

ACES: AI TechLab in Jupyter Notebooks

Accelerating AI/ML Workflows on a Composable Cyberinfrastructure

Zhenhua He

02/10/2026



High Performance
Research Computing
DIVISION OF RESEARCH



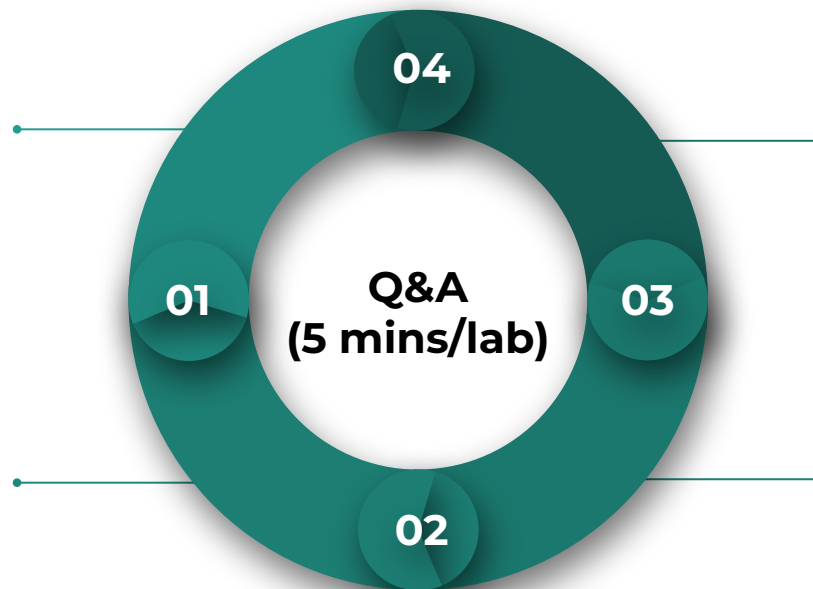
Outline

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.



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



File Edit View Run Kernel Tabs Settings Help

Files

- + notebooks
- notebooks
 - 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

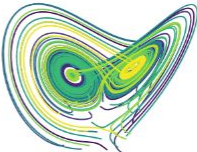
In this Notebook we explore the Lorenz system of differential equations:

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

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



```
9 def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8./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.random((N, 3))
28
```

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

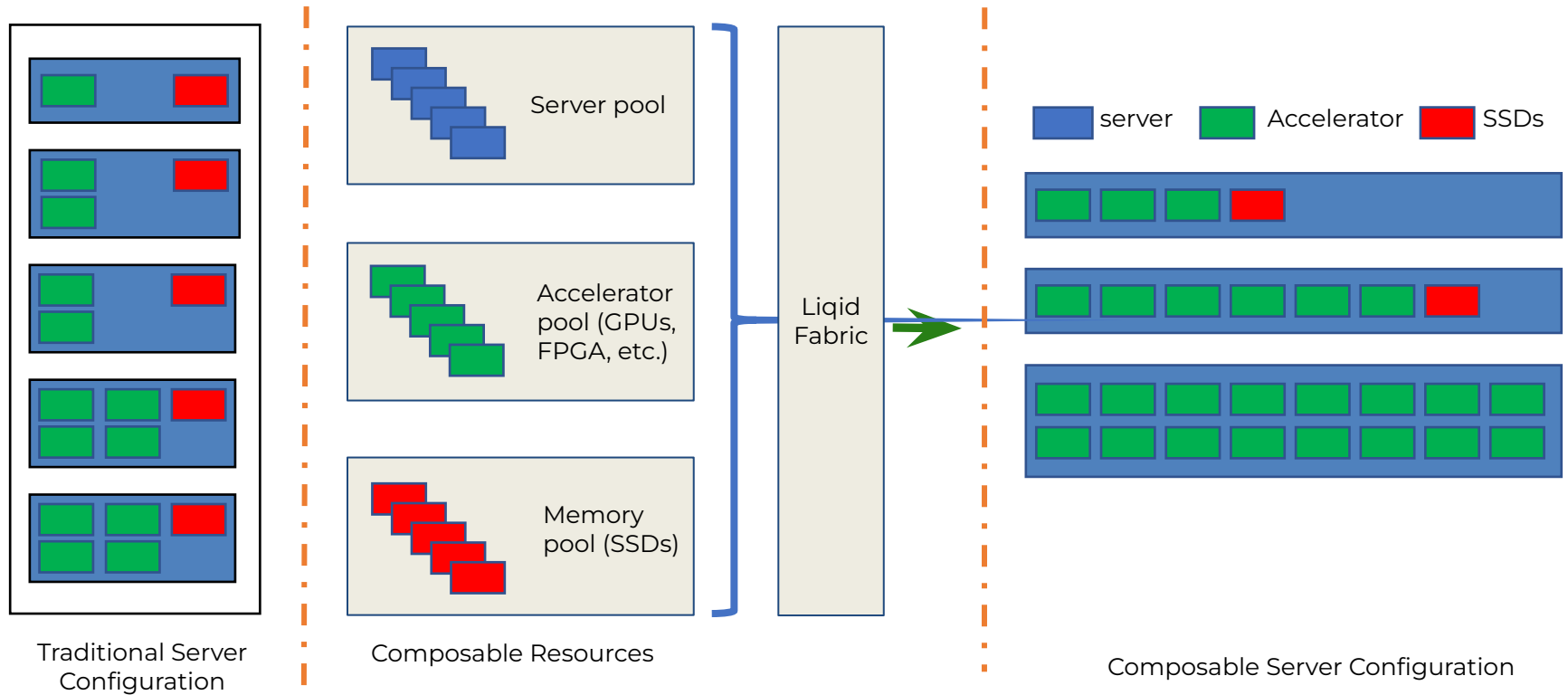
Accelerating Computing for Emerging Sciences

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.



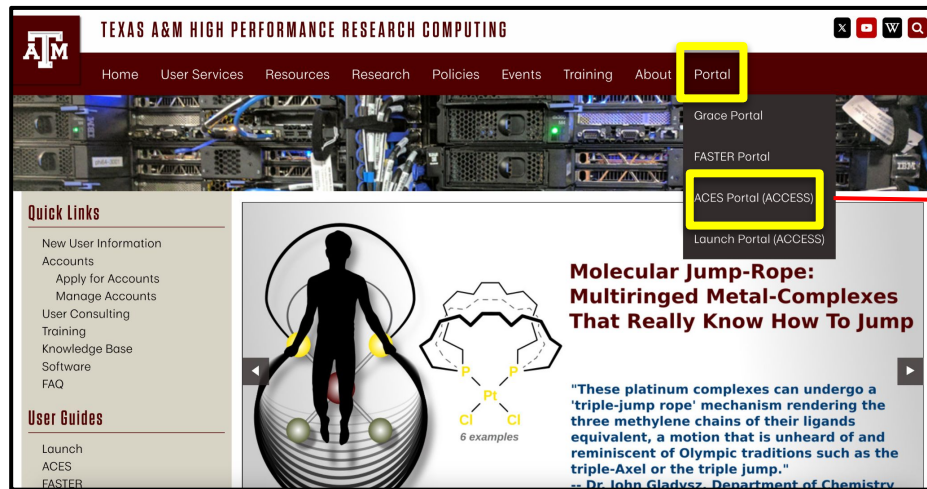
Design: Composability at the Hardware Level



ACES Accelerators

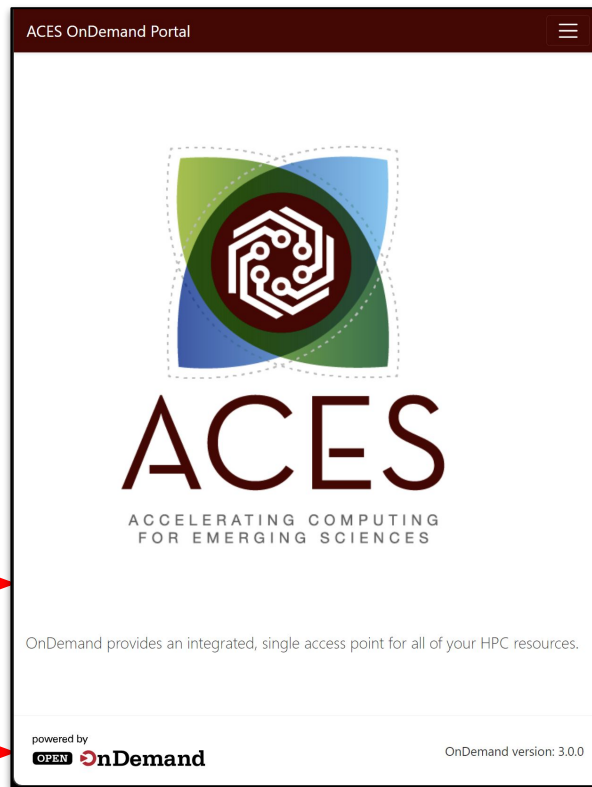
Component	Quantity	Description
Graphcore IPU: Colossus GC200 Bow	16 16	Each IPU group hosted with a CPU server as a POD16 on a 100 GbE RoCE fabric
NVIDIA GPUs: H100 A30	30 4	For HPC, DL Training, AI Inference For AI Inference and Mainstream Compute
BittWare IA-840F FPGA	3	Accelerator with Agilex AGF027 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

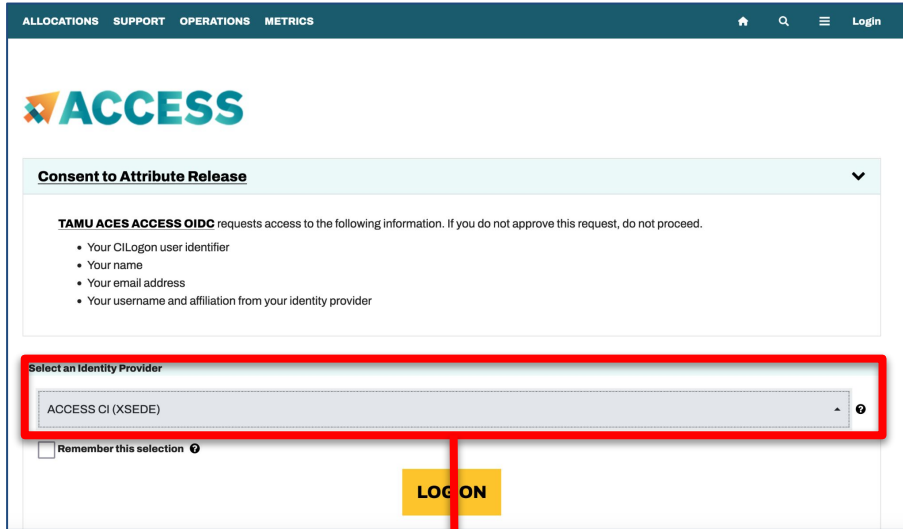


ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster.

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

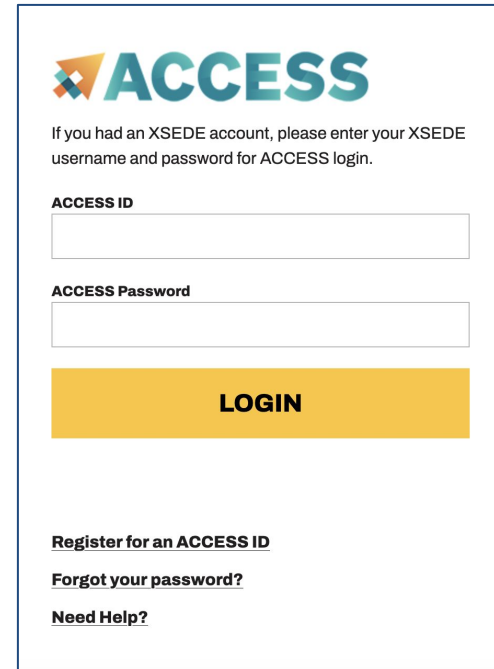


Accessing ACES via the Portal (ACCESS)



The screenshot shows the ACCESS portal interface. At the top is a navigation bar with links: ALLOCATIONS, SUPPORT, OPERATIONS, METRICS, and a Login link. Below the navigation bar is the ACCESS logo. A section titled "Consent to Attribute Release" contains a message from TAMU ACES ACCESS OIDC and a list of requested information: CI/Logon user identifier, name, email address, and username/affiliation. Below this is a "Select an Identity Provider" dropdown menu with "ACCESS CI (XSEDE)" selected. A red box highlights this dropdown. Below the dropdown is a "Remember this selection" checkbox and a yellow "LOG ON" button. A red line points from the "LOG ON" button to the text below.

Select the Identity Provider appropriate for your account.

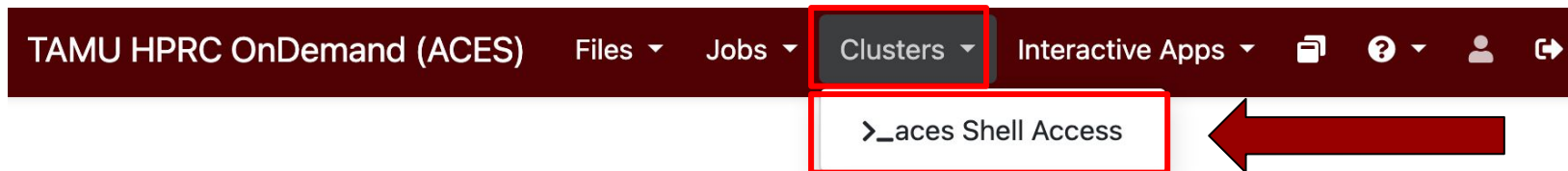


The screenshot shows the ACCESS portal login page. At the top is the ACCESS logo. Below it is a message: "If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login." There are two input fields: "ACCESS ID" and "ACCESS Password". Below these fields is a yellow "LOGIN" button. At the bottom, there are links: "Register for an ACCESS ID", "Forgot your password?", and "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:

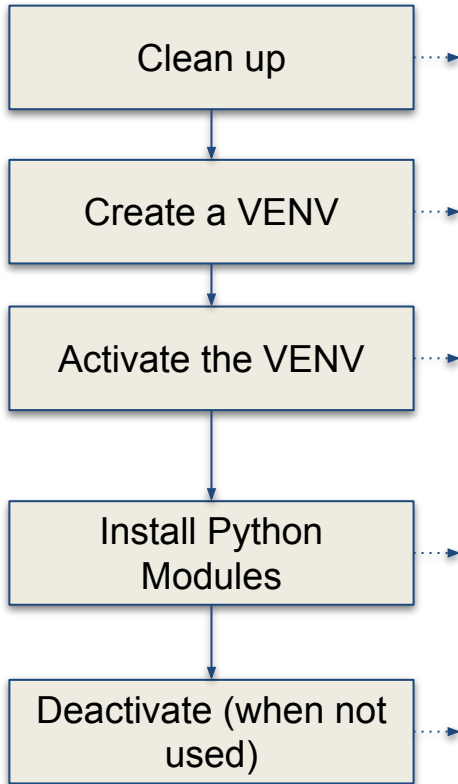
- Creating Environments (`create_venv`)
- Activating Environments (`activate_venv`)
- Listing Environments (`list_envs`)
- Deleting Environments (`delete_venv`)

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 mainter 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


 cisTEM


Servers


 Jupyter AI Assistant

 Jupyter Notebook

 Jupyter Notebook for Python Training

 JupyterLab

 RStudio

 TensorBoard

sources.

ta Center (WCDC) during 6a-8p
powered down for the electrical

number 28. HPRC will also power

ince windows.

JupyterLab Page

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)

Other fields:

- Node Type: CPU
- Number of hours: 3
- Number of cores: 4
- Total memory (GB): 20
- Advanced Params:
Reservation Name: **training**

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.

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: ac005Delete

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

Time Remaining: 2 hours and 58 minutes

Session ID: 159fe4ff-1dec-4bd7-8db0-c34ade3964cc

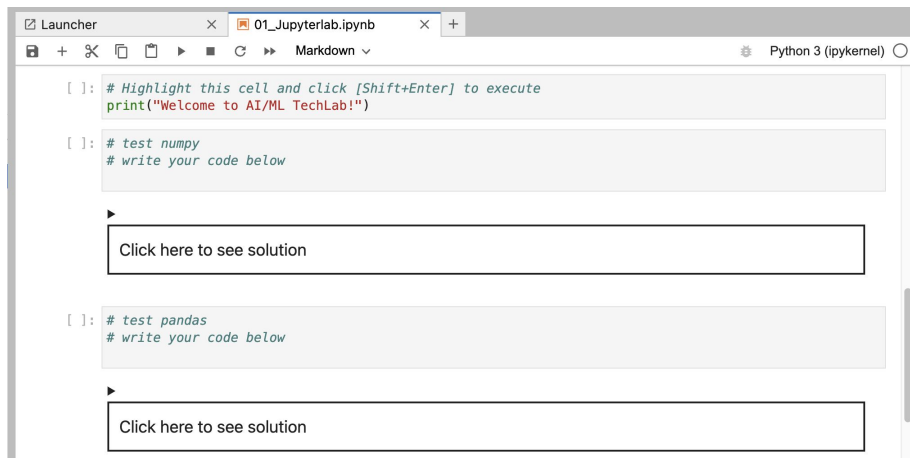
Type of environment: modularir

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.



```
[ ]: # 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) Shared Anaconda Env.

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

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"

Other fields:

- Node Type: CPU
- Number of hours: 3
- Number of cores: 4
- Total memory (GB): 20
- Advanced Params:
Reservation Name: **training**

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

Path to the shared environment:

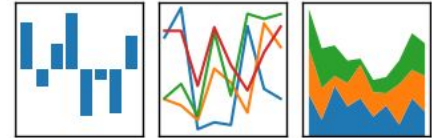
/sw/hprc/sw/Anaconda3/2024.02-1/envs/ai-labs

Lab II. Data Exploration

matplotlib

pandas

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



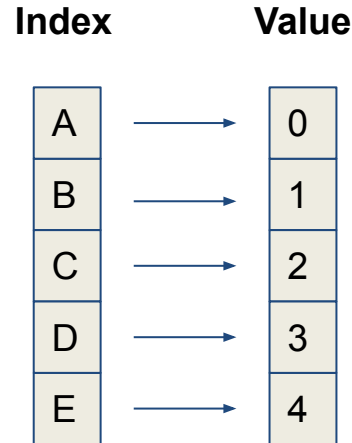
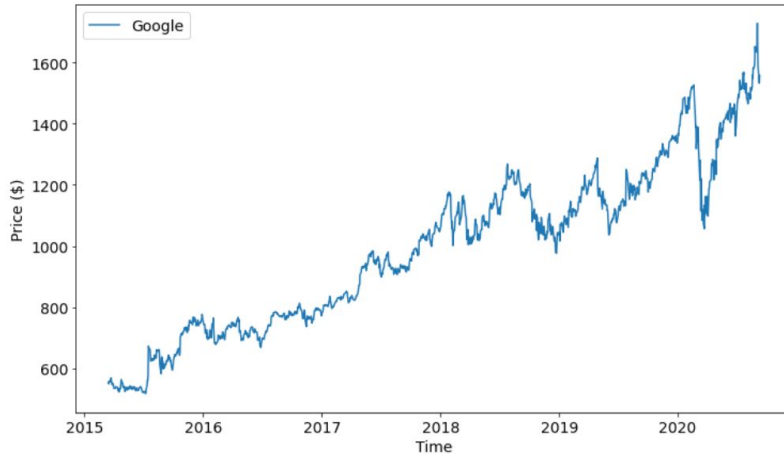
Data Structures

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	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**

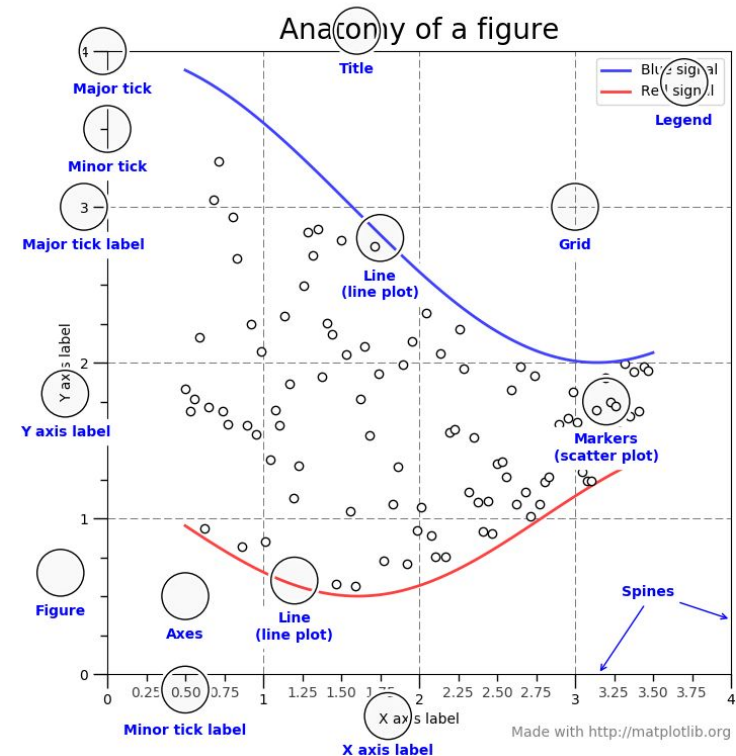
Figure is the object that keeps the whole image output. Adjustable parameters include:

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

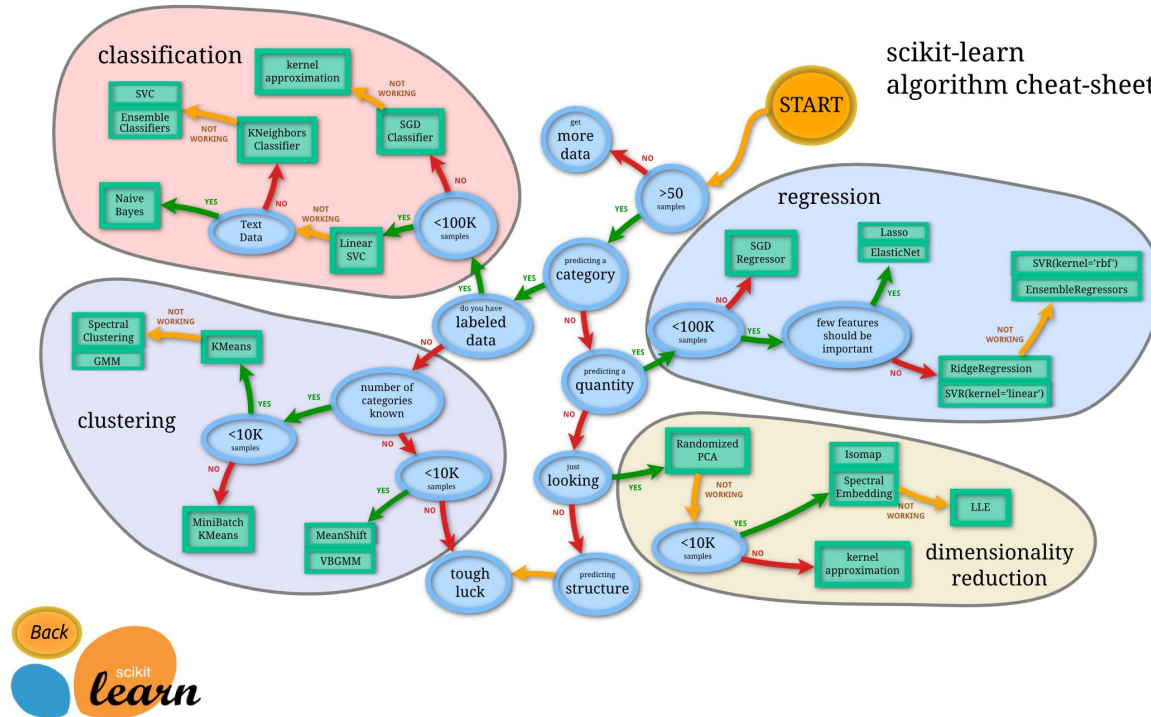
After this lesson, you will know how to create:

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



JupyterLab Exercises

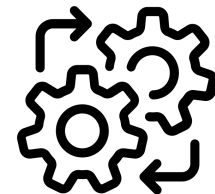
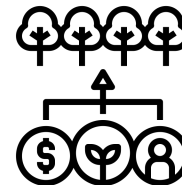
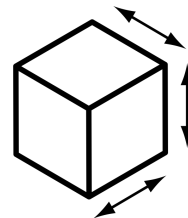
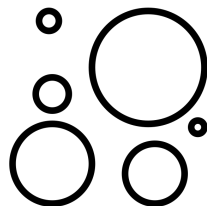
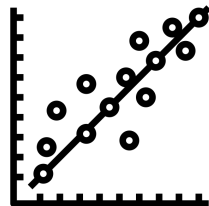
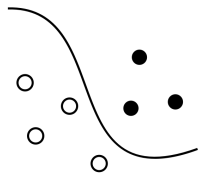
Lab III. Machine Learning



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

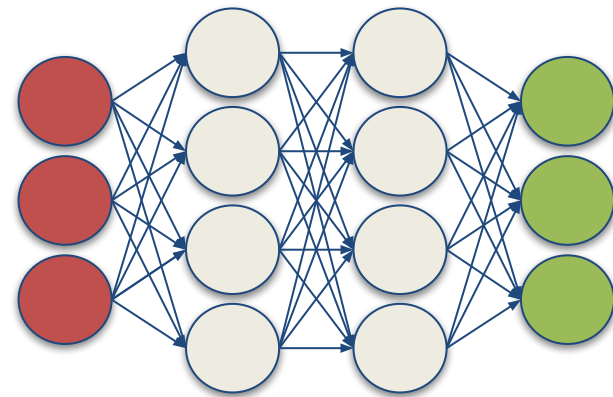
by Grant Sanderson

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

Visualization of CNN

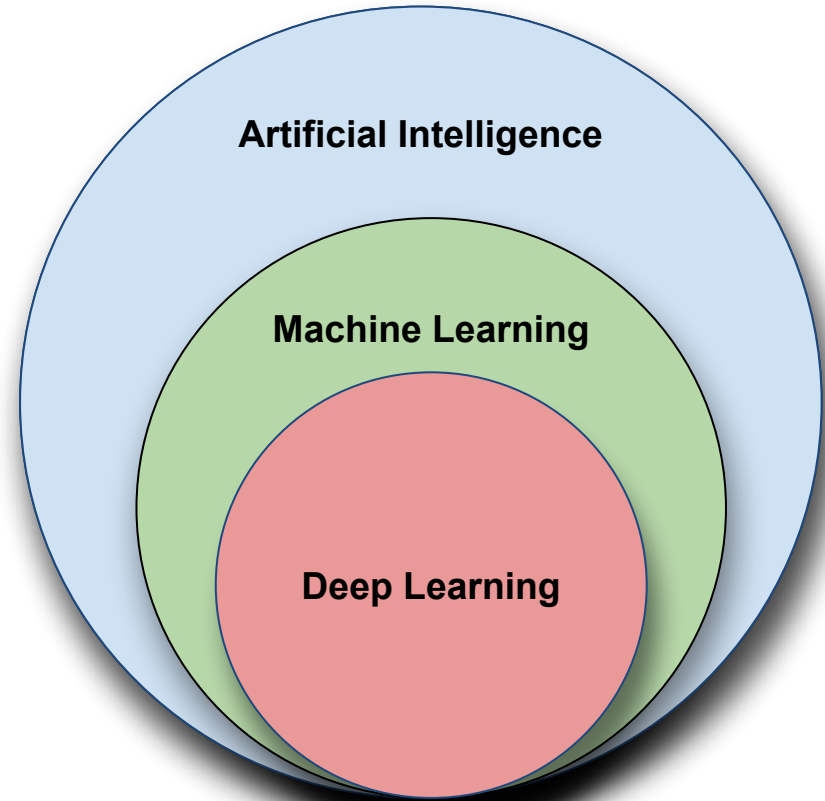
by Adam Harley

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



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**

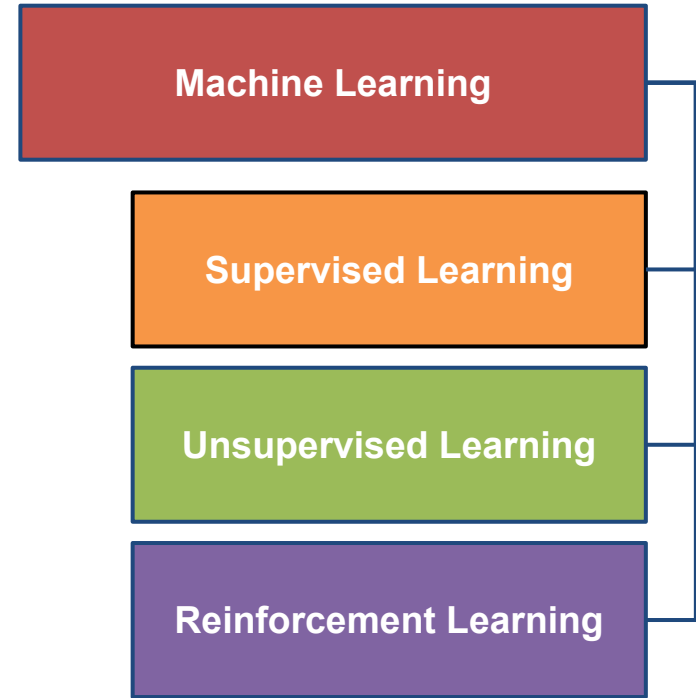
- trained with labeled data; including regression and classification problems

- **Unsupervised Learning**

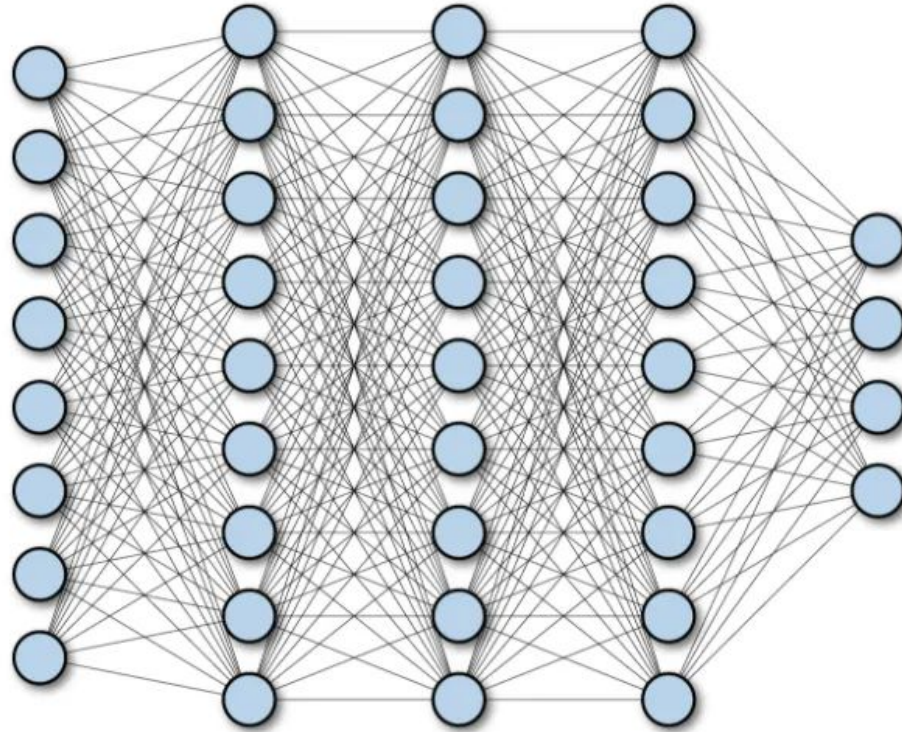
- trained with unlabeled data; clustering and association rule learning problems.

- **Reinforcement Learning**

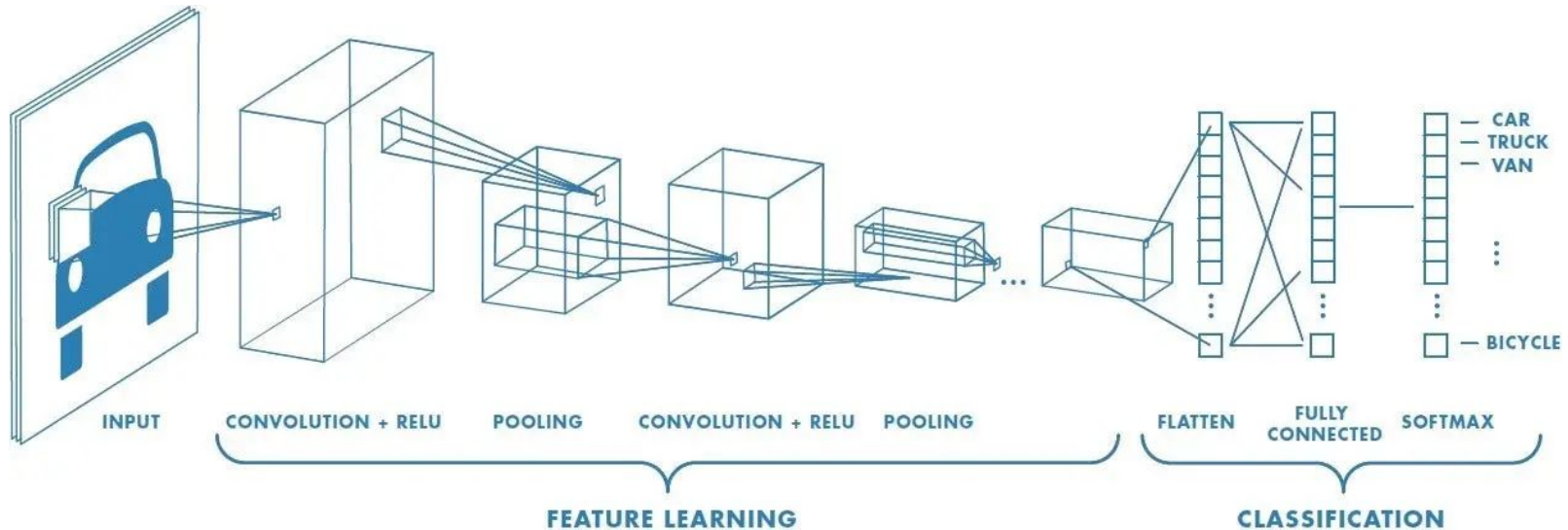
- no training data; stochastic Markov decision process; robotics and business strategy planning.



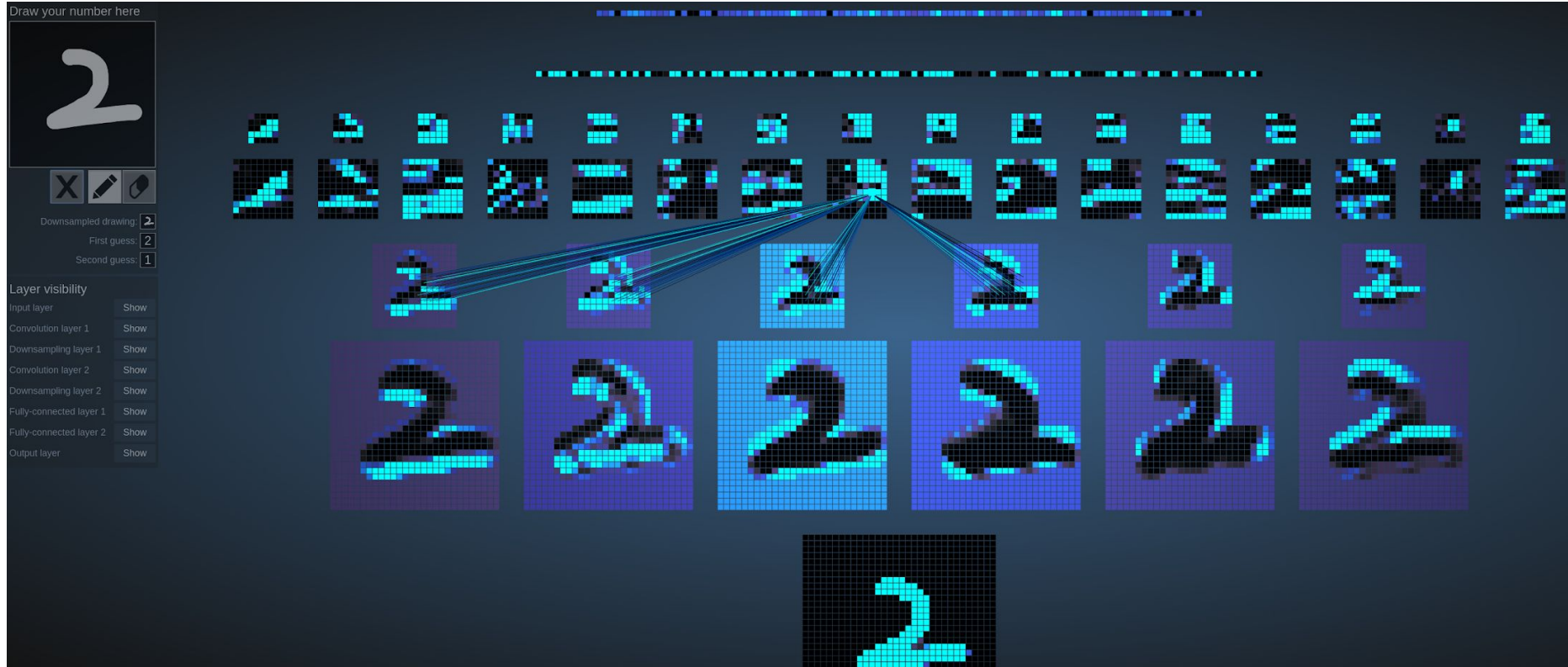
Fully Connected Neural Network



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

The image shows two overlapping screenshots of the ACES OnDemand Portal. The top screenshot displays the portal's header with navigation links (Files, Jobs, Clusters, Interactive Apps, Affinity Groups, Chatbot, Dashboard, Training, Utilities) and the ACES logo with the tagline 'ACCELERATING COMPUTING FOR EMERGING SCIENCES'. Below the logo, it states 'OnDemand provides an integrated, single access point for all of your HPC resources.' A dropdown menu for 'Dashboard' shows two options: 'ACES Dashboard (HPCMosaic)' and 'ACES Dashboard (legacy)', with the latter highlighted. The bottom screenshot shows the 'TEXAS A&M DASHBOARD (ACES)' with a 'Create Help Ticket' and 'Request Software' button. It features several widgets: 'Node Utilization' and 'Core Utilization' donut charts, 'Queue Availability' table, 'Group Memberships' table, 'Accounts' table, and 'Disk Quotas' table. The 'Disk Quotas' table has a 'Request Quota Increase' button highlighted for the 'scratch' account.

ACES OnDemand Portal

ACES Dashboard (HPCMosaic)
ACES Dashboard (legacy)

TEXAS A&M DASHBOARD (ACES)

Create Help Ticket Request Software

Node Utilization

Core Utilization

Queue Availability

Queue	Nodes Avail	CPU Avail
u.ab123456	matlab	
p.staz2004	4.000	

Group Memberships

Group	Members
u.ab123456	matlab
p.staz2004	4.000

Accounts

Account	Default	Allocation	Used	Balance
155062417651	default	1000	0	1000

Disk Quotas

Disk	Disk Usage	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.staz20004.000	4K (0.00 %)	1.0T	1 (0.00 %)	500,000

Request Quota Increase

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@hprc.tamu.edu

Phone: 979-845-0219

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https://u.tamu.edu/hprc_shortcourse_survey

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.

