# Al Tech Labs 0⇒1

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03/11/2022





High Performance Research Computing

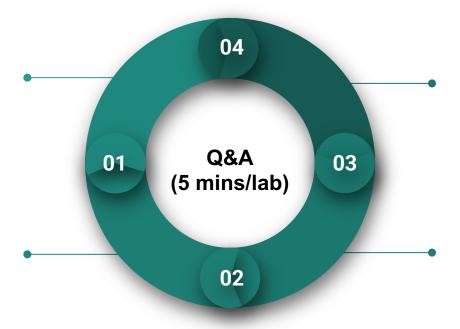
## Al Tech Labs

### Lab I. JupyterLab (30 mins)

We will set up a Python virtual environment and run JupyterLab on the HPRC Grace Portal.

### 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)

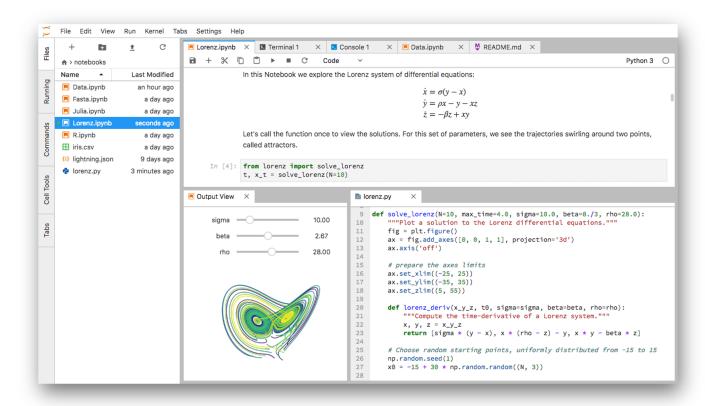
We will learn how to use Keras to build and train a simple image classification model with deep neural network (DNN).

### Lab III Machine Learning (30 minutes)

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

# Lab I. JupyterLab

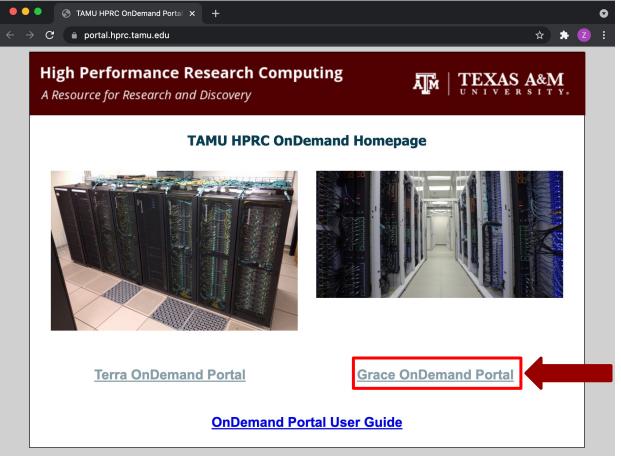




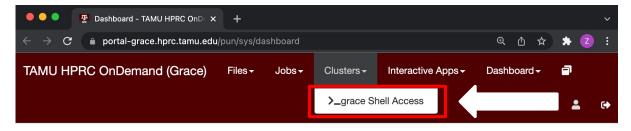
### L1 - Resources

- Texas A&M High Performance Research Computing (HPRC)
- Grace Quick Start Guide
- HPRC Portal
- HPRC YouTube Channel
- Jupyter Project
- help@hprc.tamu.edu

# **Login HPRC Portal**



### **Shell Access - I**





OnDemand provides an integrated, single access point for all of your HPC resources.

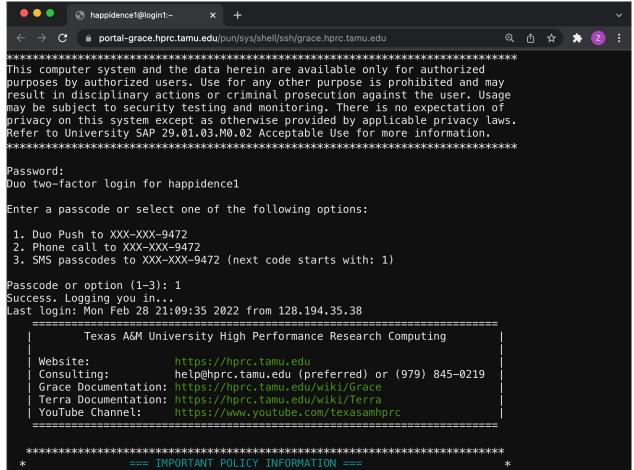
#### Message of the Day

#### Grace Cluster Status, January 30 - February 04

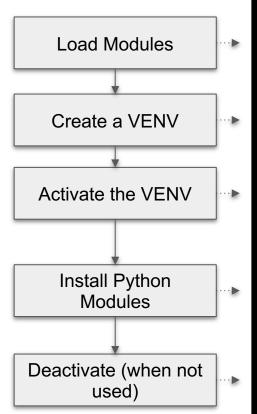
UPDATE (8:09pm 02/04/2022): The Grace storage has been recovered from the Jan. 30th, Feb. 1st, and Feb. 3rd incidents involving storage software defects. The Grace maintenance has also been completed. Quota enforcement has also been restored for the Grace storage. Some users may have storage usage that is drastically over their intended home and scratch directory quotas. Please archive and remove any unneeded data if possible. Our apologies again for the extended unavailability of the Grace cluster.

#### **IMPORTANT POLICY INFORMATION**

### **Shell Access - II**



# Python Virtual Environment (VENV)

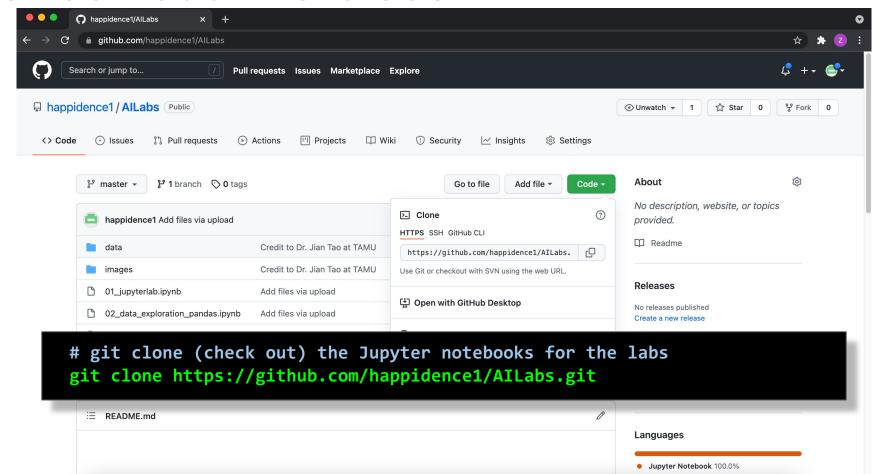


```
# clean up and load Anaconda
cd $SCRATCH
module purge
module load Anaconda3/2021.11
# create a Python virtual environment
conda create -n mylab
# activate the virtual environment
conda activate mylab
# install required packages to be used in the portal
conda install scikit-learn
conda install tensorflow
# deactivate the virtual environment
# conda deactivate
```

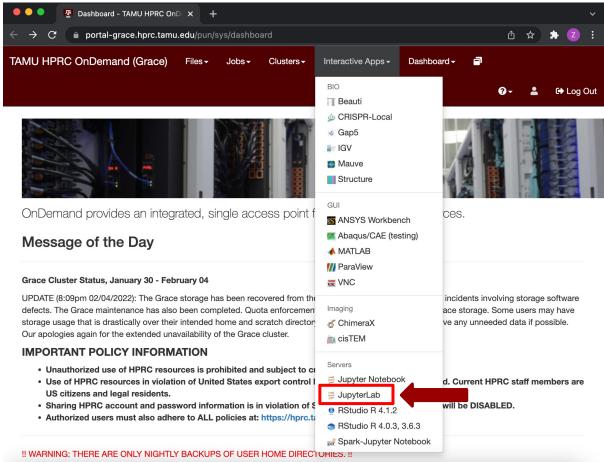
### **Common Anaconda Commands**

```
# Conda virtual environment
conda info
                                 # show Conda installation
                   # create a virtual environment
conda create -n VENV
conda create -n VENV python=3.8 # create a venv with a py version
conda env list
                                 # list installed venv
# Conda package management
                                 # list all installed packages
conda list
                                 # search a Conda package
conda search PACKAGENAME
conda install PACKAGENAME
                                 # install a Conda package
conda update PACKAGENAME
                                 # update a Conda package
conda remove PACKAGENAME
                                 # remove a Conda package
```

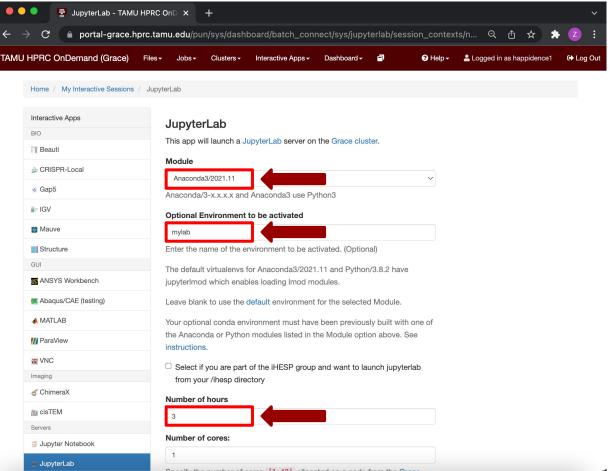
### **Check out Exercises**



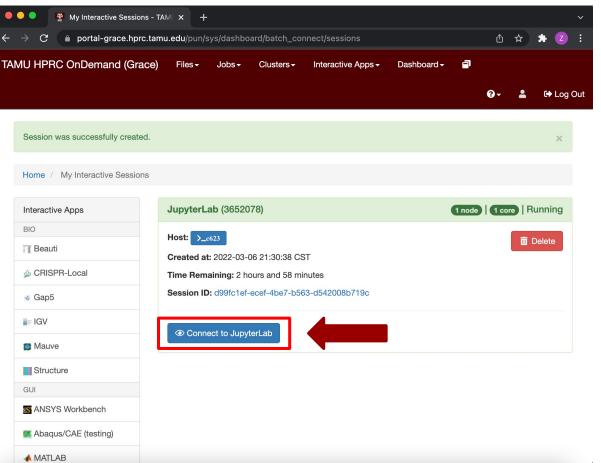
# Go to JupyterLab Page



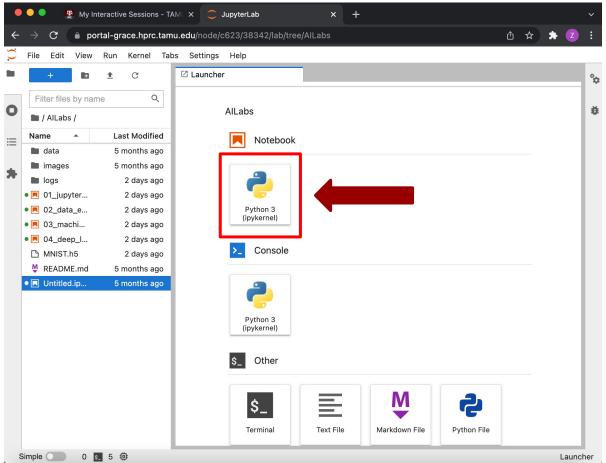
### **Set Virtual Environment**



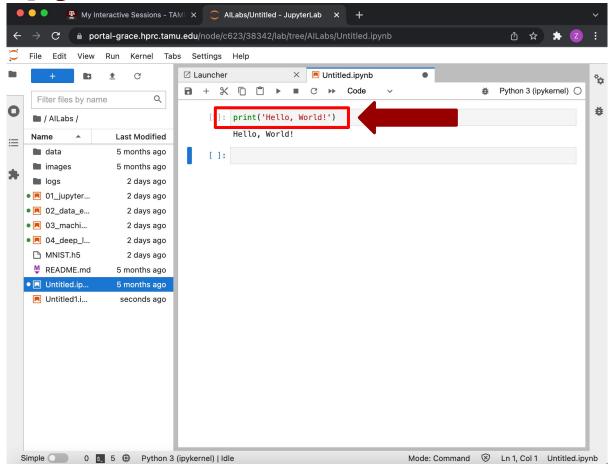
# Connect to JupyterLab



## Create a Jupyter Notebook



## Test JupyterLab



# Lab II. Data Exploration





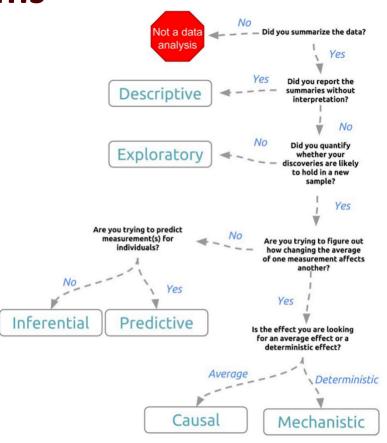






### **Types of Data Science Problems**

- Descriptive (summaries, e.g., census)
- Exploratory (search for unknowns, e.g., fourplanet 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

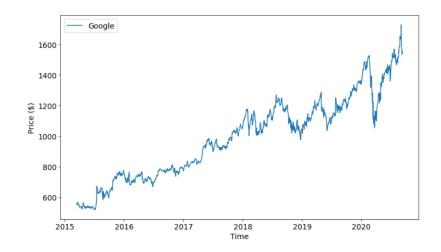
### **Data Structures**

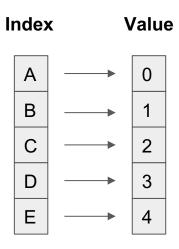
**Pandas** has two data structures that are descriptive and optimized for data with different dimensions.

- 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

Α	В	С	D	E	F	G	н
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	20150225T00	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	20140627T00	257500	3	2.25	1715	6819	2
2008000270	20150115T0	291850	3	1.5	1060	9711	1
2414600126	20150415T00	229500	3	1	1780	7470	1

#### **Columns**

Index	•	<b>C1</b>	C2	C3	C4
Α		0	x	0.1	True
В		1	У	2.4	False
С	<b></b>	2	Z	1.9	True
D	<b></b>	NA	W	8.3	False
Е		9	а	6.8	False

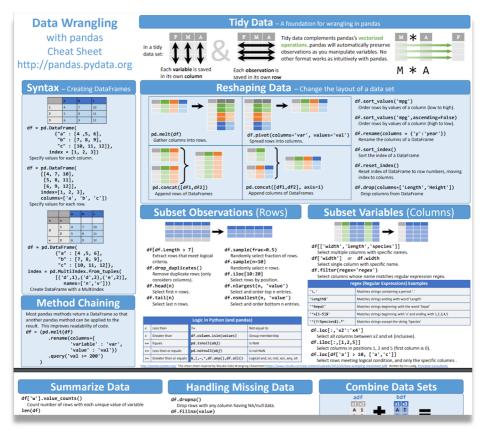
### **Pandas Learning Objectives**

#### After this lesson, you will know how to:

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



### **Pandas Cheat Sheet**



https://pandas.pydata.org/Pandas\_Cheat\_Sheet.pdf

### **Key Plotting Concepts in Matplotlib**

#### Matplotlib: Figure

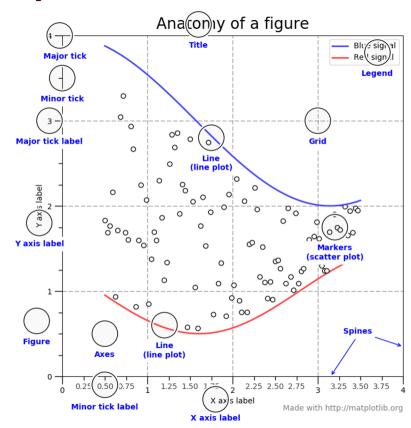
Figure is the object that keeps the whole image output. Adjustable parameters include:

- Image size (set\_size\_inches())
- 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:

- The plot frame (set\_frame\_on() or set\_frame\_off())
- 2. X-axis and Y-axis limits (set\_xlim() and set\_ylim())
- X-axis and Y-axis Labels (set\_xlabel() and set\_ylabel())
- 4. The plot title (set\_title())



(Credit: matplotlib.org)

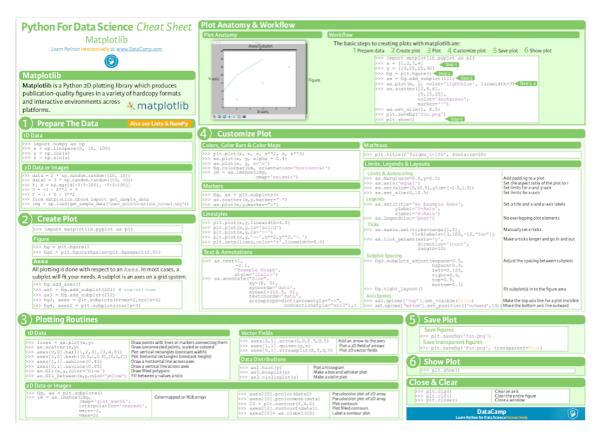
### **Matplotlib Learning Objectives**

After this lesson, you will know how to:

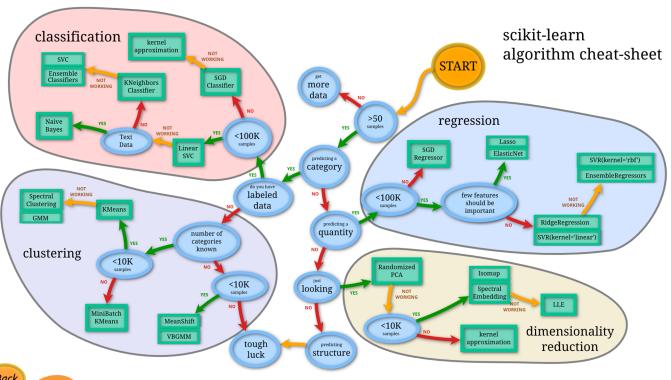
- Scatter plot and Line plot
- Subplots
- Color map
- Contour figures
- 3D figures
  - Surface plots
  - Wire-frame plot
  - Contour plots with projections



### **Matplotlib Cheat Sheet**



# Lab III. Machine Learning





### Main Features of scikit-learn



Identifying
category of an

object

Classification

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, nonnegative matrix
factorization, and
more...

## Selecting models with

parameter

search

Model Selection

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

### Preprocessing

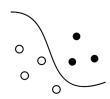
Preprocessing data to prepare for modeling

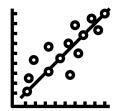
#### Applications:

Transforming input data such as text for use with machine learning algorithms.

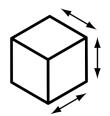
Algorithms:

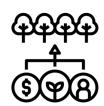
preprocessing, feature extraction, and more...













# Lab IV. Deep Learning

#### Deep Learning

by Ian Goodfellow, Yoshua Bengio, and Aaron Courville <a href="http://www.deeplearningbook.org/">http://www.deeplearningbook.org/</a>

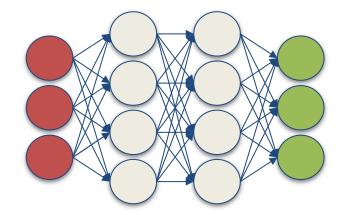
#### **Animation of Neutron Networks**

by Grant Sanderson <a href="https://www.3blue1brown.com/">https://www.3blue1brown.com/</a>

#### Visualization of CNN

by Adam Harley

https://www.cs.ryerson.ca/~aharley/vis/conv/

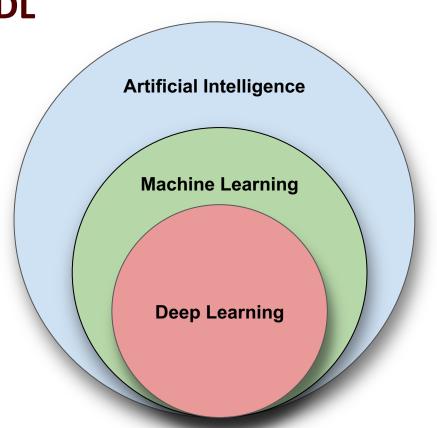






Relationship of AI, ML, and DL

- 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

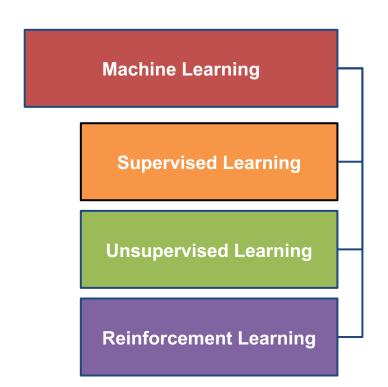
 trained with labeled data; including regression and classification problems

#### Unsupervised Learning

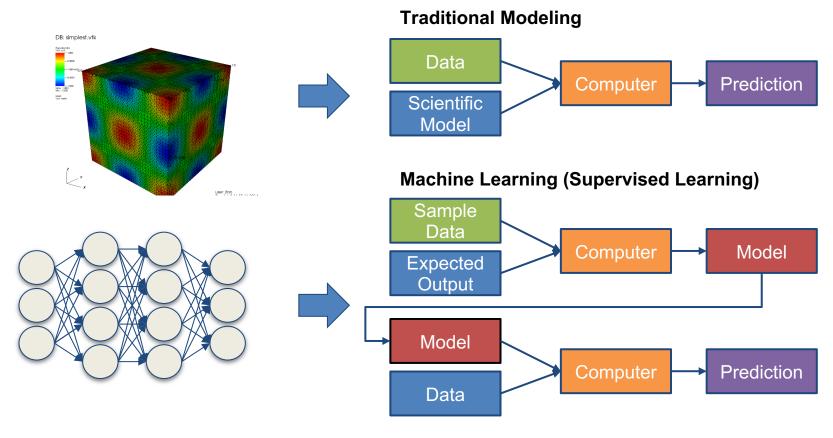
trained with unlabeled data;
 clustering and association rule
 learning problems.

#### Reinforcement Learning

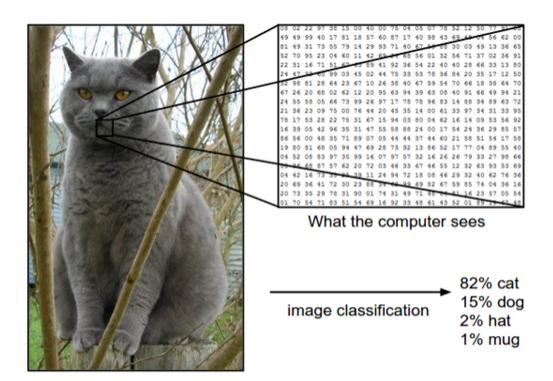
no training data; stochastic
 Markov decision process; robotics
 and self-driving cars.

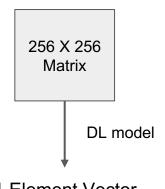


### **Machine Learning**

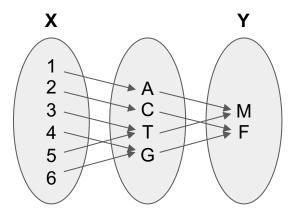


### **Inputs and Outputs**





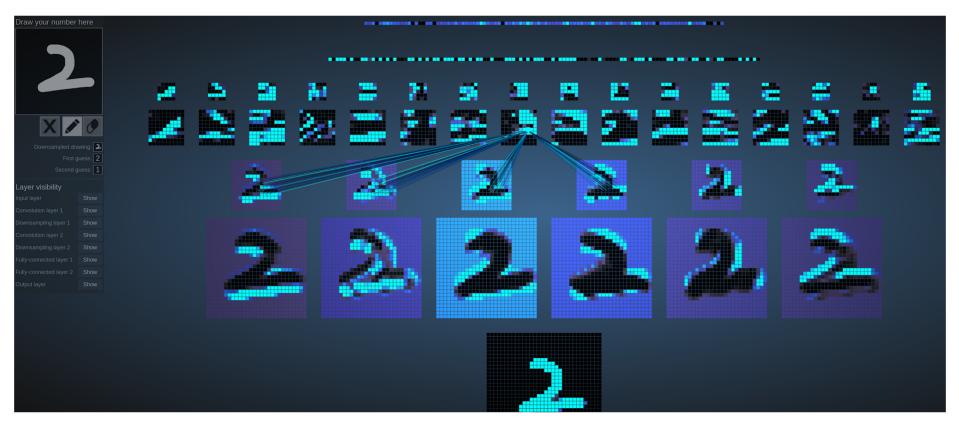
4-Element Vector



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

Image from the Stanford CS231 Course

### **MNIST - CNN Visualization**



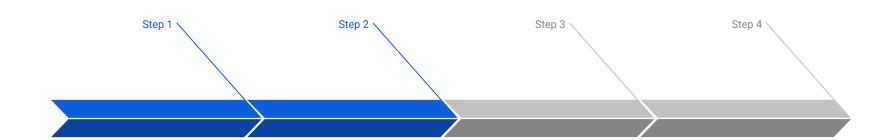
(Image Credit: <a href="http://scs.ryerson.ca/~aharley/vis/">http://scs.ryerson.ca/~aharley/vis/</a>)

### **CNN** Explainer



(Image Credit: <a href="https://poloclub.github.io/cnn-explainer/">https://poloclub.github.io/cnn-explainer/</a>)

### **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.