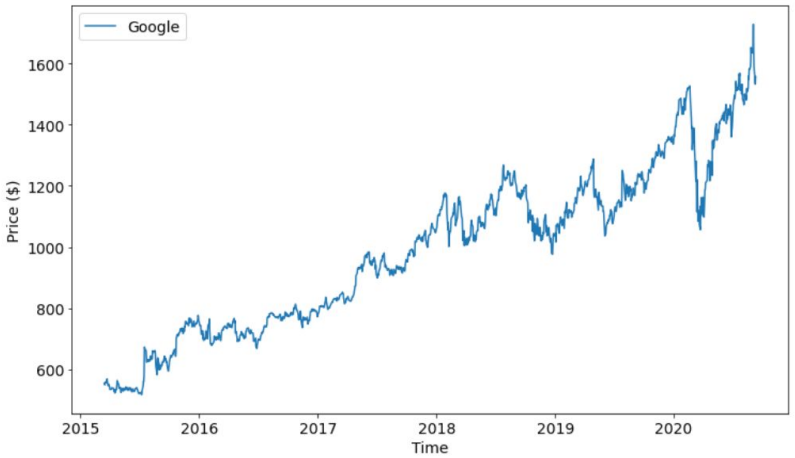
Data Structures

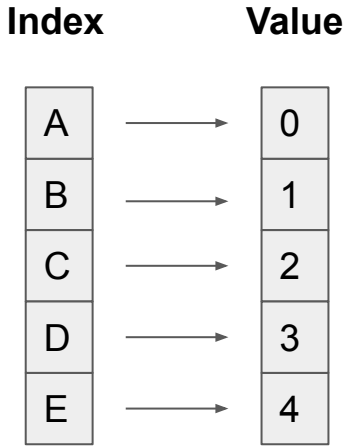
Pandas has two data structures that are descriptive and optimized for data with different dimensions.

- **Series:** 1D labeled array
- **DataFrame:** General 2D labeled, size-mutable tabular structure with potentially heterogeneously-typed columns

Series in pandas

- One-dimensional labeled array
- Capable of holding any data type (integers, strings, floating point numbers, etc.)
- Example: time-series stock price data

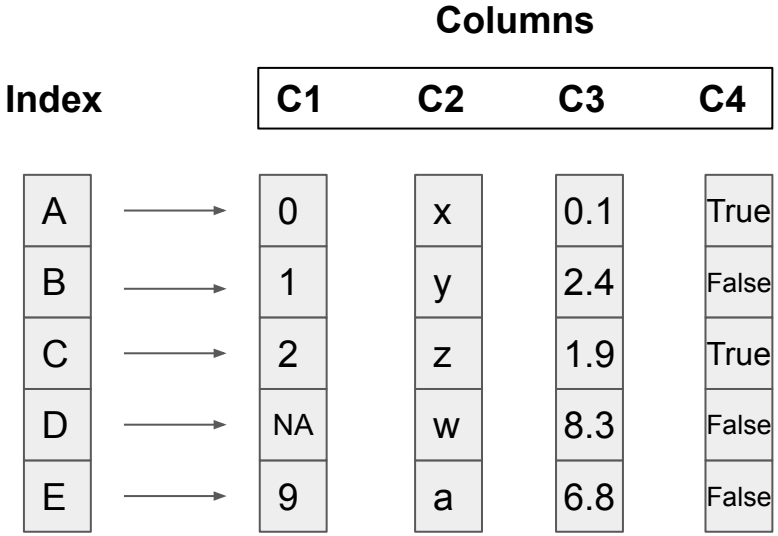




DataFrame in pandas

- Primary Pandas data structure
- A dict-like container for Series objects
- Two-dimensional size-mutable
- Heterogeneous tabular data structure

A	B	C	D	E	F	G	H
id	date	price	bedrooms	bathrooms	sqft_living	sqft_lot	floors
7129300520	20141013T0(	221900	3	1	1180	5650	1
6414100192	20141209T0(	538000	3	2.25	2570	7242	2
5631500400	20150225T0(	180000	2	1	770	10000	1
2487200875	20141209T0(	604000	4	3	1960	5000	1
1954400510	20150218T0(	510000	3	2	1680	8080	1
7237550310	20140512T0(	1.23E+06	4	4.5	5420	101930	1
1321400060	20140627T0(	257500	3	2.25	1715	6819	2
2008000270	20150115T0(	291850	3	1.5	1060	9711	1
2414600126	20150415T0(	229500	3	1	1780	7470	1



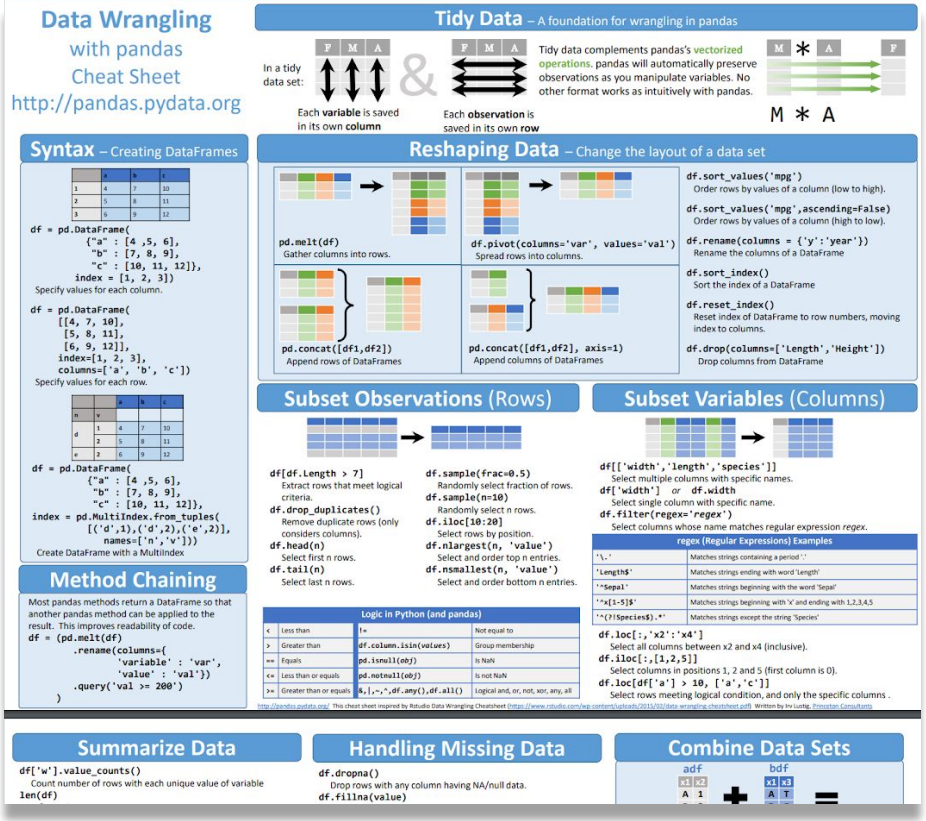
Pandas Learning Objectives

After this lesson, you will know how to:

- Create a DataFrame
- Drop Entries
- Index, Select, and Filter data
- Sort data
- Input and Output

JupyterLab Exercises

Pandas Cheat Sheet

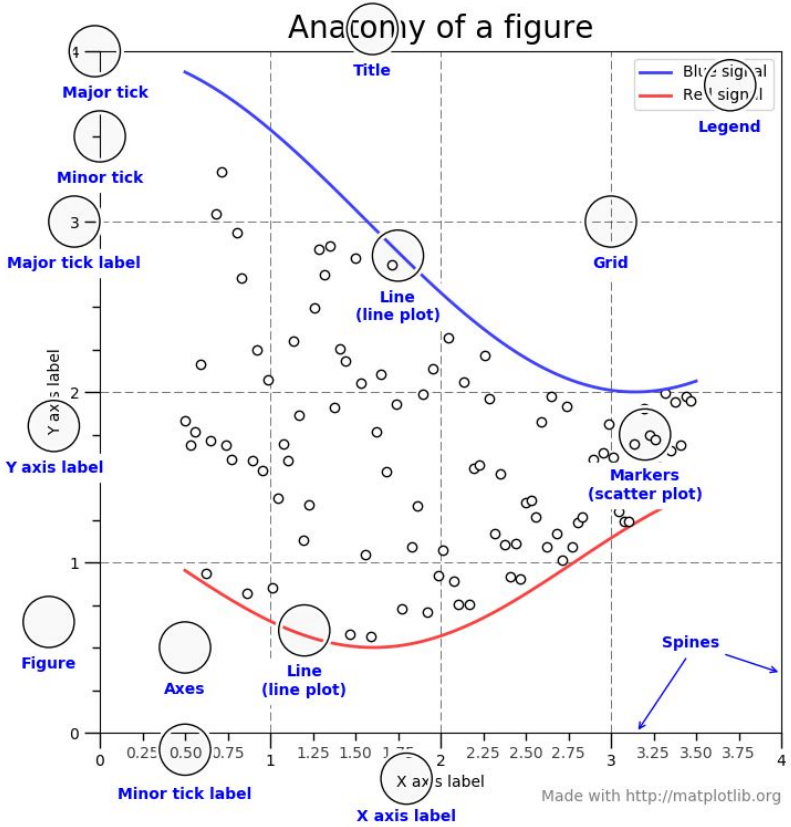


https://pandas.pydata.org/Pandas_Cheat_Sheet.pdf

Key Plotting Concepts in Matplotlib

- **Matplotlib: Figure**
  Figure is the object that keeps the whole image output. Adjustable parameters include:
  1. Image size (set_size_inches())
  2. Whether to use tight_layout (set_tight_layout())

- **Matplotlib: Axes**
  Axes object represents the pair of axis that contain a single plot (x-axis and y-axis). The Axes object also has more adjustable parameters:
  1. The plot frame (set_frame_on() or set_frame_off())
  2. X-axis and Y-axis limits (set_xlim() and set_ylim())
  3. X-axis and Y-axis Labels (set_xlabel() and set_ylabel())
  4. The plot title (set_title())



(Credit: matplotlib.org)

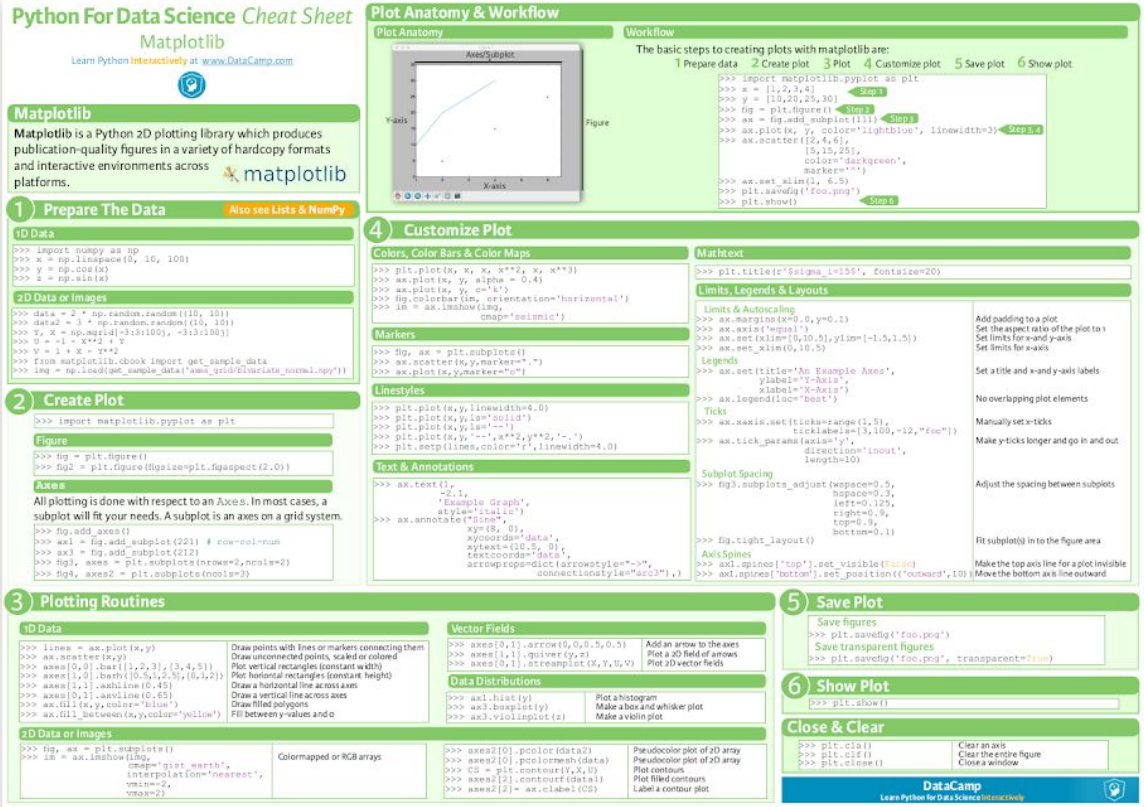
Matplotlib Learning Objectives

After this lesson, you will know how to:

- Scatter plot and Line plot
- Subplots
- Color map
- Contour figures
- 3D figures
  - Surface plots
  - Wire-frame plot
  - Contour plots with projections

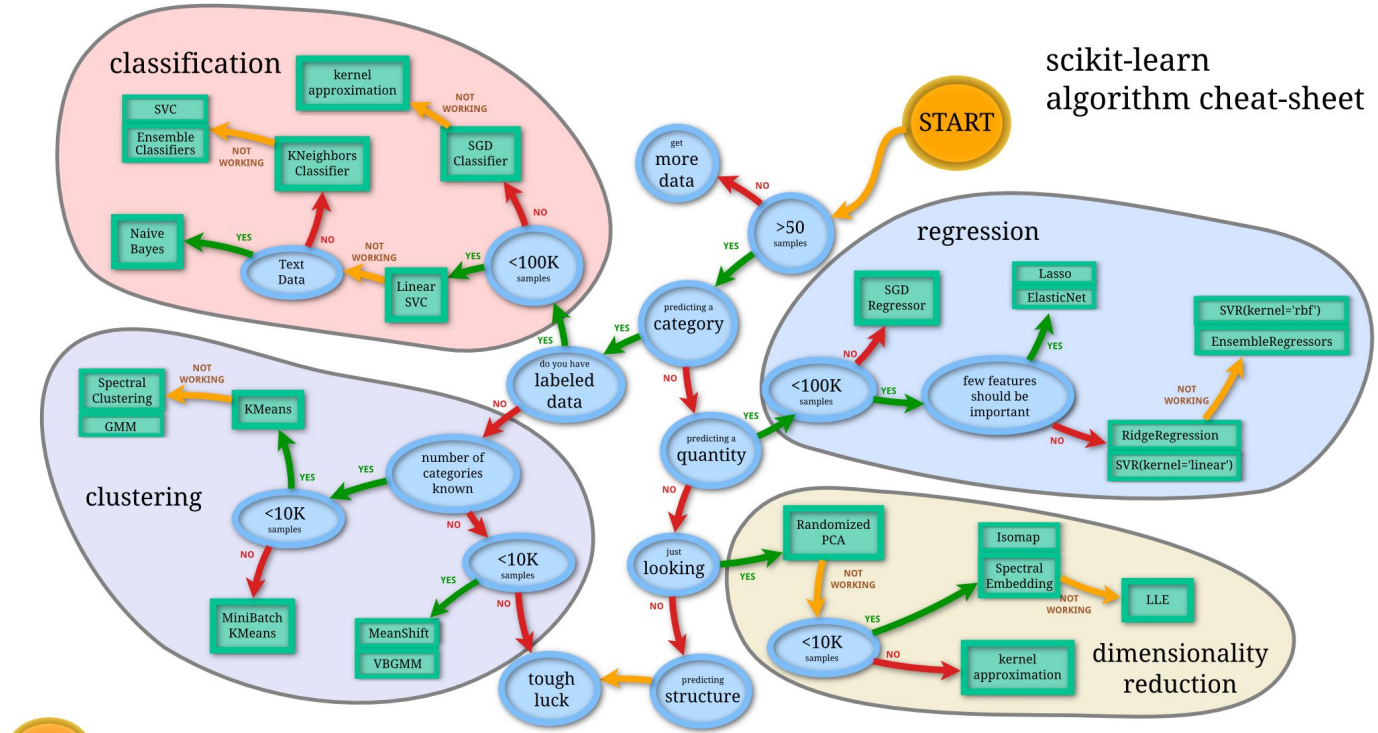
JupyterLab Exercises

Matplotlib Cheat Sheet



https://s3.amazonaws.com/assets.datacamp.com/blog_assets/Python_Matplotlib_Cheat_Sheet.pdf

Lab III. Machine Learning

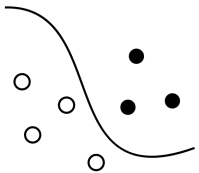


Main Features of scikit-learn

Classification

Identifying category of an object

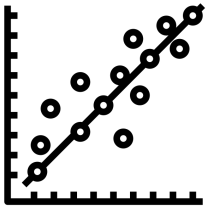
Applications: Spam detection, image recognition.
Algorithms: SVM, nearest neighbors, random forest, and more...



Regression

Predicting a attribute for an object

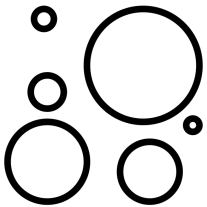
Applications: Drug response, Stock prices.
Algorithms: SVR, nearest neighbors, random forest, and more...



Clustering

Grouping similar objects into sets

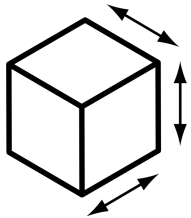
Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, and more...



Dimension Reduction

Reducing the number of dimensions

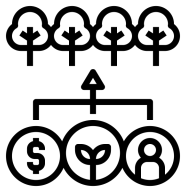
Applications: Visualization, Increased efficiency **Algorithms:** k-Means, feature selection, non-negative matrix factorization, and more...



Model Selection

Selecting models with parameter search

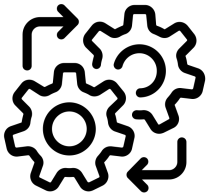
Applications: Improved accuracy via parameter tuning **Algorithms:** grid search, cross validation, metrics, and more...



Preprocessing

Preprocessing data to prepare for modeling

Applications: Transforming input data such as text for use with machine learning algorithms. **Algorithms:** preprocessing, feature extraction, and more...

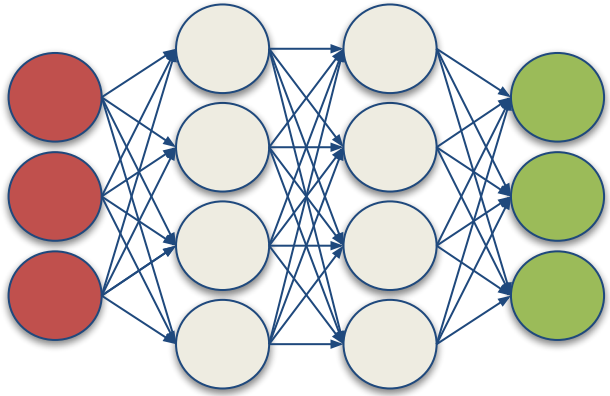


Lab IV. Deep Learning

Deep Learning
by Ian Goodfellow, Yoshua Bengio, and Aaron Courville
http://www.deeplearningbook.org/

Animation of Neutron Networks
by Grant Sanderson
https://www.3blue1brown.com/

Visualization of CNN
by Adam Harley
https://www.cs.ryerson.ca/~aharley/vis/conv/

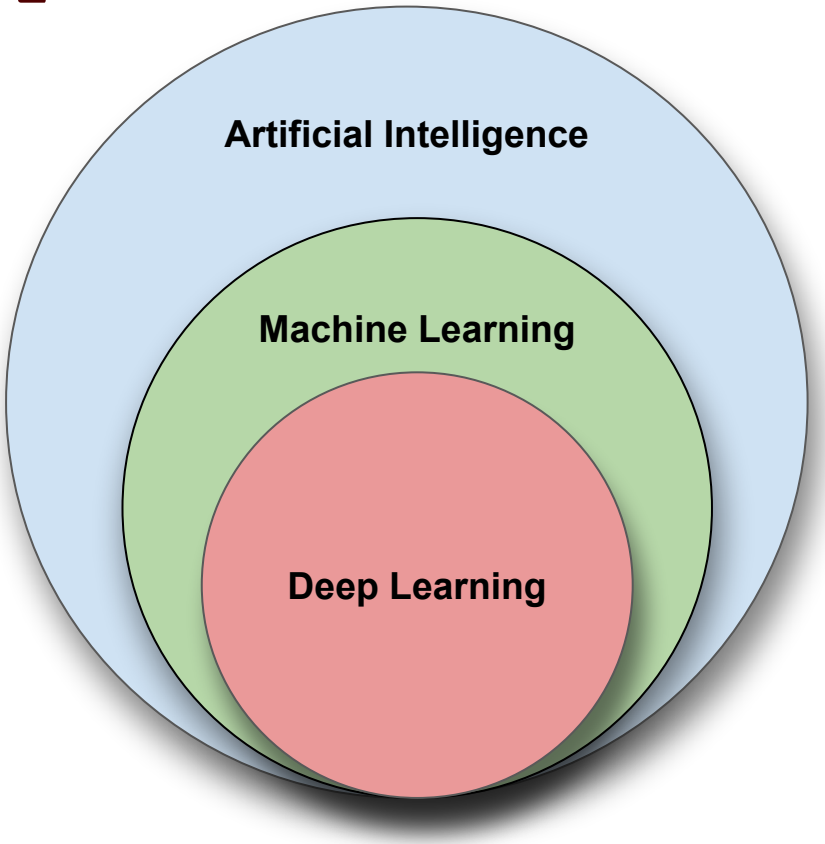


TensorFlow 2.0

Keras

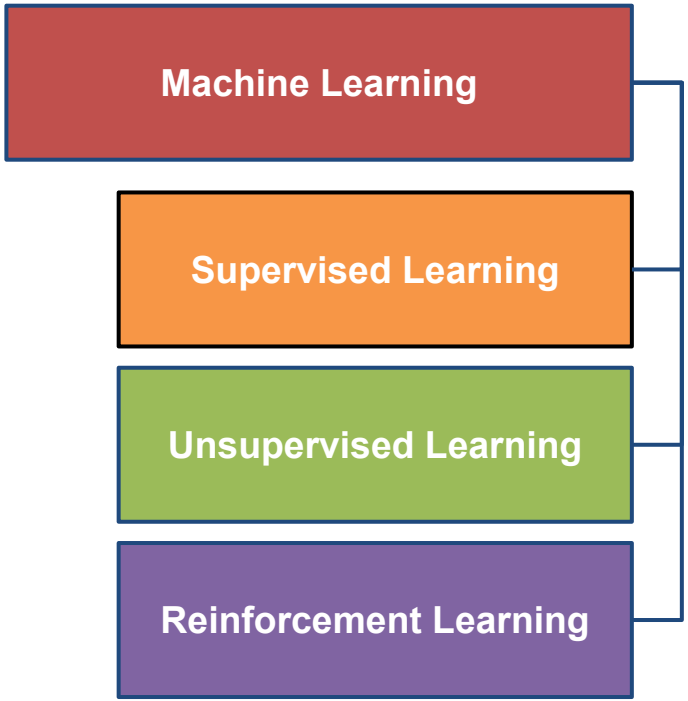
Relationship of AI, ML, and DL

- **Artificial Intelligence (AI)** is anything about man-made intelligence exhibited by machines.
- **Machine Learning (ML)** is an approach to achieve **AI**.
- **Deep Learning (DL)** is one technique to implement **ML**.

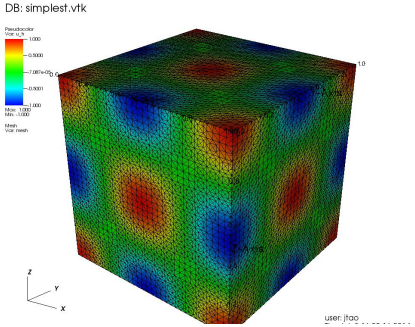


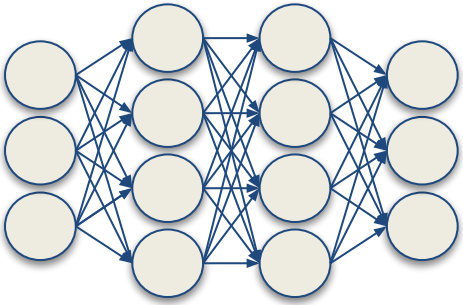
Types of ML Algorithms

- **Supervised Learning**
  - trained with labeled data; including regression and classification problems
- **Unsupervised Learning**
  - trained with unlabeled data; clustering and association rule learning problems.
- **Reinforcement Learning**
  - no training data; stochastic Markov decision process; robotics and self-driving cars.

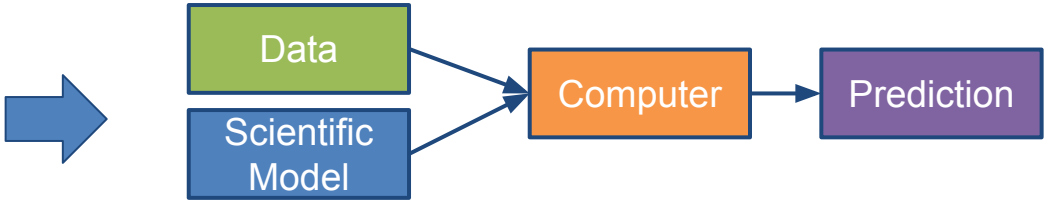


Machine Learning

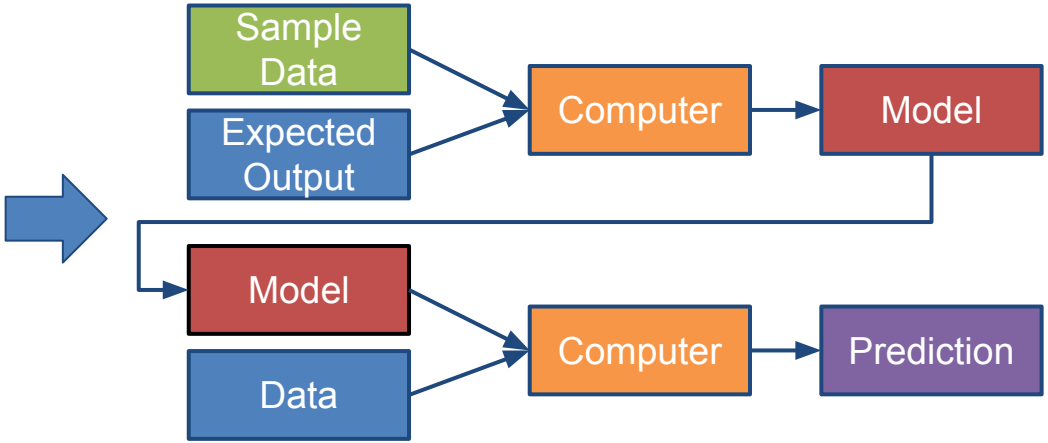




Traditional Modeling



Machine Learning (Supervised Learning)



Inputs and Outputs

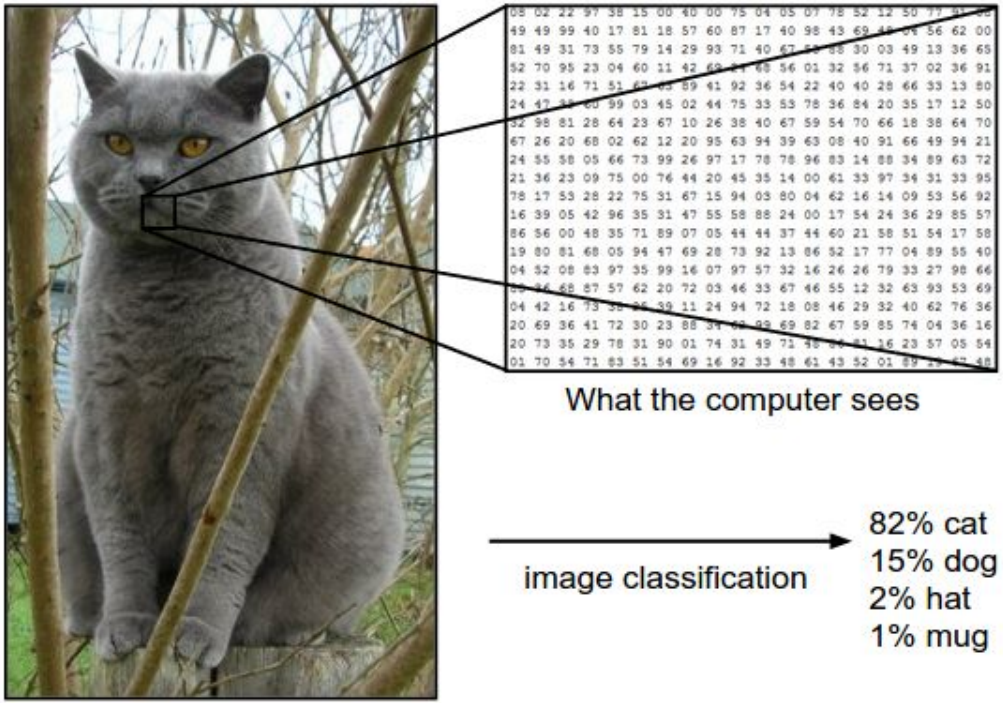
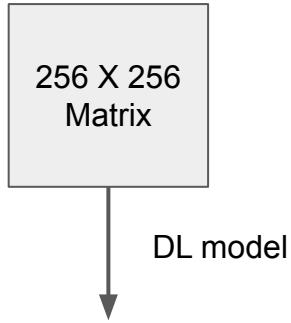
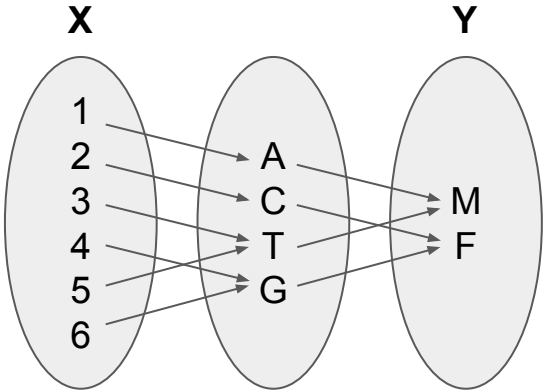


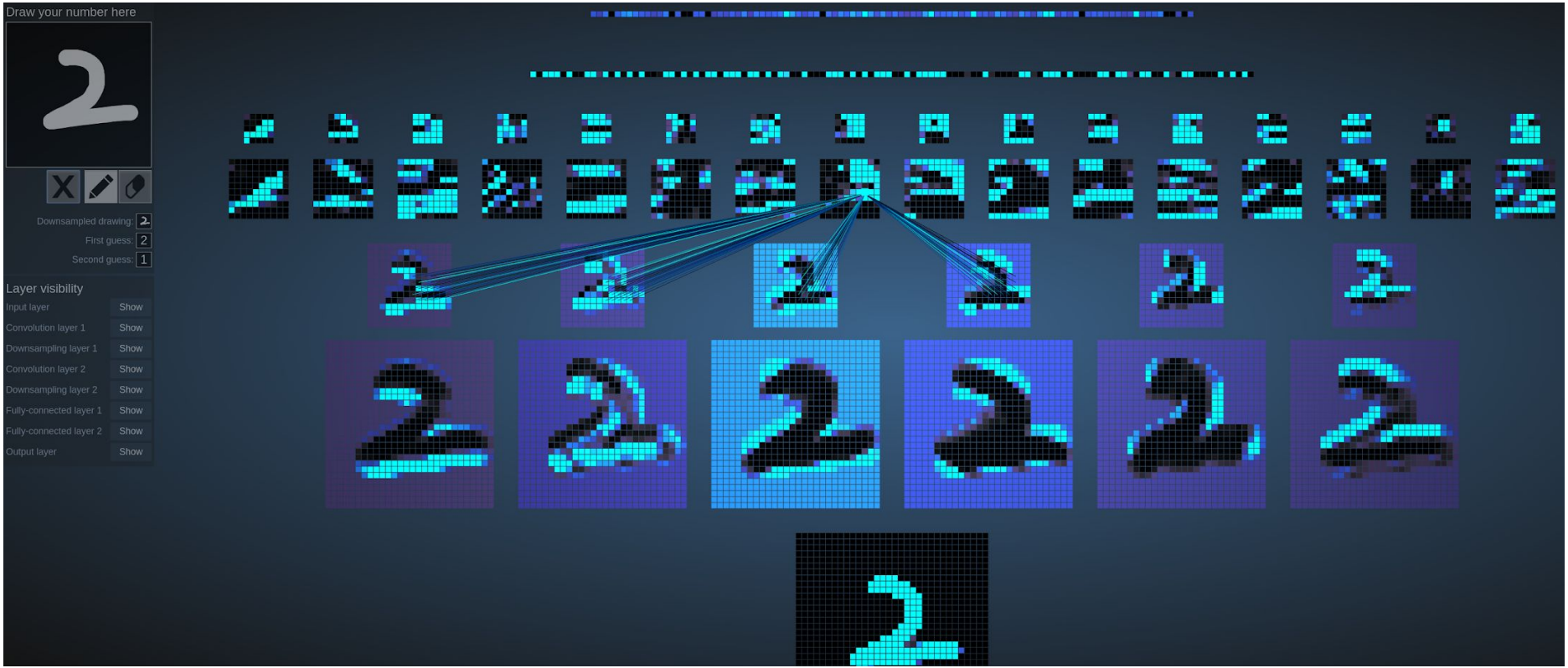
Image from the Stanford CS231 Course





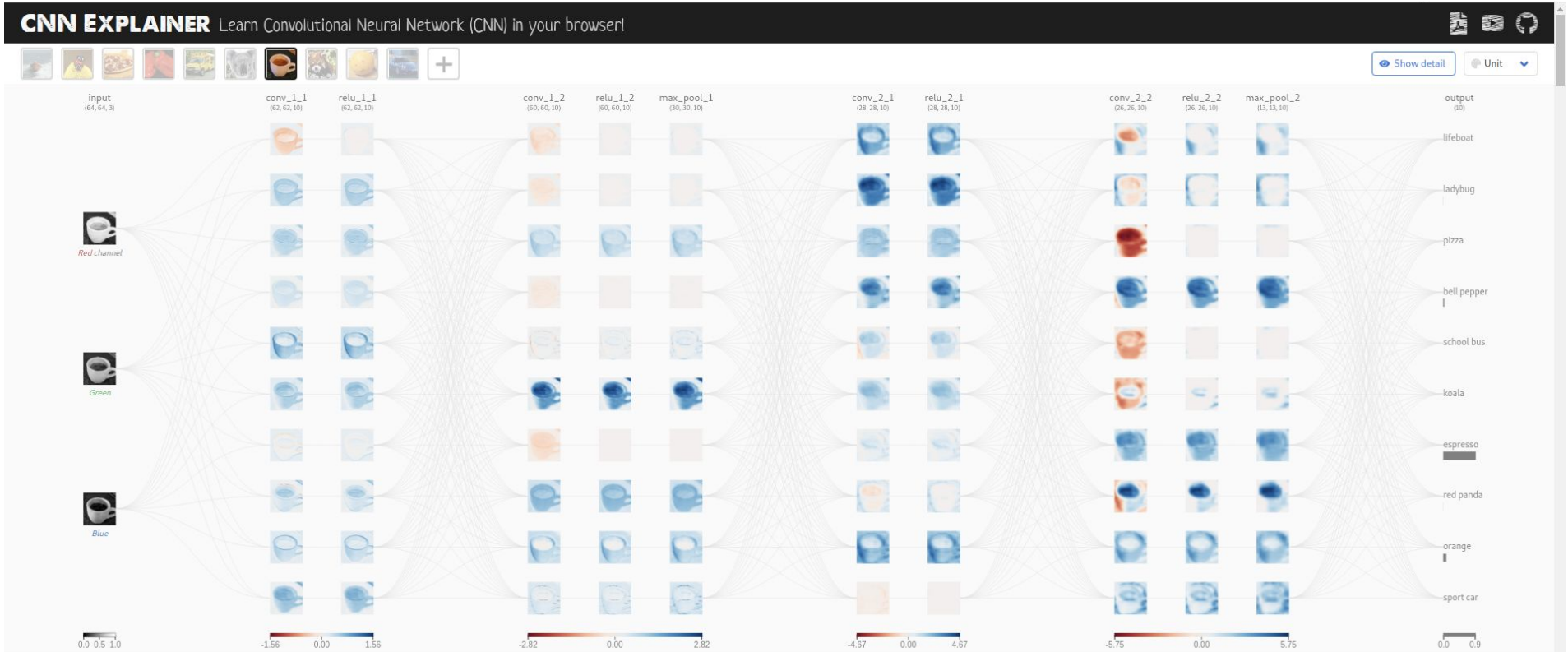
With deep learning, we are searching for a **surjective** (or **onto**) function **f** from a set **X** to a set **Y**.

MNIST - CNN Visualization



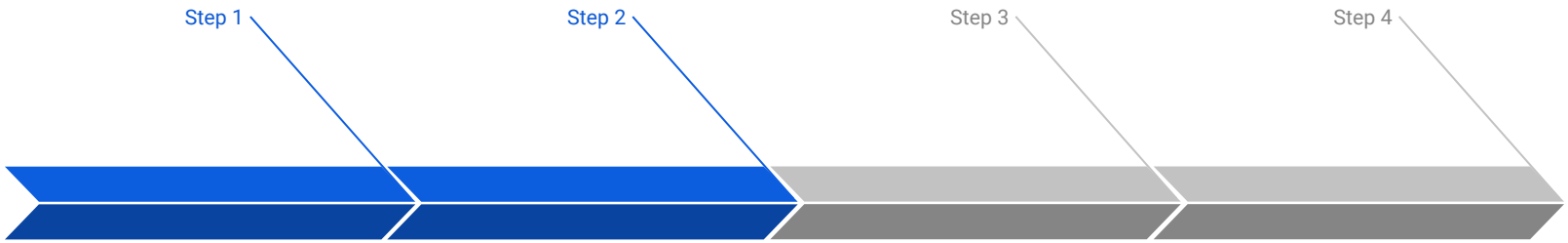
(Image Credit: http://scs.ryerson.ca/~aharley/vis/)

CNN Explainer



(Image Credit: https://poloclub.github.io/cnn-explainer/)

Machine Learning Workflow with Keras



Prepare Train Data

The preprocessed data set needs to be shuffled and splitted into training and testing data.

Define Model

A model could be defined with Keras Sequential model for a linear stack of layers or Keras functional API for complex network.

Training Configuration

The configuration of the training process requires the specification of an optimizer, a loss function, and a list of metrics.

Train Model

The training begins by calling the fit function. The number of epochs and batch size need to be set. The measurement metrics need to be evaluated.