

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



Outline

Lab I. JupyterLab (30 mins)

We will build and activate a ModuLair virtual environment and run JupyterLab on HPRC ACES portal.

Lab II. Data Exploration (30 mins)

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

04

Q&A
(5 mins/lab)

01

02

03

Lab IV. Deep Learning (30 minutes)

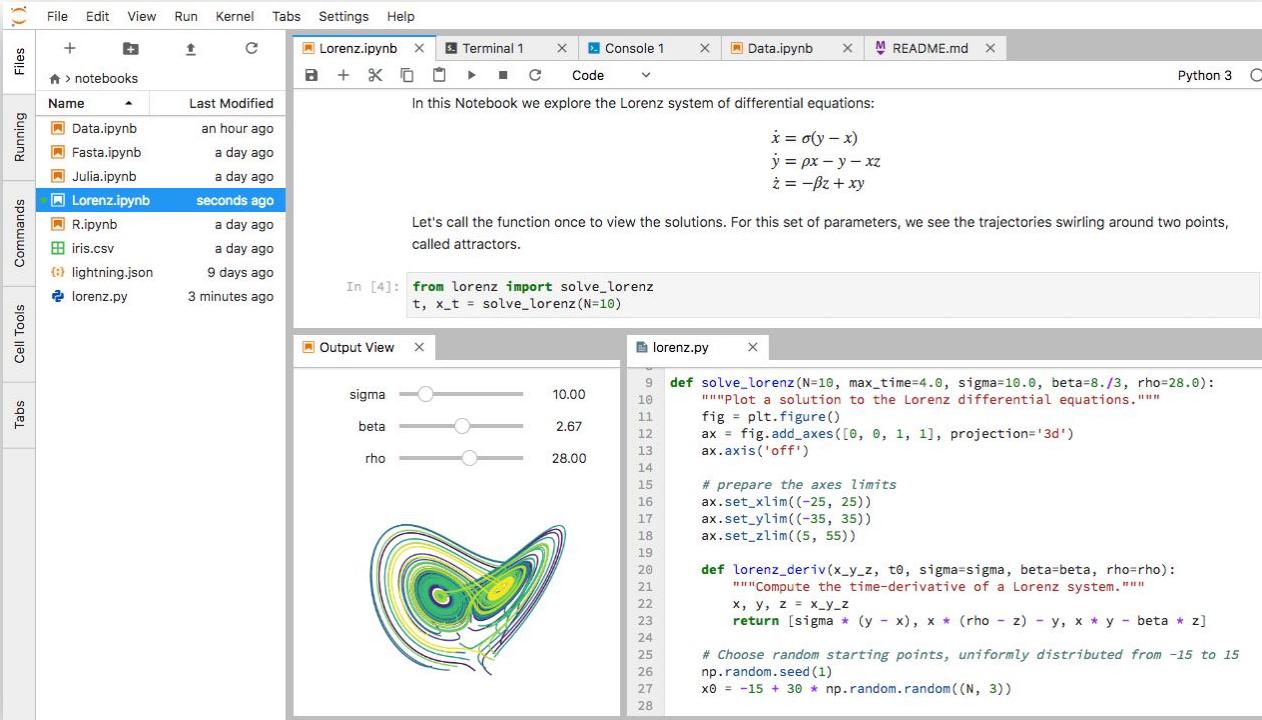
We will learn how to use PyTorch to build and train a simple image classification model with deep neural network (DNN).

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 AI TechLab.

Lab I. JupyterLab



The screenshot shows the JupyterLab interface. On the left is a sidebar with tabs for Files, Running, Commands, Cell Tools, and Tabs. The Files tab is active, showing a list of notebooks and files. The 'Running' tab shows the 'Lorenz.ipynb' notebook is currently running. The 'Commands' tab lists R.ipynb, iris.csv, lightning.json, and lorenz.py. The 'Cell Tools' tab is empty. The 'Tabs' tab shows tabs for Lorenz.ipynb, Terminal 1, Console 1, Data.ipynb, README.md, and a Code tab. The main area contains a text cell with code and a description of the Lorenz system, and a code cell with Python code. Below the code cell is an 'Output View' tab showing sliders for sigma, beta, and rho, and a 3D plot of the Lorenz attractor. The 'lorenz.py' code cell contains the following Python code:

```
9 def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8.0/3, rho=28.0):
10     """Plot a solution to the Lorenz differential equations."""
11     fig = plt.figure()
12     ax = fig.add_axes([0, 0, 1, 1], projection='3d')
13     ax.axis('off')
14
15     # prepare the axes limits
16     ax.set_xlim((-25, 25))
17     ax.set ylim((-35, 35))
18     ax.set_zlim((5, 55))
19
20     def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
21         """Compute the time-derivative of a Lorenz system."""
22         x, y, z = x_y_z
23         return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]
24
25     # Choose random starting points, uniformly distributed from -15 to 15
26     np.random.seed(1)
27     x0 = -15 + 30 * np.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:

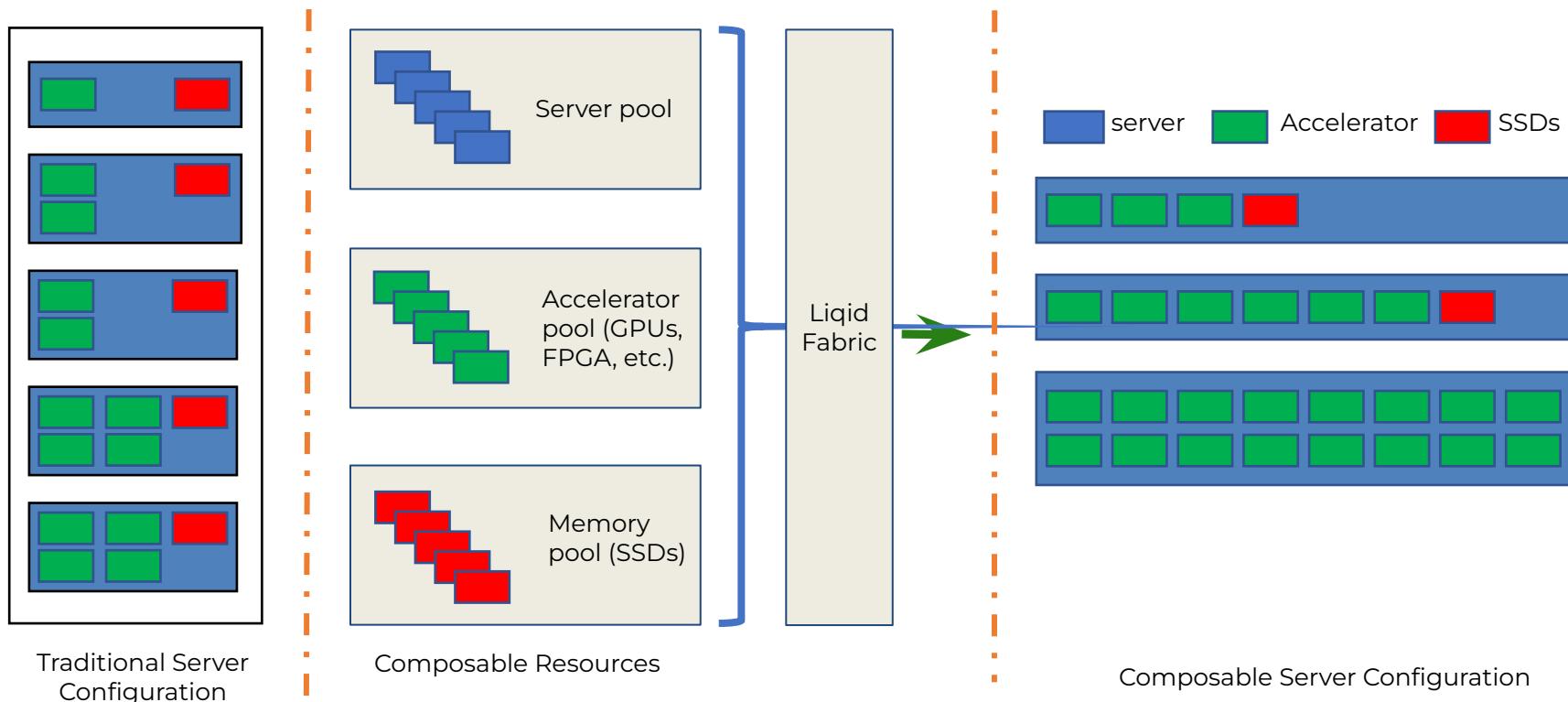
- Develop an NSF ACSS CI testbed
- Offer an accelerator testbed for numerical simulations and AI/ML workloads
- Provide consulting, technical guidance, and training to researchers
- Collaborate on computational and data-enabled research.



ACES

ACCELERATING COMPUTING
FOR EMERGING SCIENCES

Design: Composability at the Hardware Level



ACES Accelerators

Component	Quantity	Description
Graphcore IPU: Colossus GC200 Bow	16 16	Each IPU group hosted with a CPU server as a POD16 on a 100 GbE RoCE fabric
NVIDIA GPUs: H100 A30	30 4	For HPC, DL Training, AI Inference For AI Inference and Mainstream Compute
BittWare IA-840F FPGA	3	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 SSDs addressable as memory w/ MemVerge Memory Machine.
Intel PVC GPUs	120	Intel GPUs for HPC, DL Training, AI Inference

ACES Portal

The screenshot shows the Texas A&M High Performance Research Computing website. The top navigation bar includes links for Home, User Services, Resources, Research, Policies, Events, Training, About, and Portal. The 'Portal' link is highlighted with a yellow box. Below the navigation is a photograph of server racks. To the right of the photograph is a 'Quick Links' sidebar with sections for New User Information, Accounts, User Consulting, Training, Knowledge Base, Software, and FAQ. The main content area features a graphic of a person jumping rope and a chemical structure of a platinum complex. Text on the right reads: 'Molecular Jump-Rope: Multiringed Metal-Complexes That Really Know How To Jump'. A quote below states: 'These platinum complexes can undergo a 'triple-jump rope' mechanism rendering the three methylene chains of their ligands equivalent, a motion that is unheard of and reminiscent of Olympic traditions such as the triple-Axel or the triple jump.' - Dr. John Gladysz, Department of Chemistry. A red arrow points from the 'ACES Portal (ACES)' link in the sidebar to the 'ACES OnDemand Portal' window.

The screenshot shows the ACES OnDemand Portal. The top navigation bar includes links for Home, User Services, Resources, Research, Policies, Events, Training, About, and Portal. The 'Portal' link is highlighted with a yellow box. Below the navigation is a photograph of server racks. To the right of the photograph is a 'Quick Links' sidebar with sections for New User Information, Accounts, User Consulting, Training, Knowledge Base, Software, and FAQ. The main content area features a graphic of a person jumping rope and a chemical structure of a platinum complex. Text on the right reads: 'Molecular Jump-Rope: Multiringed Metal-Complexes That Really Know How To Jump'. A quote below states: 'These platinum complexes can undergo a 'triple-jump rope' mechanism rendering the three methylene chains of their ligands equivalent, a motion that is unheard of and reminiscent of Olympic traditions such as the triple-Axel or the triple jump.' - Dr. John Gladysz, Department of Chemistry. A red arrow points from the 'ACES Portal (ACES)' link in the sidebar to the 'ACES OnDemand Portal' window.

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

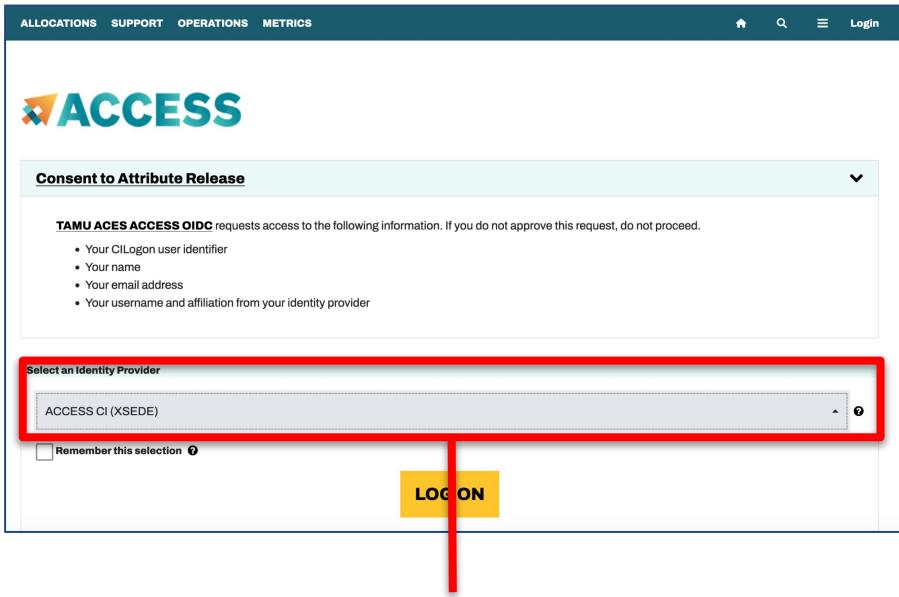
Open OnDemand (OOD) is an advanced web-based graphical interface framework for HPC users.

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

powered by
 OnDemand

OnDemand version: 3.0.0

Accessing ACES via the Portal (ACCESS)



ALLOCATIONS SUPPORT OPERATIONS METRICS Home Search Menu Login

ACCESS

Consent to Attribute Release

TAMU ACES ACCESS OIDC requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

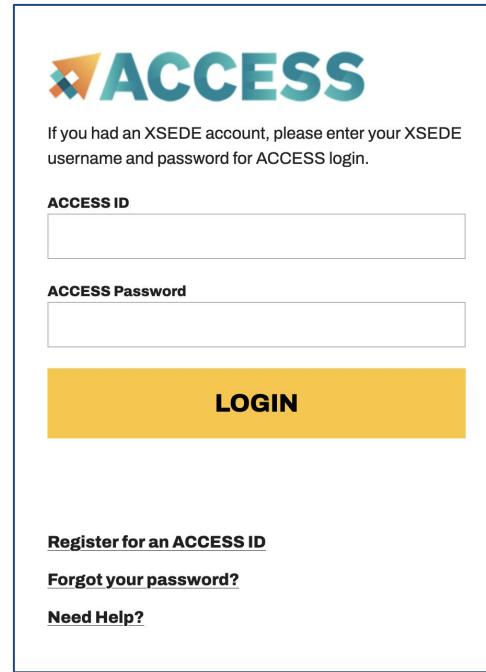
Select an Identity Provider

ACCESS CI (XSEDE)

Remember this selection ?

LOG ON

Select the Identity Provider appropriate for your account.



ACCESS

If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login.

ACCESS ID

ACCESS Password

LOGIN

[Register for an ACCESS ID](#)

[Forgot your password?](#)

[Need Help?](#)

Log in using your ACCESS or institutional credentials.

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
```

(Option 1) Environment Setup: ModuLair

- The ModuLair Framework is designed to streamline the management of Python environments on HPC clusters.

Core Functionalities:

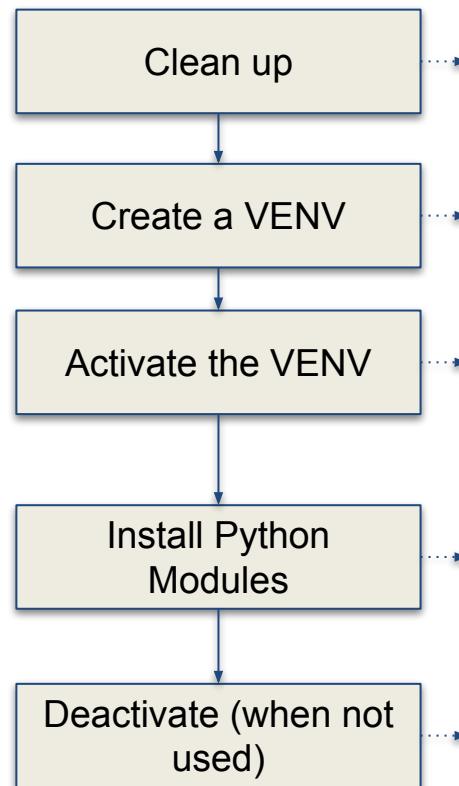
- Creating Environments (`create_venv`)
- Activating Environments (`activate_venv`)
- Listing Environments (`list_envs`)
- Deleting Environments (`delete_venv`)

hprc.tamu.edu/kb/Software/ModuLair

Advantages of ModuLair

- ModuLair builds virtual environments in \$SCRATCH (at \$SCRATCH/virtual_envs) instead of using \$HOME to avoid filling your home directory space quickly.
- ModuLair automatically records the toolchain and Python modules used to create each environment, so you don't need to keep track of them yourself.

ModuLair



```
# clean up
cd $SCRATCH
module purge

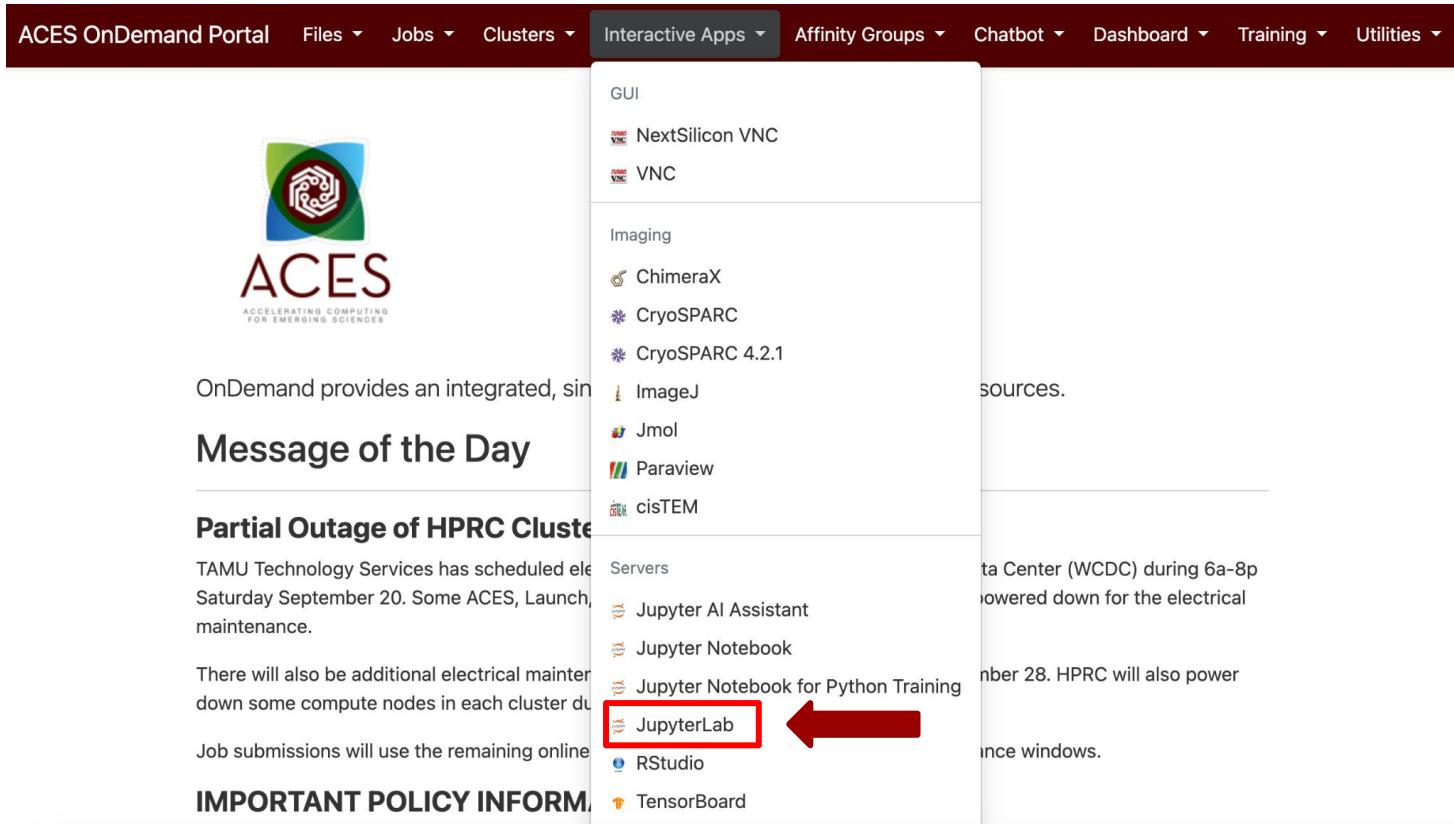
# create a ModuLair virtual environment
create_venv ai_labs_env -d "Environment for \
AI TechLab" -t "GCCcore/12.2.0 Python/3.10.8"

# activate the virtual environment
source activate_venv ai_labs_env

# install required packages
pip3 install jupyter
pip3 install pandas matplotlib
pip3 install scikit-learn
pip3 install torch torchvision \
--index-url https://download.pytorch.org/whl/cu126
pip3 install transformers

# deactivate the virtual environment
# deactivate
```

Go to JupyterLab Page



ACES OnDemand Portal Files ▾ Jobs ▾ Clusters ▾ **Interactive Apps ▾** Affinity Groups ▾ Chatbot ▾ Dashboard ▾ Training ▾ Utilities ▾

OnDemand provides an integrated, sin

Message of the Day

Partial Outage of HPRC Cluste

TAMU Technology Services has scheduled ele Saturday September 20. Some ACES, Launch, maintenance.

There will also be additional electrical mainte down some compute nodes in each cluster du

Job submissions will use the remaining online

IMPORTANT POLICY INFORM

GUI

- NextSilicon VNC
- VNC

Imaging

- ChimeraX
- CryoSPARC
- CryoSPARC 4.2.1
- ImageJ
- Jmol
- Paraview
- cisSTEM

Servers

- Jupyter AI Assistant
- Jupyter Notebook
- Jupyter Notebook for Python Training
- JupyterLab** ←
- RStudio
- TensorBoard

JupyterLab Page

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Home / My Interactive Sessions / JupyterLab

Interactive Apps

- GUI
 - NextSilicon VNC
 - VNC
 - Imaging
 - ChimeraX
 - CryoSPARC
 - CryoSPARC 4.2.1
 - ImageJ
 - Jmol
 - Paraview
 - cisTEM
 - Servers
 - Jupyter AI Assistant
 - Jupyter Notebook
 - Jupyter Notebook

JupyterLab

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

Type of environment

TAMU ModuLair (Python virtualenv manager) 

Select the type of environment in which Jupyter is installed.
[Help me choose](#)

TAMU ModuLair environment (required)

ai_labs_env 

Select the name of the TAMU ModuLair environment to be activated.

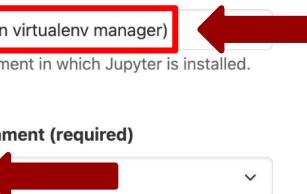
Your TAMU ModuLair environment is expected to have a Jupyter package installed. Please see [instructions](#)

Node type

CPU only

- cpuavail gpuavail select a non-CPU node type only if your software supports the Accelerator

Number of hours (max 72)



Option 1: Use own created ModuLair environment

Connect to JupyterLab

ACES OnDemand Portal Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Affinity Groups ▾ Chatbot ▾ Dashboard ▾ Training ▾ Utilities ▾ 📁

Session was successfully deleted. X

Home / My Interactive Sessions

Interactive Apps

- Desktops
- 💻 VNC
- GUI
- 💻 NextSilicon VNC
- Imaging
- 🌀 ChimeraX
- ✳️ CryoSPARC
- ✳️ CryoSPARC 4.2.1
- 💡 ImageJ
- 🧬 Jmol

JupyterLab (1438080) 1 node 4 cores | Running

Host: > ac005 ✖ Delete

Created at: 2026-02-05 13:54:53 CST

Time Remaining: 2 hours and 58 minutes

Session ID: [159fe4ff-1dec-4bd7-8db0-c34ade3964cc](#)

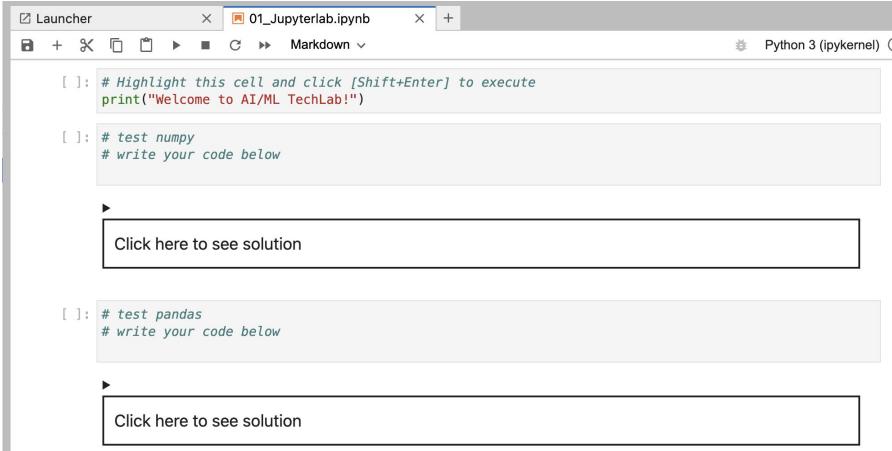
Type of environment: modular

Node type: CPU

🔗 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.



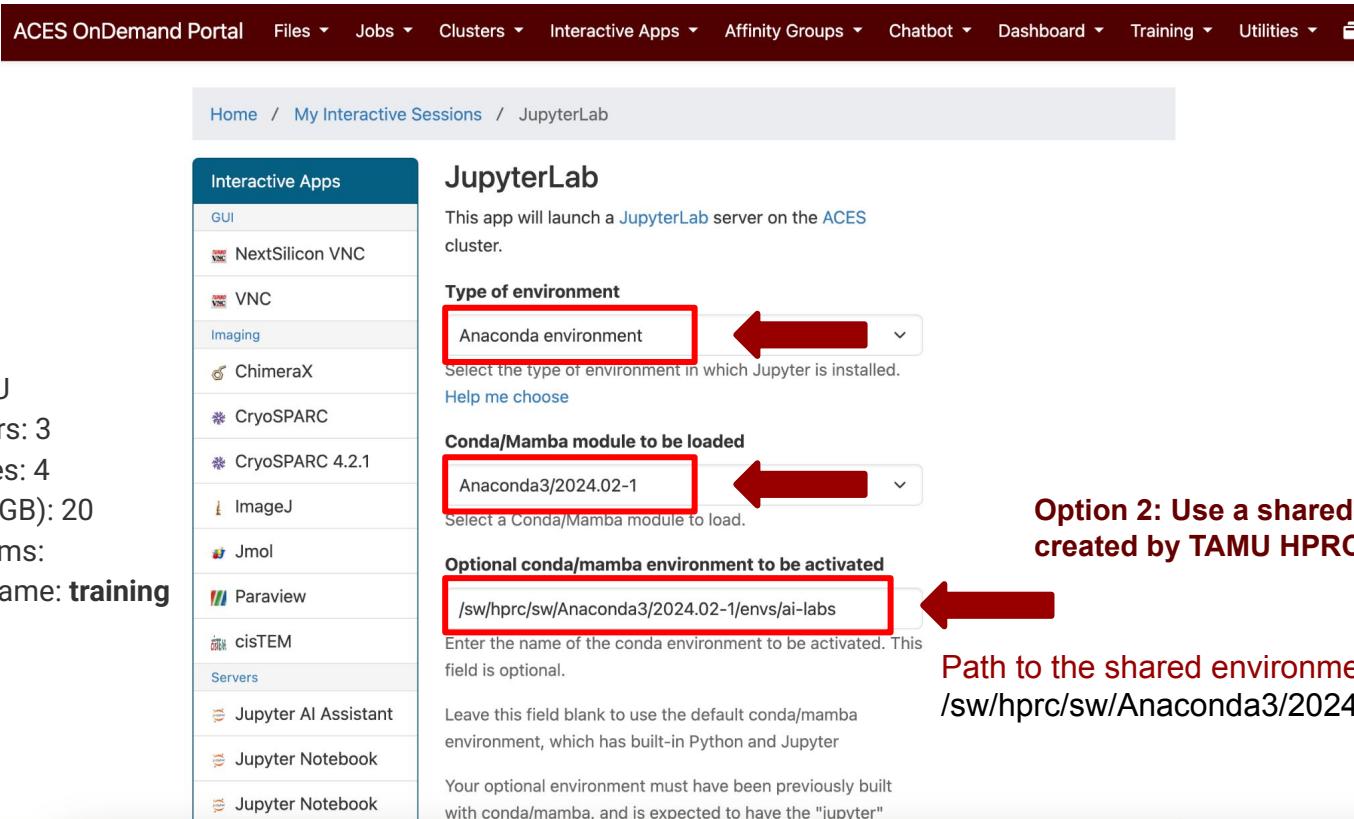
The screenshot shows a JupyterLab interface with a tab bar at the top labeled 'Launcher' and '01_Jupyterlab.ipynb'. The main area contains two code cells and two 'Click here to see solution' buttons.

- Cell 1:** Contains the following code:

```
[ ]: # Highlight this cell and click [Shift+Enter] to execute
print("Welcome to AI/ML TechLab!")
```
- Cell 2:** Contains the following code:

```
[ ]: # test numpy
# write your code below
```
- Solution Buttons:** Below each code cell is a button labeled 'Click here to see solution'.
- Kernel Information:** In the top right corner, it shows 'Python 3 (ipykernel)'.

(Option 2) Shared Anaconda Env.



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

Home / My Interactive Sessions / JupyterLab

Interactive Apps

- GUI
- NextSilicon VNC
- VNC
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- ChimeraX
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- CryoSPARC 4.2.1
- ImageJ
- Jmol
- Paraview
- cisTEM
- Servers
- Jupyter AI Assistant
- Jupyter Notebook
- Jupyter Notebook

JupyterLab

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

Type of environment

Anaconda environment

Select the type of environment in which Jupyter is installed.
[Help me choose](#)

Conda/Mamba module to be loaded

Anaconda3/2024.02-1

Select a Conda/Mamba module to load.

Optional conda/mamba environment to be activated

/sw/hprc/sw/Anaconda3/2024.02-1/envs/ai-labs

Enter the name of the conda environment to be activated. This field is optional.

Leave this field blank to use the default conda/mamba environment, which has built-in Python and Jupyter

Your optional environment must have been previously built with conda/mamba, and is expected to have the "jupyter"

Option 2: Use a shared environment created by TAMU HPRC for this course

Path to the shared environment:
`/sw/hprc/sw/Anaconda3/2024.02-1/envs/ai-labs`

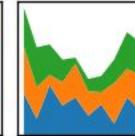
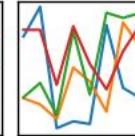
Lab II. Data Exploration

matplotlib



pandas

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



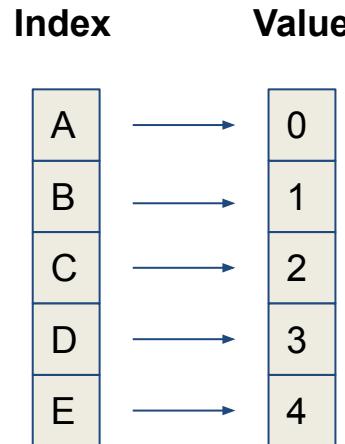
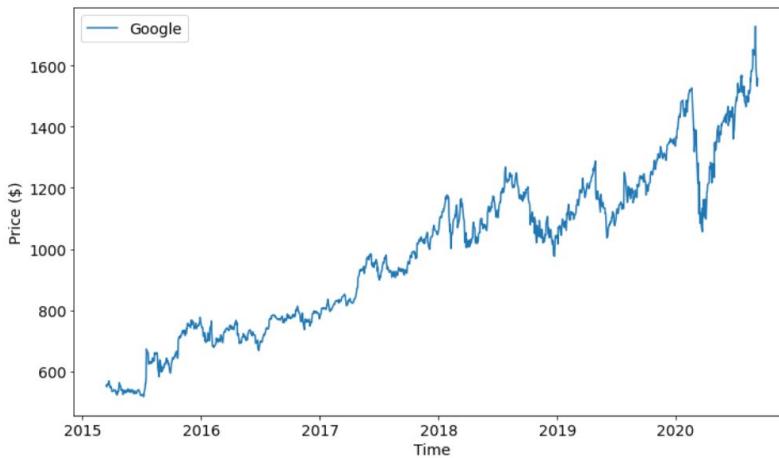
Data Structures

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

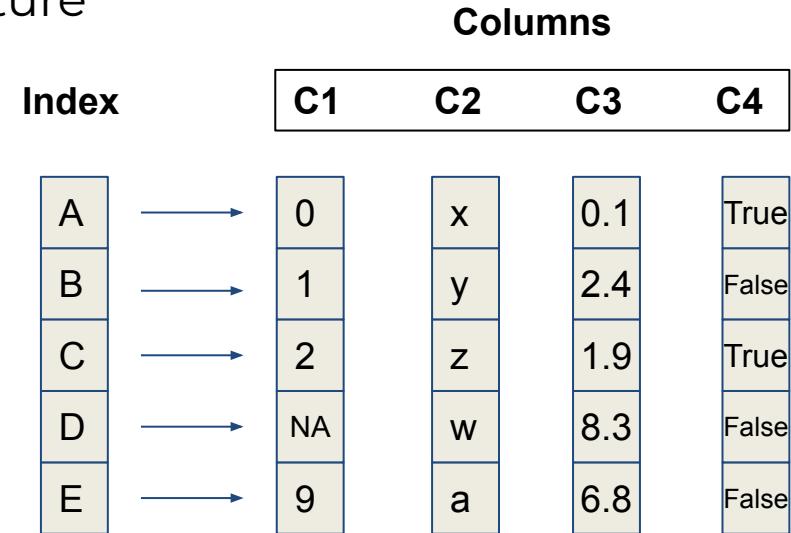
- One-dimensional labeled array
- Capable of holding any data type (integers, strings, floating point numbers, etc.)
- Example: time-series stock price data



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	20141013T000000	221900	3	1	1180	5650	1
6414100192	20141209T000000	538000	3	2.25	2570	7242	2
5631500400	20150225T000000	180000	2	1	770	10000	1
2487200875	20141209T000000	604000	4	3	1960	5000	1
1954400510	20150218T000000	510000	3	2	1680	8080	1
7237550310	20140512T000000	1.23E+06	4	4.5	5420	101930	1
1321400060	20140627T000000	257500	3	2.25	1715	6819	2
2008000270	20150115T000000	291850	3	1.5	1060	9711	1
2414600126	20150415T000000	229500	3	1	1780	7470	1



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**

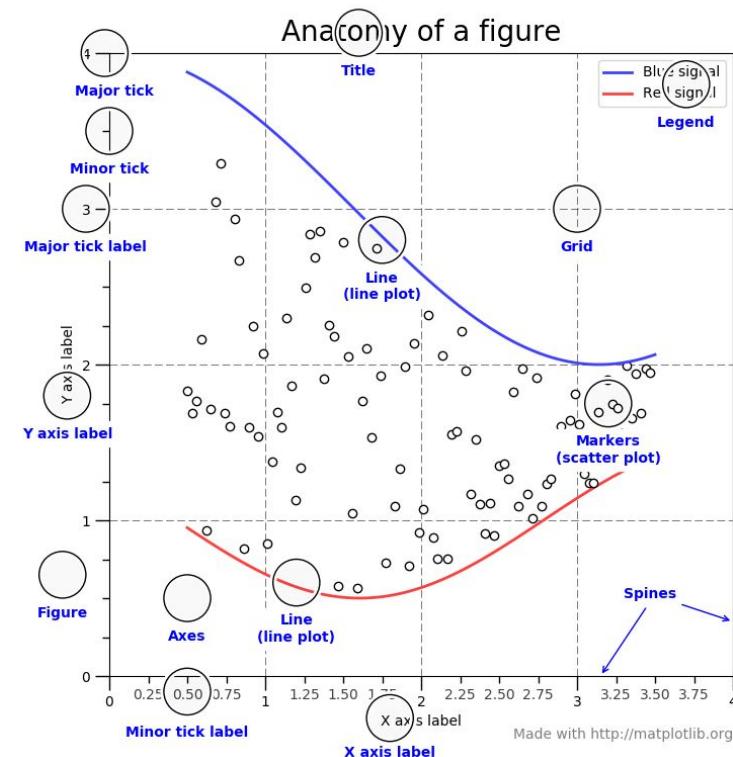
Figure is the object that keeps the whole image output. Adjustable parameters include:

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

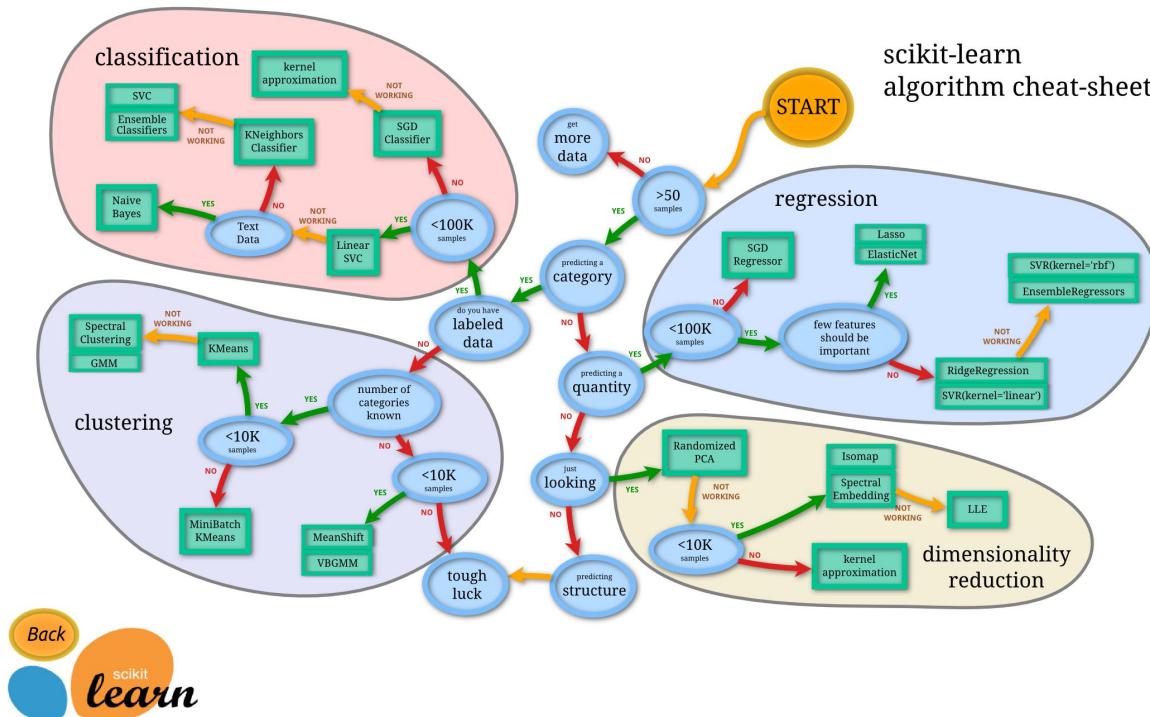
After this lesson, you will know how to create:

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



JupyterLab Exercises

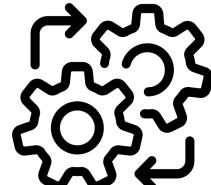
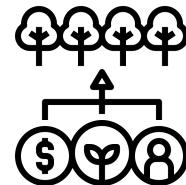
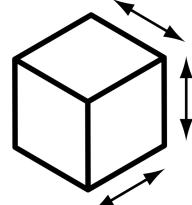
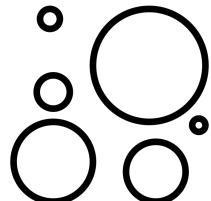
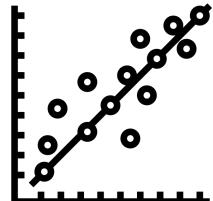
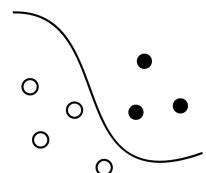
Lab III. Machine Learning



Main Features of scikit-learn



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



JupyterLab Exercises

Credit: icons are from [The Noun Project](#) under Creative Commons Licenses

Lab IV. Deep Learning

Deep Learning

by Ian Goodfellow, Yoshua Bengio, and Aaron Courville

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

Animation of Neuron Networks

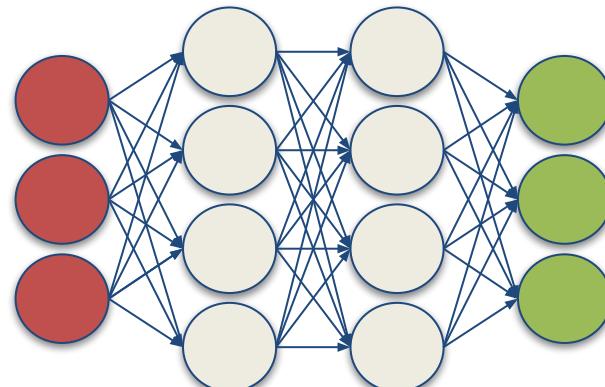
by Grant Sanderson

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

Visualization of CNN

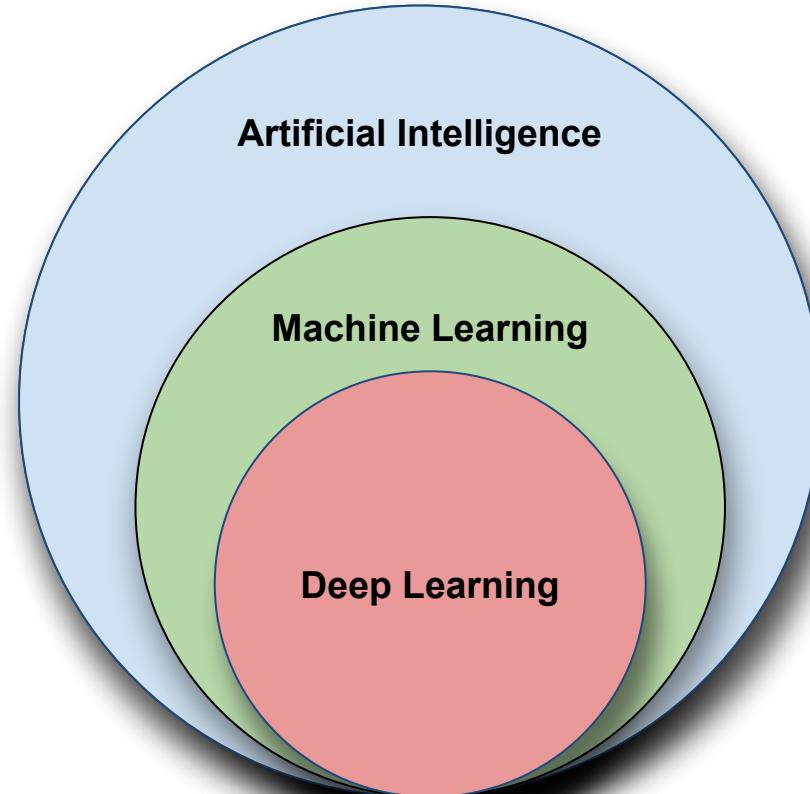
by Adam Harley

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



Introduction to AI/ML/DL

- **AI (Artificial Intelligence):**
Machines simulating human intelligence
- **ML (Machine Learning):**
A method to enable AI through data learning
- **DL (Deep Learning):**
A type of ML using layered neural networks



Types of ML Algorithms

- **Supervised Learning**

- trained with labeled data; including regression and classification problems

Machine Learning

- **Unsupervised Learning**

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

Supervised Learning

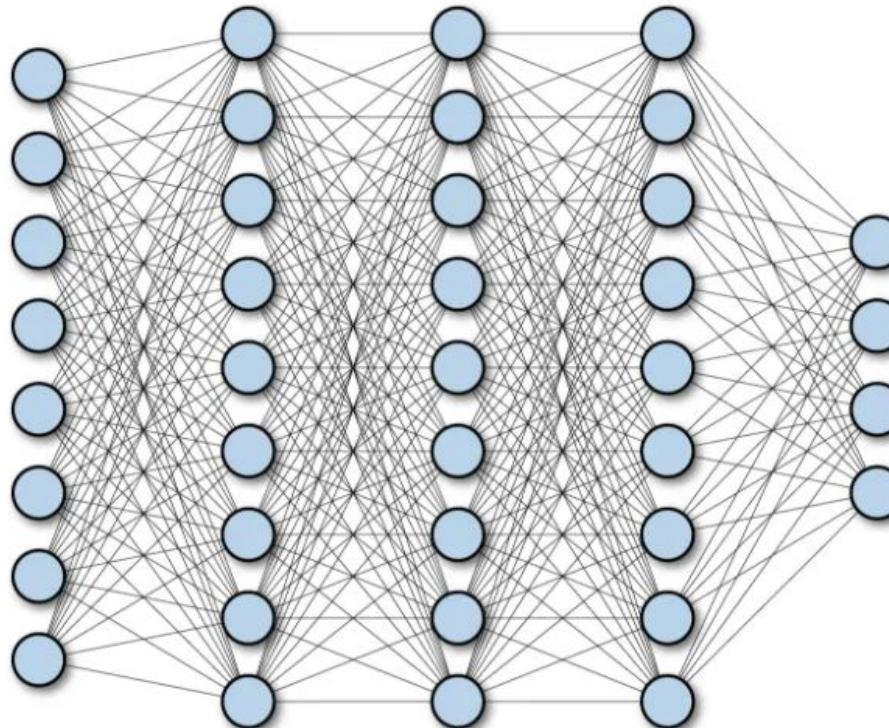
- **Reinforcement Learning**

- no training data; stochastic Markov decision process; robotics and business strategy planning.

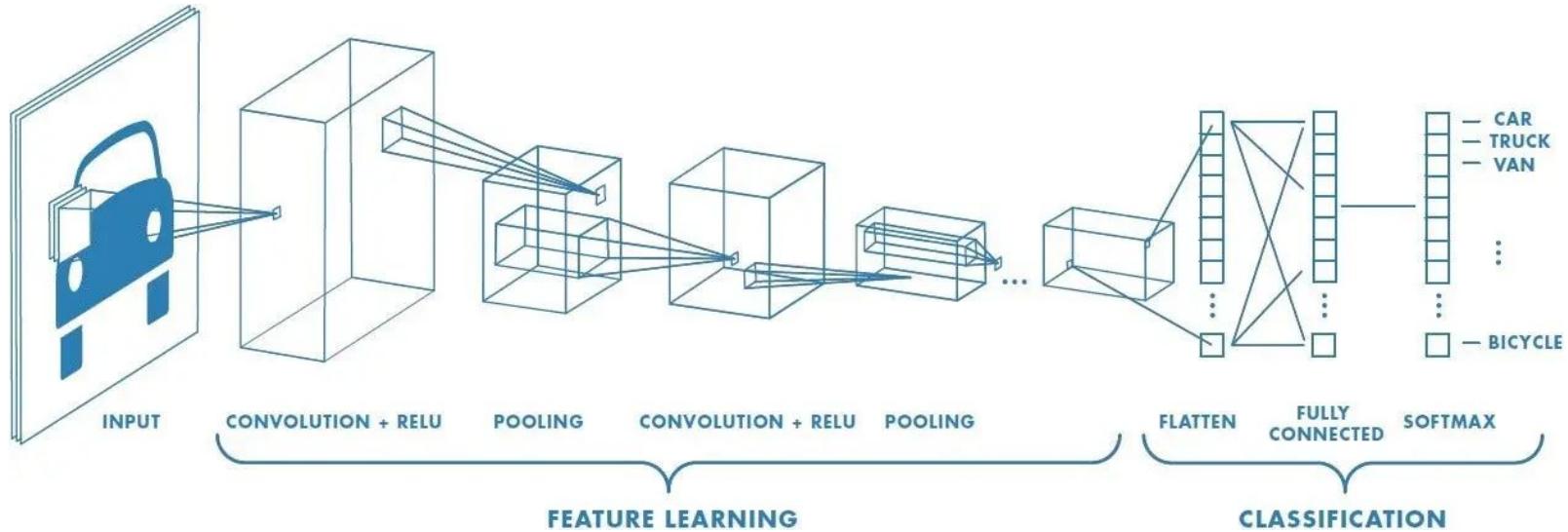
Unsupervised Learning

Reinforcement Learning

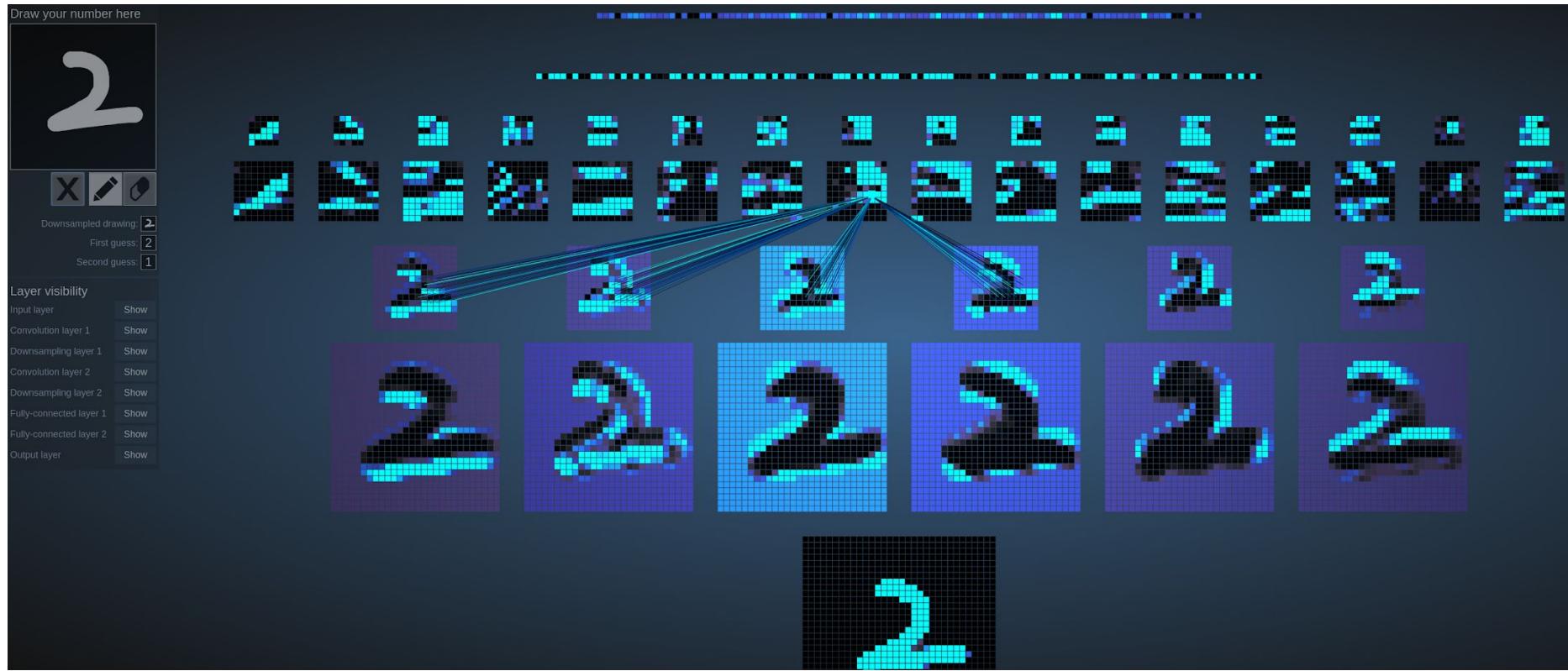
Fully Connected Neural Network



Convolutional Neural Network (CNN)



MNIST - Convolutional Neural Network Visualization

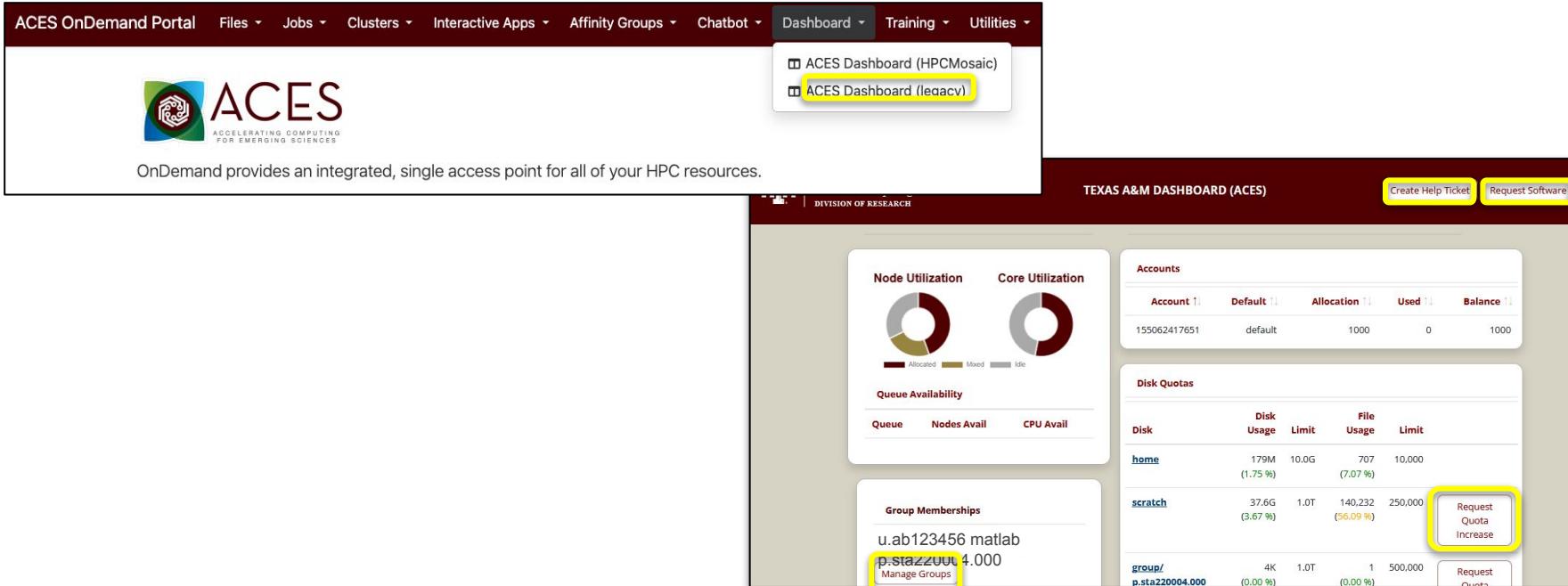


(Image Credit: https://adamharley.com/nn_vis/cnn/3d.html)

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



ACES OnDemand Portal

Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Affinity Groups ▾ Chatbot ▾

Dashboard ▾ Training ▾ Utilities ▾

ACES Dashboard (HPCMosaic)

ACES Dashboard (legacy)

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

TEXAS A&M DASHBOARD (ACES)

Create Help Ticket Request Software

Node Utilization

Core Utilization

Queue Availability

Accounts

Account	Default	Allocation	Used	Balance
155062417651	default	1000	0	1000

Disk Quotas

Disk	Disk Usage	File Limit	File Usage	Limit
home	179M (1.75 %)	10.0G	707 (7.07 %)	10,000
scratch	37.6G (3.67 %)	1.0T	140,232 (56.09 %)	250,000
group/p.stazzu04.000	4K (0.00 %)	1.0T	1 (0.00 %)	500,000

Request Quota Increase

Group Memberships

u.ab123456 matlab
p.stazzu04.000
Manage Groups

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



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Help us help you. Please include details in your request for support, such as, Cluster (ACES, FASTER, Grace, Launch), NetID (UserID), Job information (JobID(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.



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