

ACES: AI TechLab in Jupyter Notebooks

Accelerating AI/ML Workflows on a Composable Cyberinfrastructure

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High Performance
Research Computing
DIVISION OF RESEARCH



AI TechLab

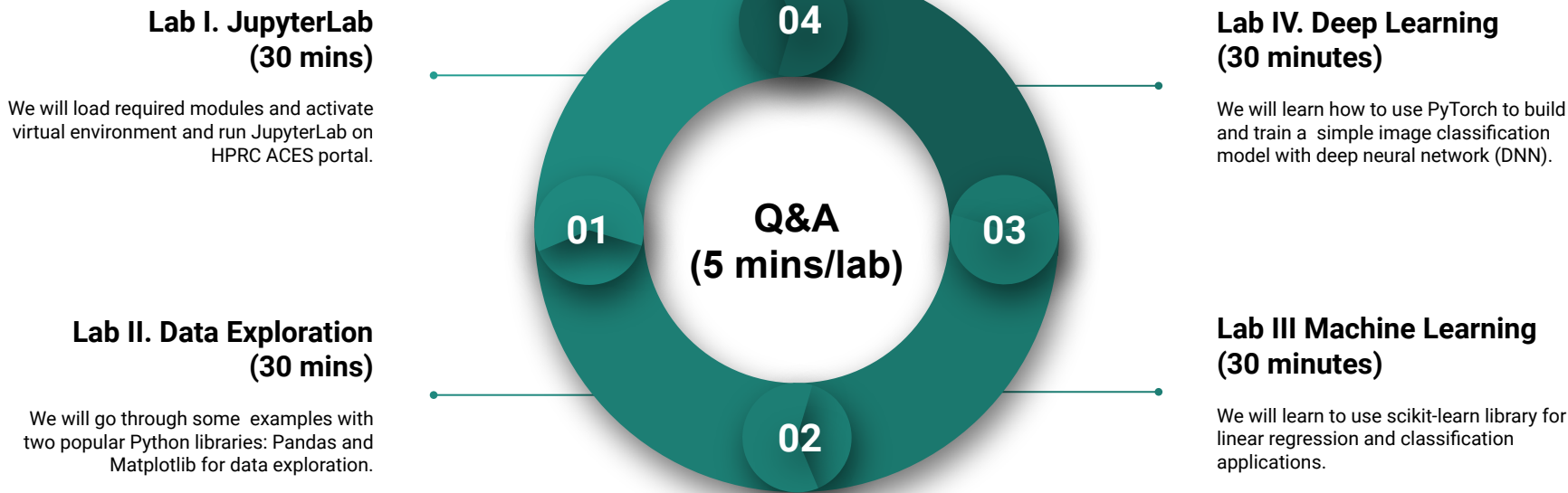


Figure 1. Structure of the AI TechLab.

Lab I. JupyterLab



File Edit View Run Kernel Tabs Settings Help

Files

- + notebooks
- Name Last Modified
- Data.ipynb an hour ago
- Fasta.ipynb a day ago
- Julia.ipynb a day ago
- Lorenz.ipynb seconds ago
- R.ipynb a day ago
- iris.csv a day ago
- lightning.json 9 days ago
- lorenz.py 3 minutes ago

Running

Commands

Cell Tools

Output View

lorenz.py

In this Notebook we explore the Lorenz system of differential equations:

$$\begin{aligned}\dot{x} &= \sigma(y - x) \\ \dot{y} &= \rho x - y - xz \\ \dot{z} &= -\beta z + xy\end{aligned}$$

Let's call the function once to view the solutions. For this set of parameters, we see the trajectories swirling around two points, called attractors.

```
In [4]: from lorenz import solve_lorenz
t, x_t = solve_lorenz(N=10)
```

sigma 10.00
beta 2.67
rho 28.00

A 3D plot of the Lorenz attractor, showing a complex, swirling trajectory in a 3D space. The plot is rendered with a green and blue color scheme, and the axes are labeled x, y, and z.

```
def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8./3, rho=28.0):
    """Plot a solution to the Lorenz differential equations."""
    fig = plt.figure()
    ax = fig.add_axes([0, 0, 1, 1], projection='3d')
    ax.axis('off')

    # prepare the axes limits
    ax.set_xlim((-25, 25))
    ax.set_ylim((-35, 35))
    ax.set_zlim((5, 55))

    def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
        """Compute the time-derivative of a Lorenz system."""
        x, y, z = x_y_z
        return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]

    # Choose random starting points, uniformly distributed from -15 to 15
    np.random.seed(1)
    x0 = -15 + 30 * np.random.random((N, 3))
```


L1 - Resources

- [Texas A&M High Performance Research Computing \(HPRC\)](#)
- [ACES Quick Start Guide](#)
- [ACES Portal \(ACCESS\)](#)
- [ACCESS Documentation](#)
- [HPRC YouTube Channel](#)
- help@hprc.tamu.edu

NSF ACES

Accelerating Computing for Emerging Sciences

Our Mission:

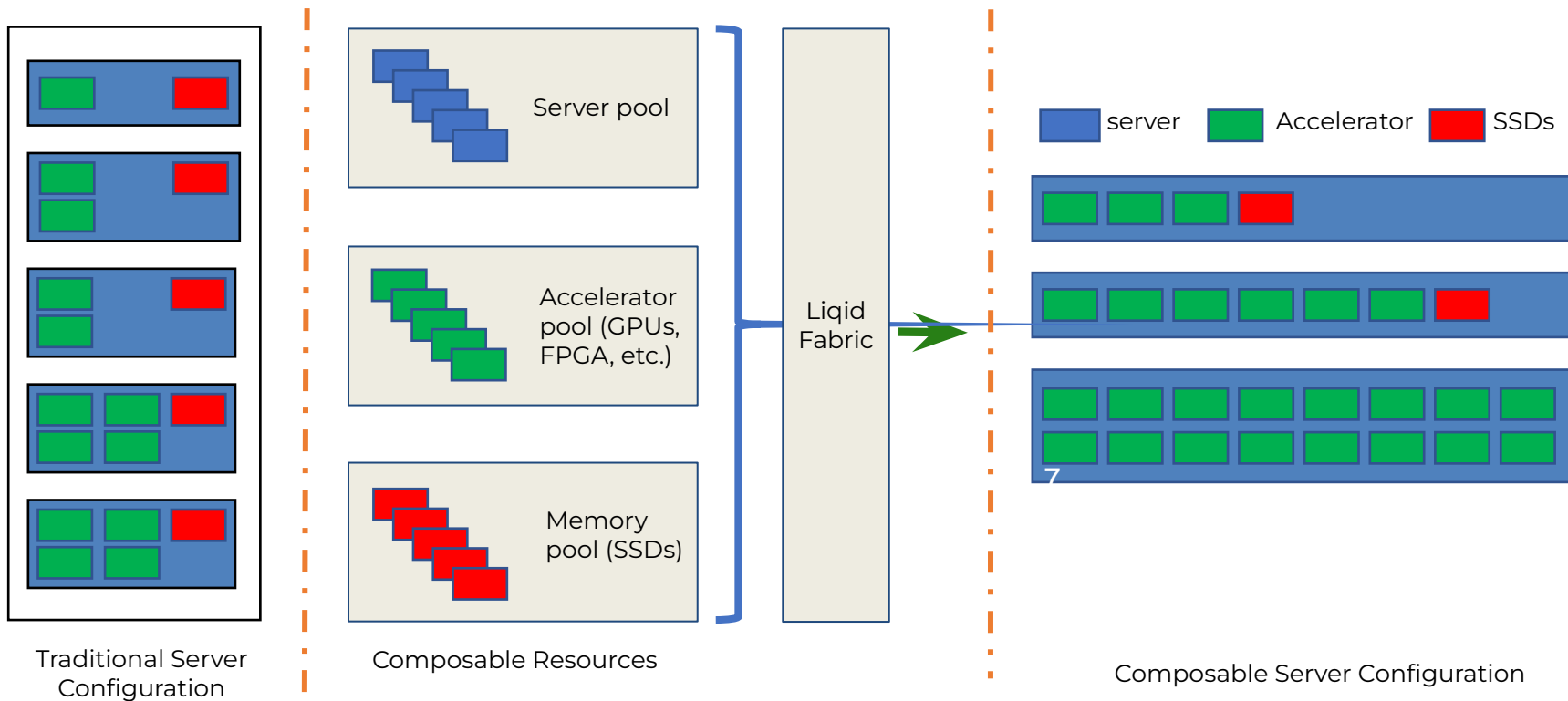
- Offer an accelerator testbed for numerical simulations and **AI/ML workloads**
- Provide consulting, technical guidance, and training to researchers
- Collaborate on computational and data-enabled research.



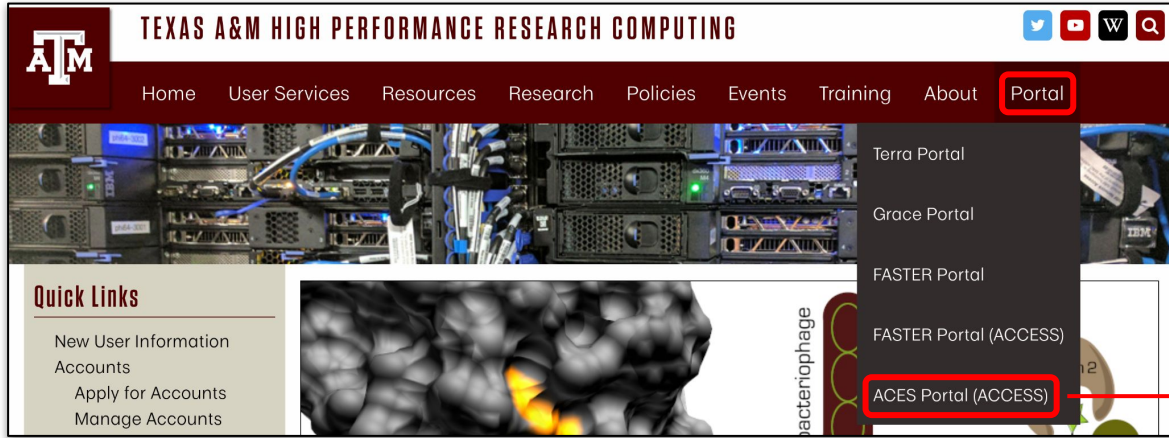
ACES Accelerators

Component	Quantity	Description
Graphcore IPU	32	16 Colossus GC200 IPU, 16 Bow IPU. Each IPU group hosted with a CPU server as a POD16 on a 100 GbE RoCE fabric
Intel PAC D5005 FPGA	2	Accelerator with Intel Stratix 10 GX FPGA and 32 GB DDR4
BittWare IA-840F FPGA	2	Accelerator with Agilex AGF027 FPGA and 64 GB of DDR4
NextSilicon Coprocessor	2	Reconfigurable accelerator with an optimizer continuously evaluating application behavior.
NEC Vector Engine	8	Vector computing card (8 cores and HBM2 memory)
Intel Optane SSD	48	18 TB of Intel Optane SSDs addressable as memory w/ MemVerge Memory Machine.
NVIDIA H100 + A30	30 + 4	NVIDIA GPUs for HPC, DL Training, AI Inference
Intel PVC + ATS-P	120	Intel GPUs for HPC, DL Training, AI Inference

Design: Composability at the Hardware Level

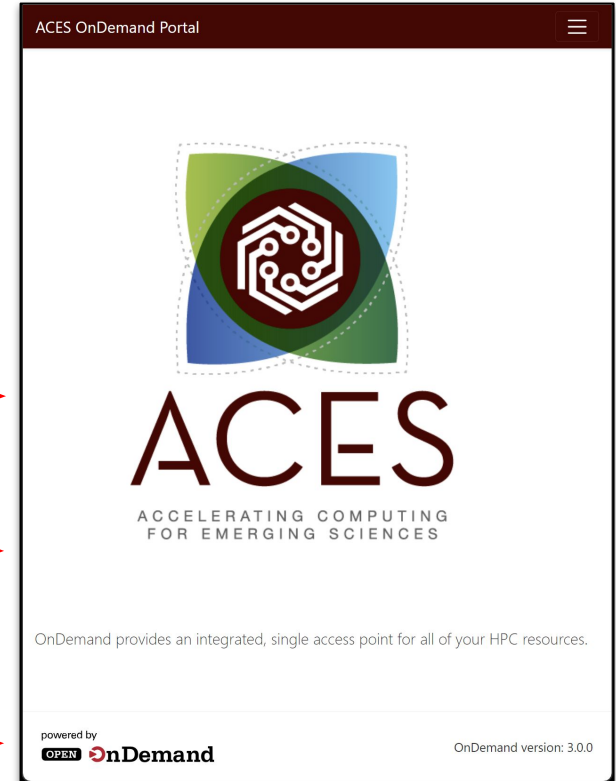


ACES Portal



ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based
graphical interface framework for HPC users



Authentication via CILogon

Log-in using your ACCESS CI credentials.

The screenshot shows the ACCESS CI login interface. At the top, there's a 'Consent to Attribute Release' section with a dropdown arrow. Below it, a list of attributes being requested: 'Your CILogon user identifier', 'Your name', 'Your email address', and 'Your username and affiliation from your identity provider'. The main section is titled 'Select an Identity Provider' and contains a dropdown menu with 'ACCESS CI (XSEDE)' selected. Below the dropdown is a 'Remember this selection' checkbox and a 'Log On' button. A red box highlights the 'Select an Identity Provider' section. At the bottom, there's a footer with links for 'FAQs' and 'help@clilogon.org'.

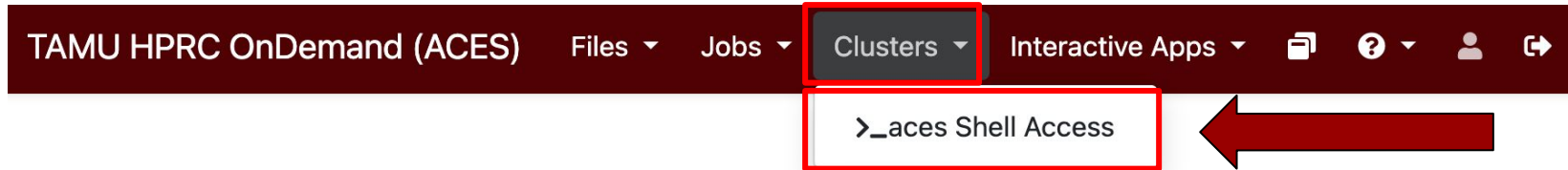
The screenshot shows the ACCESS CI login interface. At the top, there's a 'Login to CILogon' section with a 'ACCESS Username' field and a 'ACCESS Password' field. Below the password field is a 'Don't Remember Login' checkbox and a 'Login' button. To the right of the login fields is the CILogon logo and a brief description: 'CILogon facilitates secure access to CyberInfrastructure (CI)'. Below the logo, there are links for 'Register for an ACCESS Account', 'Forgot your password?', and 'Need Help?'. A red box highlights the 'Login to CILogon' section.

This is a close-up of the 'Select an Identity Provider' dropdown menu. It shows the text 'Select an Identity Provider' in a teal header. Below the header, there's a dropdown menu with 'ACCESS CI (XSEDE)' selected. A red box highlights the entire dropdown menu.

Select the Identity Provider appropriate for your account.

Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access



Success!

Welcome to the ACES login node.

Check which login node you are on.

```
Host: login.aces Themes: Default
| Consulting:      help@hprc.tamu.edu (preferred) or (979) 845-0219 |
| ACES Documentation: https://hprc.tamu.edu/kb/User-Guides/ACES |
| FASTER Documentation: https://hprc.tamu.edu/kb/User-Guides/FASTER |
| Grace Documentation: https://hprc.tamu.edu/kb/User-Guides/Grace |
| Terra Documentation: https://hprc.tamu.edu/kb/User-Guides/Terra |
| YouTube Channel: https://www.youtube.com/texasamhprc |
|=====|

*****
*                               *****
*                               === IMPORTANT POLICY INFORMATION ===
*                               *****
* - Unauthorized use of HPRC resources is prohibited and subject to
*   criminal prosecution.
* - Use of HPRC resources in violation of United States export control
*   laws and regulations is prohibited. Current HPRC staff members are
*   US citizens and legal residents.
* - Sharing HPRC account and password information is in violation of
*   Texas State Law. Any shared accounts will be DISABLED.
* - Authorized users must also adhere to ALL policies at:
*   https://hprc.tamu.edu/policies/
*                               *****
*                               !! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!
*                               *****

Please restrict usage to 8 CORES across ALL login nodes.
Users found in violation of this policy will be SUSPENDED.

To see these messages again, run the motd command.
Your current disk quotas are:
Disk                               Disk Usage      Limit      File Usage      Limit
/home/u.zh108696                   4.0G           10.0G       2361             10000
/scratch/user/u.zh108696          275.4G         1.0T        352057           1000000
Type 'showquota' to view these quotas again.
[u.zh108696@aces-login1 ~]$
```


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
```

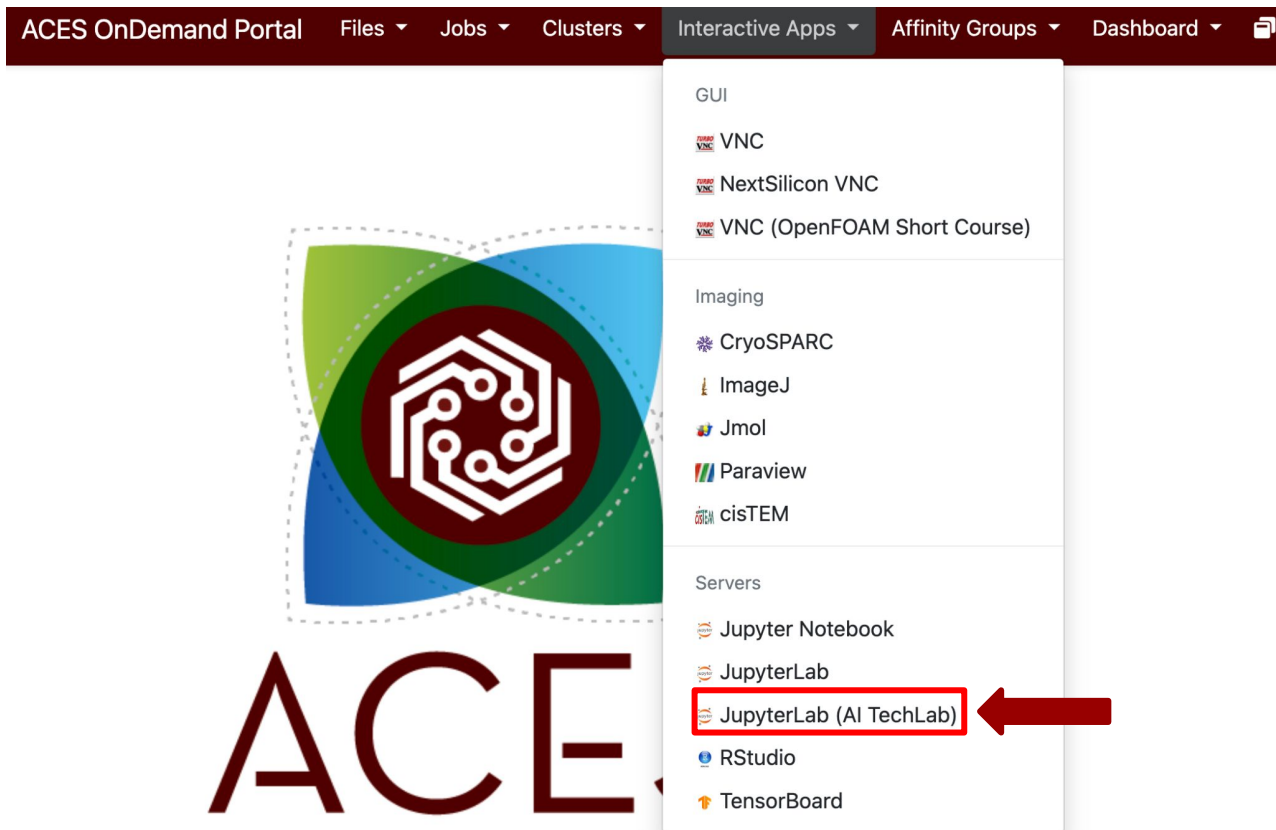
Make a copy in your personal scratch directory

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

- Enter this directory (your local copy)

```
$ cd ai_tech_labs
```


Go to JupyterLab Page



The screenshot shows the ACES OnDemand Portal interface. The top navigation bar includes links for 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Affinity Groups', and 'Dashboard'. The 'Interactive Apps' dropdown menu is open, displaying a list of applications categorized into GUI, Imaging, and Servers. The 'JupyterLab (AI TechLab)' option is highlighted with a red box and a red arrow pointing to it.

ACES OnDemand Portal Files Jobs Clusters Interactive Apps Affinity Groups Dashboard

GUI

- VNC
- NextSilicon VNC
- VNC (OpenFOAM Short Course)

Imaging

- CryoSPARC
- ImageJ
- Jmol
- Paraview
- cisTEM

Servers

- Jupyter Notebook
- JupyterLab
- JupyterLab (AI TechLab)**
- RStudio
- TensorBoard

JupyterLab Page

ACES OnDemand Portal Files Jobs Clusters Interactive Apps Affinity Groups Dashboard

Home / My Interactive Sessions / JupyterLab (AI TechLab)

Interactive Apps

- GUI
- VNC
- NextSilicon VNC
- VNC (OpenFOAM Short Course)
- Imaging
- CryoSPARC
- ImageJ
- Jmol
- Paraview
- cisTEM
- Servers
- Jupyter Notebook

JupyterLab (AI TechLab)

This app will launch a [JupyterLab](#) server on the [ACES cluster](#).

Module

Anaconda3/2022.05

Optional Environment to be activated

/sw/hprc/sw/Anaconda3/2022.05/envs/ai-labs

Enter the name of the environment to be activated.

Leave blank to use the [default](#) environment for the selected Module.

Your optional conda environment must have been previously built with one of the Anaconda or Python modules listed in the Module option above. See [instructions](#).

Node type

First available GPU

- Select a GPU node for software that supports GPU processing.

7 lucky attendees

Other fields:

Node Type: First available GPU
Number of GPUs: 1

Node Type: CPU only

Number of hours: 3
Number of cores: 3
Total memory (GB): 5

The remaining attendees

Option 1: Use a shared environment created by TAMU HPRC for this course

Path to the shared environment:
`/sw/hprc/sw/Anaconda3/2022.05/envs/ai-labs`

Connect to JupyterLab


ACES OnDemand Portal Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Affinity Groups ▾ Dashboard


Session was successfully deleted. ✕


[Home](#) / [My Interactive Sessions](#)

Interactive Apps


GUI


 VNC


 NextSilicon VNC


 VNC (OpenFOAM Short Course)


Imaging

 CryoSPARC

 ImageJ

 Jmol

 Paraview

 cisTEM


JupyterLab (AI TechLab) (245093) 1 node | 3 cores | Running

Host: >_ac064 ✕ Delete

Created at: 2024-09-16 20:50:24 CDT

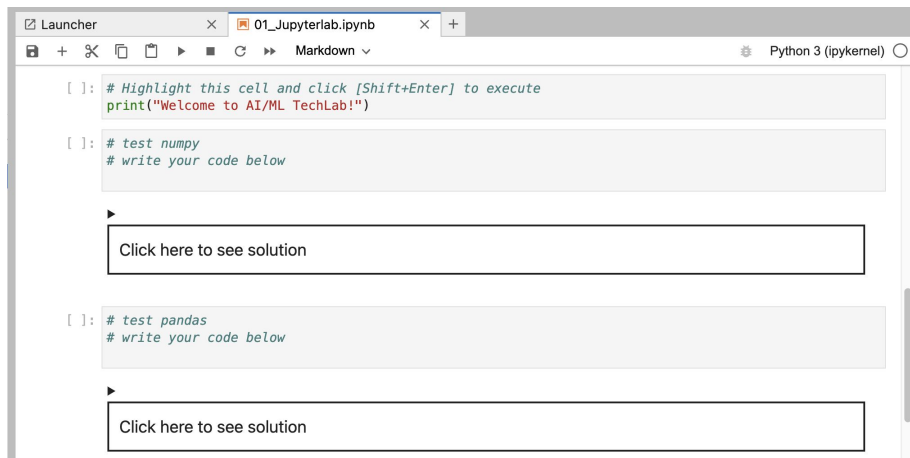
Time Remaining: 58 minutes

Session ID: ef26613c-c4f0-4766-b098-c12edfb5184c

👁 Connect to JupyterLab 

Review and Exercise

- Log into ACES through ACES Portal (ACCESS)
- Copy the training materials to your \$SCRATCH directory
- Launch JupyterLab app
- In the notebook named *01_Jupyterlab.ipynb*, follow the instructions to import the required modules to make sure they have been loaded properly.



```
[ ]: # Highlight this cell and click [Shift+Enter] to execute
print("Welcome to AI/ML TechLab!")

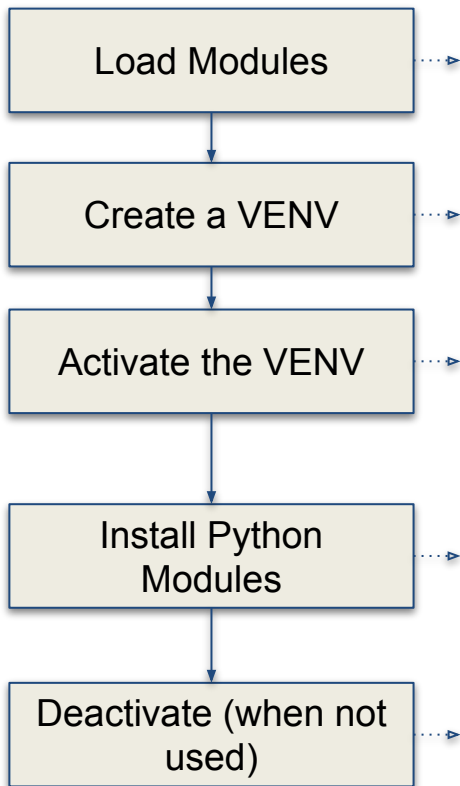
[ ]: # test numpy
# write your code below

Click here to see solution

[ ]: # test pandas
# write your code below

Click here to see solution
```


Option 2



```
# clean up and load Anaconda
cd $SCRATCH
module purge
module load Anaconda3/2022.05
```

```
# create a Python virtual environment
conda create -n ai-labs
```

```
# activate the virtual environment
source activate ai-labs
```

```
# install required package to be used in the portal
conda install -c anaconda jupyter
conda install -c anaconda pandas
conda install -c conda-forge matplotlib
conda install -c anaconda scikit-learn
conda install pytorch torchvision torchaudio
pytorch-cuda=11.8 -c pytorch -c nvidia
```

1 line

```
# deactivate the virtual environment
# source deactivate
```


JupyterLab Page

The screenshot shows a web browser window with the URL `portal-aces.hprc.tamu.edu/pun/sys/dashboard/batch_connect/dev/jupyterlab_shortcourse/ses...`. The page title is "JupyterLab (Short Course)".

Interactive Apps

- GUI
- VNC
- Nextsilicon VNC
- Imaging
- CryoSPARC
- ImageJ
- cisTEM
- Servers
- Jupyter Notebook
- JupyterLab
- RStudio

JupyterLab (Short Course)

This app will launch a [JupyterLab](#) server on the [ACES cluster](#).

Module

←

Optional Environment to be activated

←

Enter the name of the environment to be activated.

Leave blank to use the [default](#) environment for the selected Module.

Your optional conda environment must have been previously built with one of the Anaconda or Python modules listed in the Module option above. See [instructions](#).

Node type

Other fields:

Node Type: First available GPU

Number of GPUs: 1

Number of hours: 3

Number of cores: 3

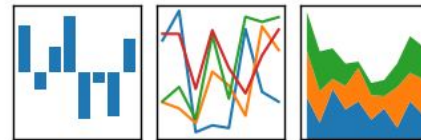
Total memory (GB): 5

Lab II. Data Exploration

matplotlib

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



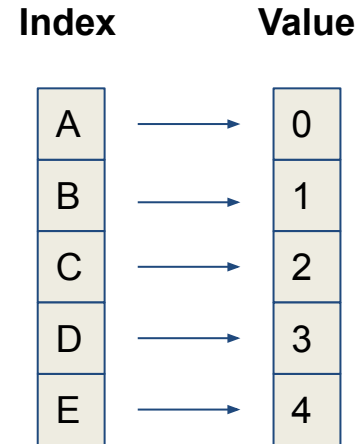
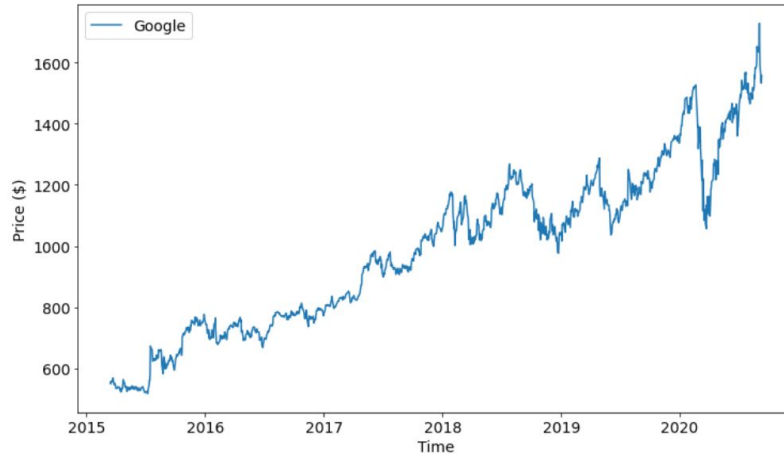
Data Structures

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	20141013T00	221900	3	1	1180	5650	1
6414100192	20141209T00	538000	3	2.25	2570	7242	2
5631500400	20150225T00	180000	2	1	770	10000	1
2487200875	20141209T00	604000	4	3	1960	5000	1
1954400510	20150218T00	510000	3	2	1680	8080	1
7237550310	20140512T00	1.23E+06	4	4.5	5420	101930	1
1321400060	20140627T00	257500	3	2.25	1715	6819	2
2008000270	20150115T00	291850	3	1.5	1060	9711	1
2414600126	20150415T00	229500	3	1	1780	7470	1

		Columns			
Index		C1	C2	C3	C4
A	→	0	x	0.1	True
B	→	1	y	2.4	False
C	→	2	z	1.9	True
D	→	NA	w	8.3	False
E	→	9	a	6.8	False

Pandas Learning Objectives

After this lesson, you will know how to:

- Create a DataFrame
- Retrieve a Row or Column
- Drop Entries
- Index, Select, and Filter data
- Sort data
- Input and Output



JupyterLab Exercises

Key Plotting Concepts in Matplotlib

- **Matplotlib: Figure**

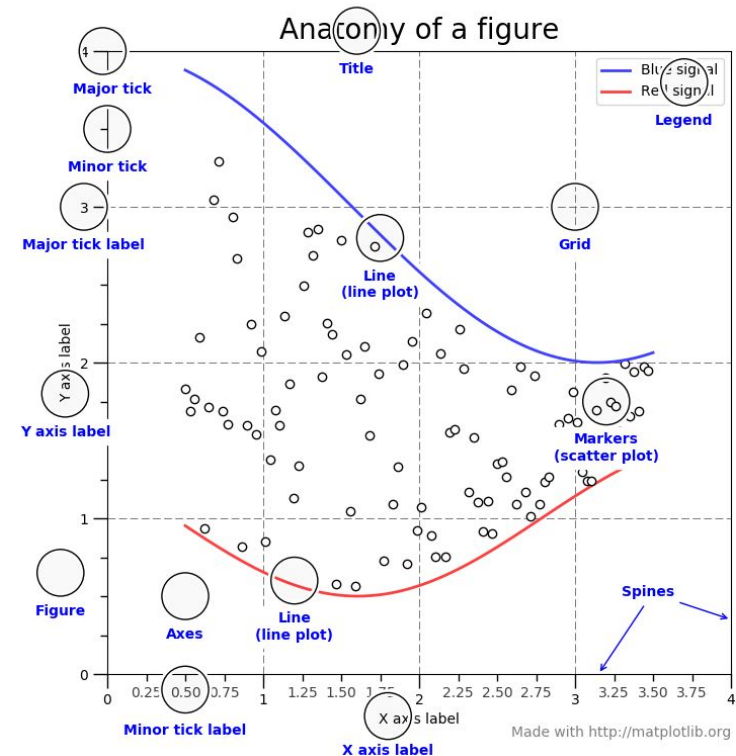
Figure is the object that keeps the whole image output. Adjustable parameters include:

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

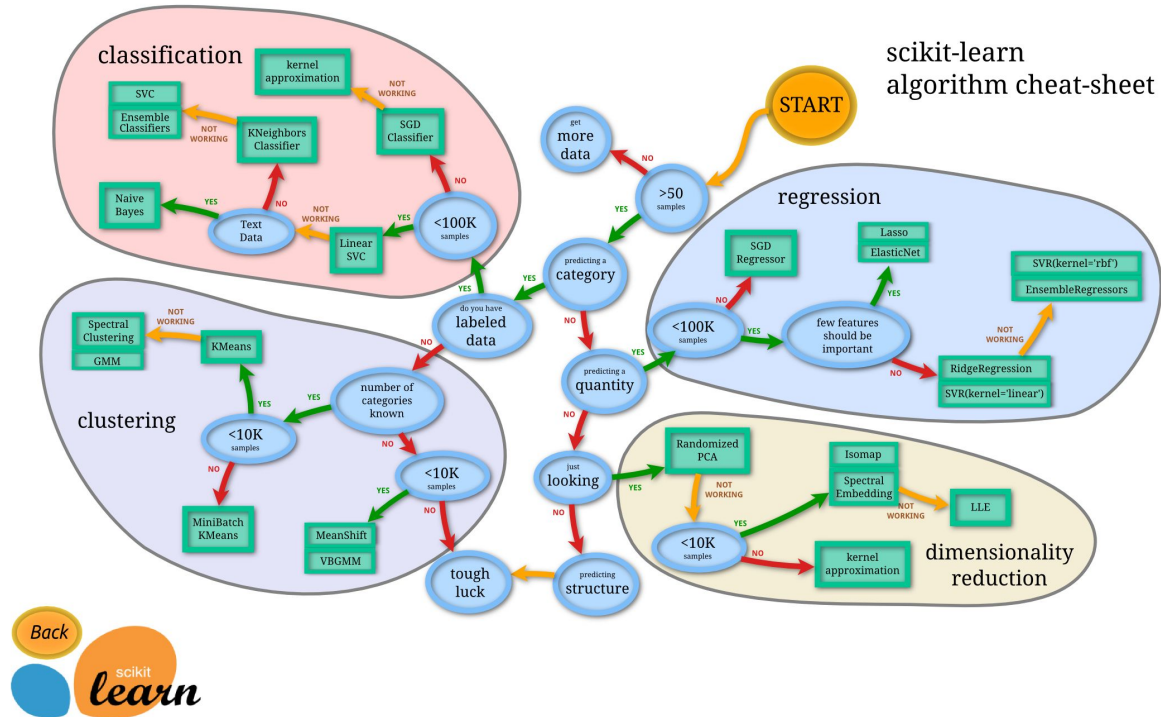
After this lesson, you will know how to create:

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



JupyterLab Exercises

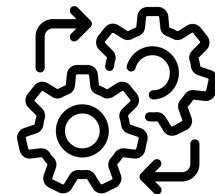
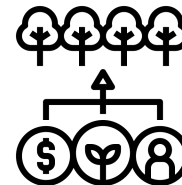
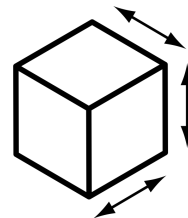
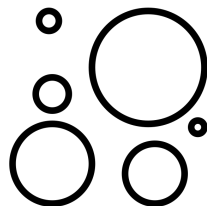
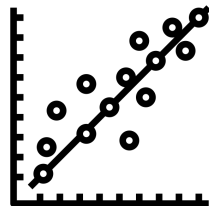
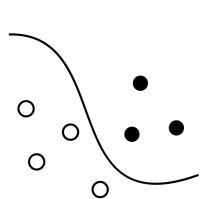
Lab III. Machine Learning



Main Features of scikit-learn



Classification	Regression	Clustering	Dimension Reduction	Model Selection	Preprocessing
Identifying category of an object Applications: Spam detection, image recognition. Algorithms: SVM, nearest neighbors, random forest, and more...	Predicting a attribute for an object Applications: Drug response, Stock prices. Algorithms: SVR, nearest neighbors, random forest, and more...	Grouping similar objects into sets Applications: Customer segmentation, Grouping experiment outcomes Algorithms: k-Means, spectral clustering, mean-shift, and more...	Reducing the number of dimensions Applications: Visualization, Increased efficiency Algorithms: k-Means, feature selection, non-negative matrix factorization, and more...	Selecting models with parameter search Applications: Improved accuracy via parameter tuning Algorithms: grid search, cross validation, metrics, and more...	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...



JupyterLab Exercises

Credit: icons are from [The Noun Project](https://thenounproject.com/) under Creative Commons Licenses

Lab IV. Deep Learning

Deep Learning

by Ian Goodfellow, Yoshua Bengio, and Aaron Courville

<http://www.deeplearningbook.org/>

Animation of Neutron Networks

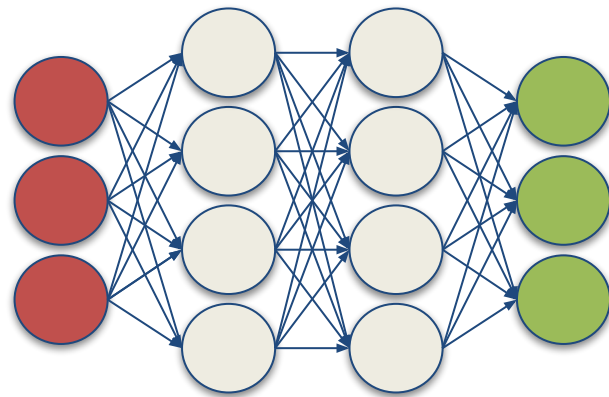
by Grant Sanderson

<https://www.3blue1brown.com/>

Visualization of CNN

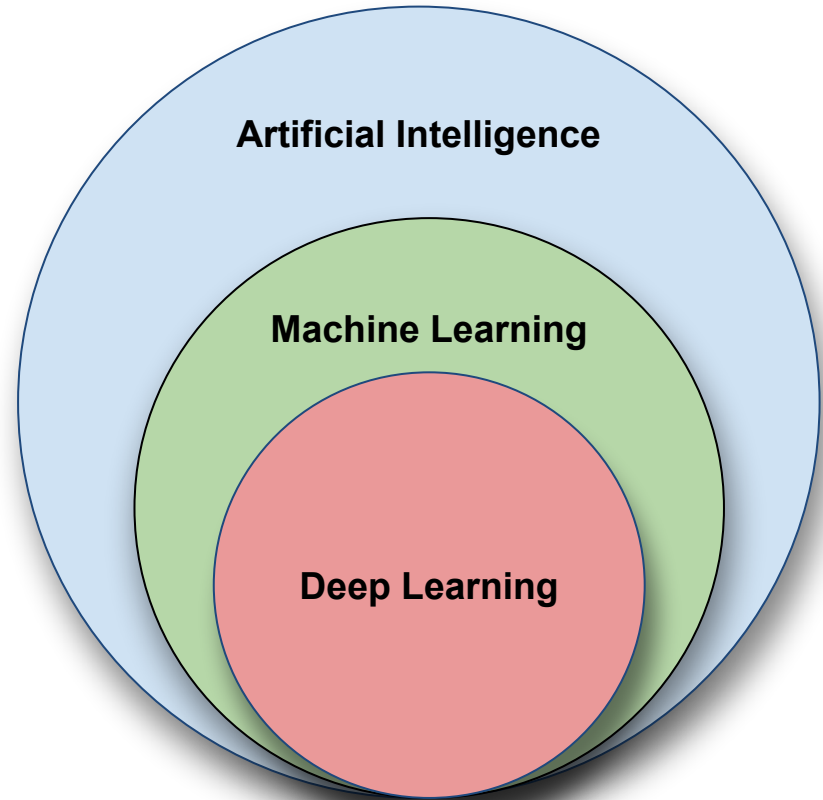
by Adam Harley

https://adamharley.com/nn_vis/cnn/3d.html



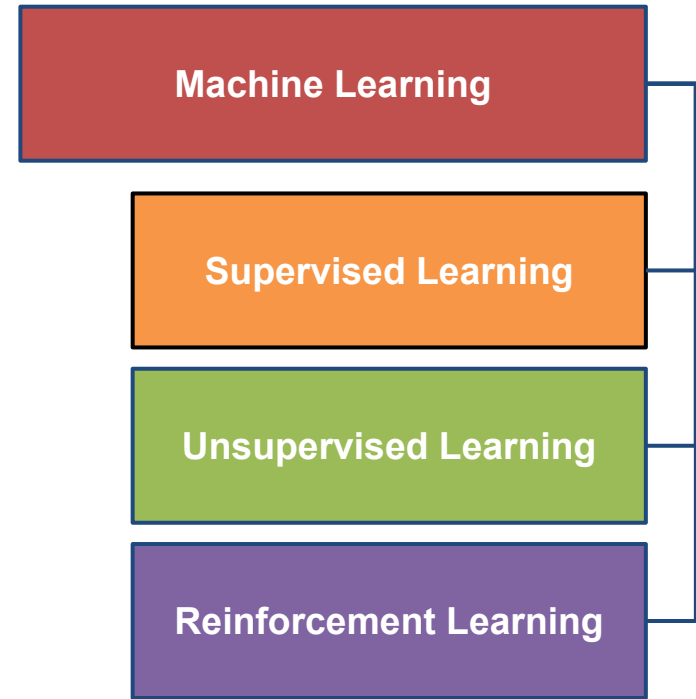
Relationship of AI, ML, and DL

- **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**.



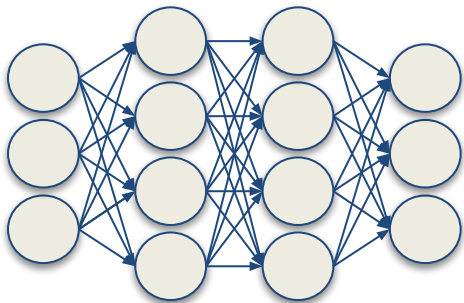
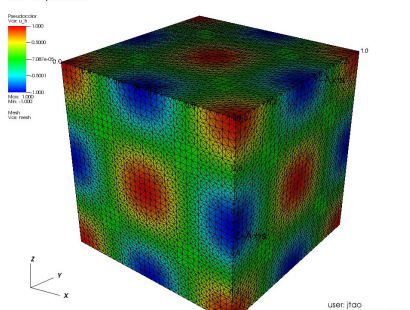
Types of ML Algorithms

- **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 business strategy planning.

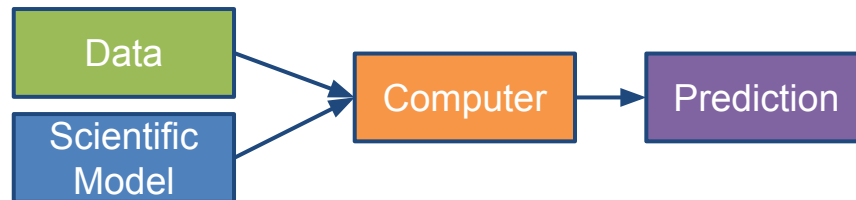


Machine Learning

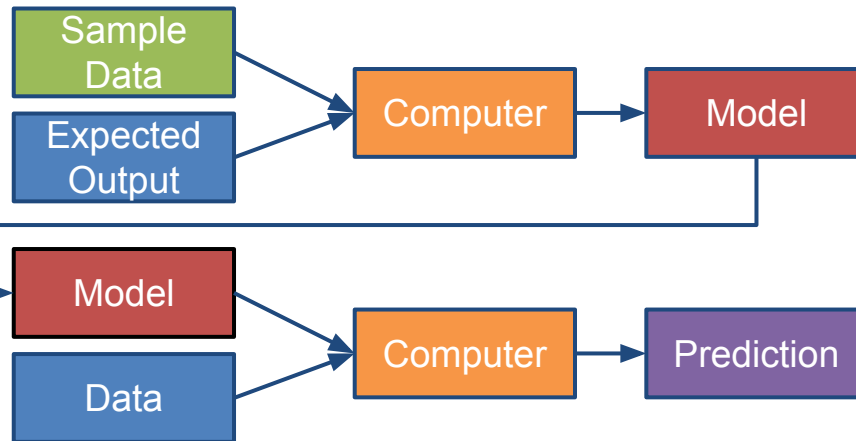
DB: simplest.vtk



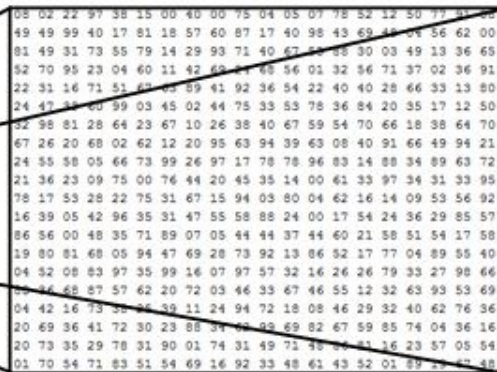
Traditional Modeling



Machine Learning (Supervised Learning)



Inputs and Outputs



What the computer sees

image classification

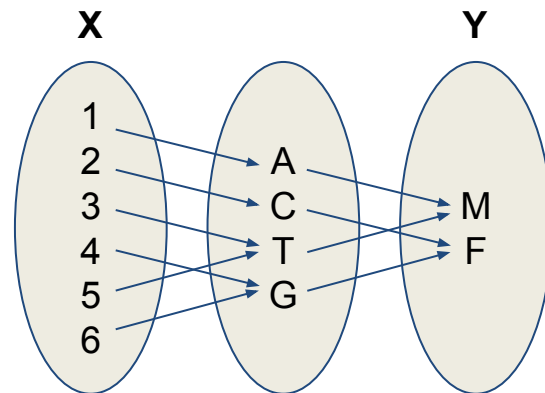
82% cat
15% dog
2% hat
1% mug

Image from the [Stanford CS231 Course](#)

256 X 256
Matrix

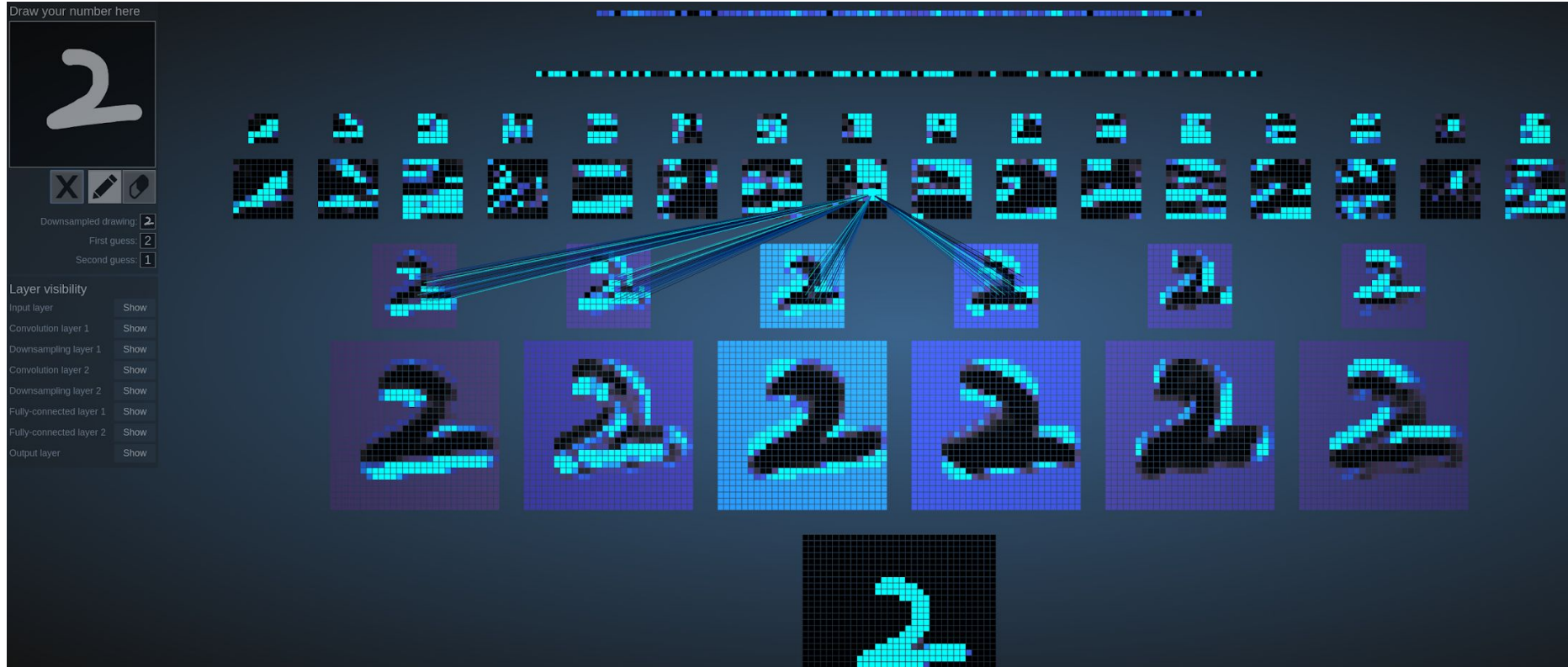
DL model

4-Element Vector



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

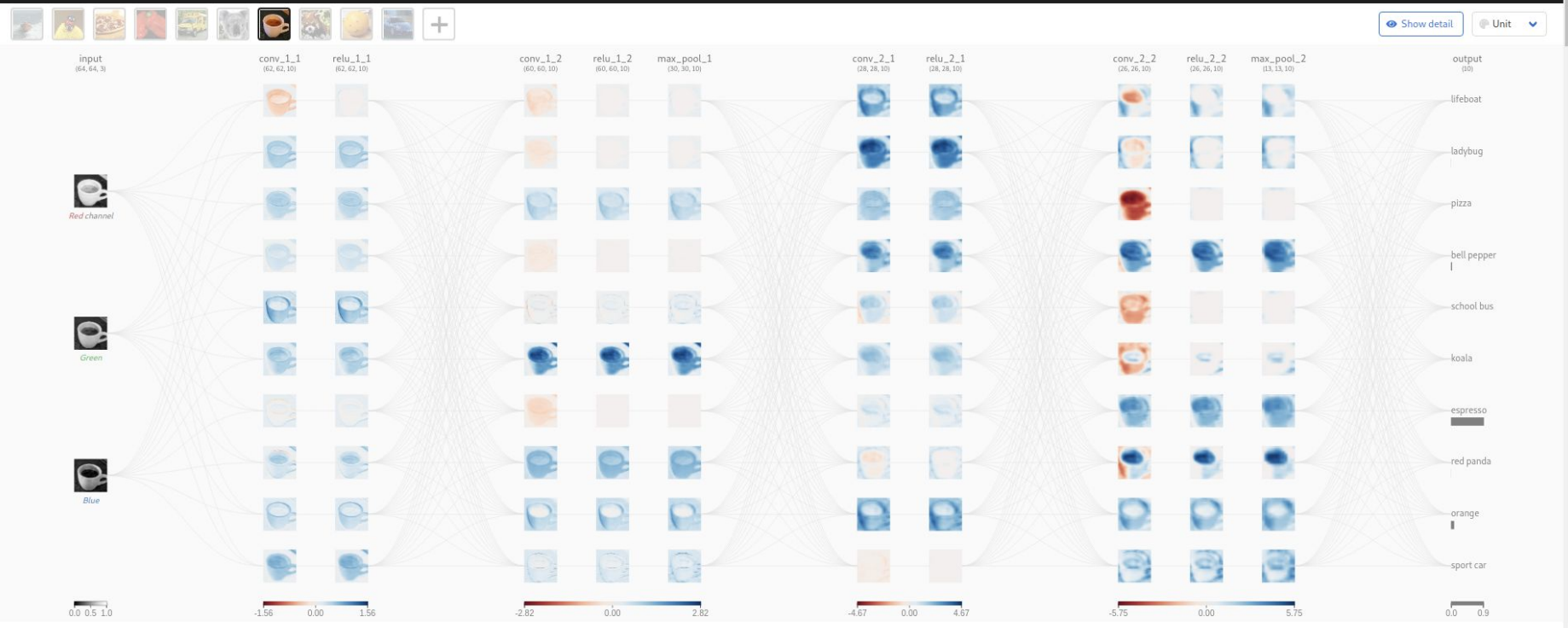
MNIST - CNN Visualization



(Image Credit: https://adamharley.com/nn_vis/cnn/3d.html)

CNN Explainer

CNN EXPLAINER Learn Convolutional Neural Network (CNN) in your browser!



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



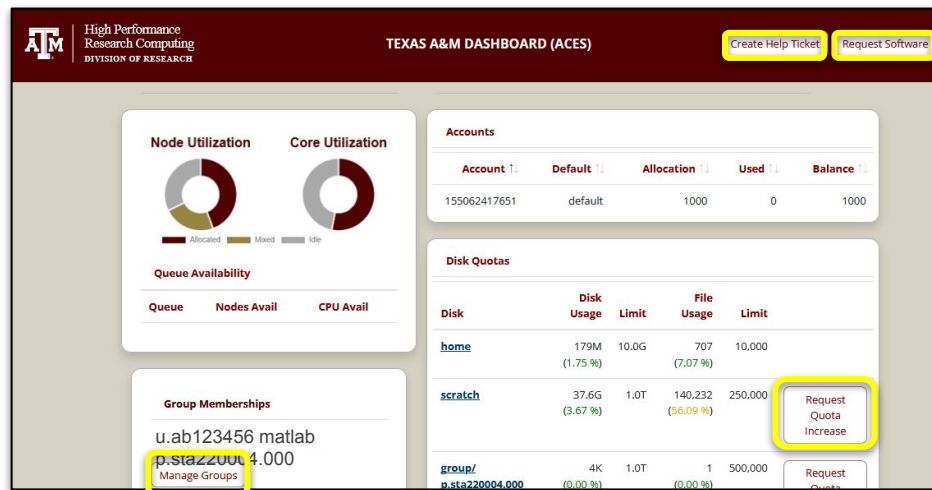
JupyterLab Exercises

Need Help?

First check the FAQ: <https://hprc.tamu.edu/kb/FAQ/Accounts>

- ACES user Guide: <https://hprc.tamu.edu/kb/User-Guides/ACES>
- Email your questions to help@hprc.tamu.edu

Remember the
Dashboard!



Need Help?

Help us help you -- tell us:

- Which cluster
- Username
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- Steps you have taken, so we can reproduce the problem



High Performance
Research Computing
DIVISION OF RESEARCH

Thank you
Questions?

Give us feedback on the class with this survey:
https://u.tamu.edu/hprc_shortcourse_survey



HPRC Survey