# Technology Lab: Using Al Frameworks in Jupyter Notebook

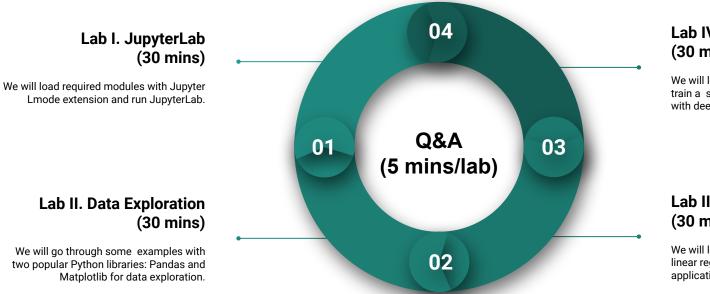
#### Zhenhua He 11/29/2022





High Performance Research Computing DIVISION OF RESEARCH

# **AI Tech Labs**



#### Lab IV. Deep Learning (30 minutes)

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

#### Lab III Machine Learning (30 minutes)

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

Figure 1. Structure of the Technology Lab.

We will go through some examples with two popular Python libraries: Pandas and

Matplotlib for data exploration.

# Lab I. JupyterLab



ß	+ 🗈	± C	Lorenz.ipynb		× Console	1 × 🗷 Data	a.ipynb × ♥ README.md ×		
2	♠ > notebooks				Code ~			Python 3	
	Name 🔺	Last Modified		In this Notebook we ex	xplore the Loren	z system of differe	ential equations:		
	📃 Data.ipynb	an hour ago				i	$\dot{x} = \sigma(y - x)$		
	📃 Fasta.ipynb	a day ago					$\dot{y} = \rho x - y - xz$		
_	📃 Julia.ipynb	a day ago					$\dot{z} = -\beta z + xy$		
	Lorenz.ipynb	seconds ago							
1	🖪 R.ipynb	a day ago		Let's call the function	once to view the	e solutions. For this	s set of parameters, we see the trajectories	swirling around two points,	
	🖽 iris.csv	a day ago		called attractors.					
	(:) lightning.json	9 days ago							
	🍦 lorenz.py	3 minutes ago	In [4]:	<pre>from lorenz import t, x_t = solve_lore</pre>					
				t, x_t - solve_ton	enz(N-10)				
			Output View	×	Di l	orenz.py ×			
			- output non			oronizipy			
			sigma =		10.00 9		enz(N=10, max_time=4.0, sigma=10.0,		
			Signia		10		<pre>solution to the Lorenz differential figure()</pre>	equations."""	
			beta =		2.67 12		add_axes([0, 0, 1, 1], projection='3	d')	
			rho =	:	28.00 13		off')		
					14		the axes limits		
					16		im((-25, 25))		
			-	_	17		im((-35, 35))		
					18		im((5, 55))		
					19 20		z_deriv(x_y_z, t0, sigma=sigma, beta	=beta, rho=rho):	
					21		mpute the time-derivative of a Loren		
					22		$z = x_y_z$		
					23	return	n [sigma * (y - x), x * (rho - z) -	y, x * y - beta * z]	
					24	# Choose i	random starting points, uniformly di	stributed from -15 to 15	5
				- K	26				
					27		+ 30 * np.random.random((N, 3))		

# L1 - Resources

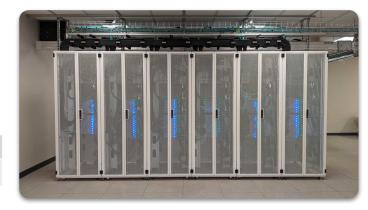
- Texas A&M High Performance Research Computing (HPRC)
- FASTER Quick Start Guide
- ACES Phase I Guide
- ACCESS Documentation
- FASTER Portal
- HPRC YouTube Channel
- help@hprc.tamu.edu

# Getting Started with FASTER and ACES

# **FASTER Cluster**

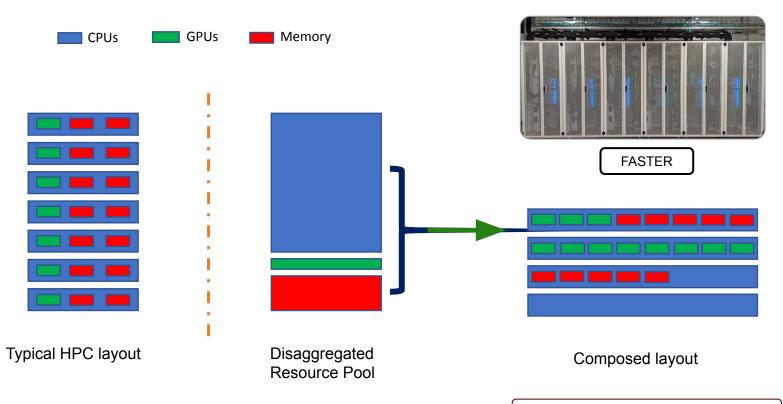
hprc.tamu.edu/wiki/FASTER:Intro

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



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

# Composability at the Hardware Level



hprc.tamu.edu/resources

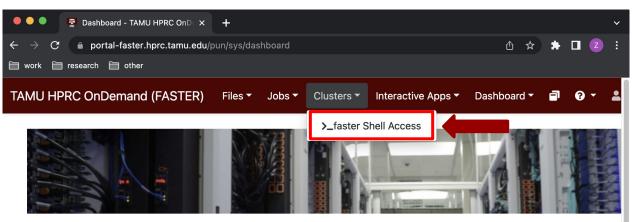
# ACES - Accelerating Computing for Emerging Sciences (Phase I)



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

ACES Phase I components are available through <u>FASTER</u>

# Shell Access - I



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

#### Message of the Day

#### **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 State Law. Any shared accounts will be DISABLED.
- · Authorized users must also adhere to ALL policies at: https://hprc.tamu.edu/policies

# Shell Access - II

● ● ● 📱 Dashboard - TAMU HPRC OnD × 🚱 happidence1@login2:~ × +					~
← → C 🌢 portal-faster.hprc.tamu.edu/pun/sys/shell/ssh/faster.hprc.tamu.edu	Û	☆	* 🗆		
🗎 work 🗎 research 🗎 other					
Host: faster.hprc.tamu.edu	Themes:	Default		```	2
Website:       https://hprc.tamu.edu                 Consulting:       help@hprc.tamu.edu (preferred) or (979) 845-0219         FASTER Documentation:https://hprc.tamu.edu/wiki/FASTER         Grace Documentation: https://hprc.tamu.edu/wiki/Grace         YouTube Channel:       https://www.youtube.com/texsamhprc					
*******					
* === IMPORTANT POLICY INFORMATION === *					
<ul> <li>* - Unauthorized use of HPRC resources is prohibited and subject to</li> <li>* criminal prosecution.</li> </ul>					
st – Use of HPRC resources in violation of United States export control $st$					
* laws and regulations is prohibited. Current HPRC staff members are *					
<ul> <li>* US citizens and legal residents.</li> <li>* - Sharing HPRC account and password information is in violation of</li> </ul>					
* Texas State Law. Any shared accounts will be DISABLED. *					
* - Authorized users must also adhere to ALL policies at:					
<pre>* https://hprc.tamu.edu/policies/ * ***********************************</pre>					
<pre>!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES, !!</pre>					
Please restrict usage to <u>8 CORES</u> across ALL login nodes. Users found in violation of this policy will be <u>SUSPENDED</u> .					
To see these messages again, run the <u>motd</u> command. Your current disk quotas are: Disk Disk Usage Limit File Usage Limit /home/happidence1 56K 10.0G 26 10000 /scratch/user/happidence1 631.0G 2.0T 450644 1000000					
<pre>* Quota increase for /scratch/user/happidence1 will expire on May 21, 2023 /scratch/group/benchmark_prj 325.1G 5.0T 1333878 500000 /scratch/group/hprc 3.9T 10.0T 615489 1000000 * Quota increase for /scratch/group/hprc will expire on Dec 31, 2026 Type 'showquota' to view these quotas again. (base) [happidence1@faster2 ~]\$</pre>					

# Commands to copy the materials

• Navigate to your personal scratch directory

\$cd \$SCRATCH

• Files for this course are located at

/scratch/training/ai\_tech\_labs

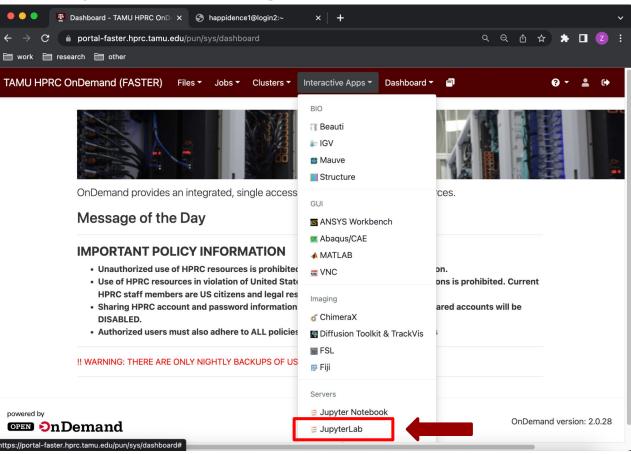
Make a copy in your personal scratch directory

\$ cp -r /scratch/training/ai\_tech\_labs \$SCRATCH

• Enter this directory (your local copy)

\$cd ai\_tech\_labs

# Go to JupyterLab Page

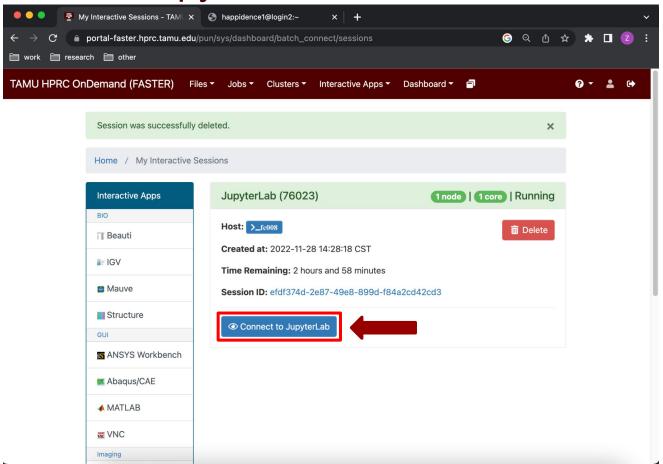


# JupyterLab Page

work 🗎 research 🗎	] other				
MU HPRC OnDema	and (FASTER) Fil	es 👻 Jobs 👻 Clusters 👻 Interactive Apps 👻 Dashboard 👻 🗐	<b>?</b> •	<b>≗</b> ເ+	1.
Hon	ne / My Interactive S	essions / JupyterLab			
Inte	eractive Apps	JupyterLab			
BIO		This app will launch a JupyterLab server on the FASTER			
TE E	Beauti	cluster. Module			
i i	GV	Python/3.8.2			
😂 N	Mauve	Anaconda3 uses Python3			
<b>I</b> S	Structure	Optional Environment to be activated			
GUI			Numb	er of h	ours
A 20	ANSYS Workbench	Enter the name of the environment to be activated. (Optional)	i turrio		ouro.
_	1015	The default virtualenvs for Anaconda3/2021.11 and	Numb	er of co	ores:
<b>E</b> <i>F</i>	Abaqus/CAE	Python/3.8.2 have jupyterImod which enables loading Imod modules.	Total	nemor	v (CF
📣 N	MATLAB		Total I	nemor	y (01
1000 \ 1000	/NC	Leave blank to use the default environment for the selected Module.	Node	type: A	NY
Imag	ging	Your optional conda environment must have been previously			
\$ C	ChimeraX	built with one of the Anaconda or Python modules listed in the Module option above. See instructions.			

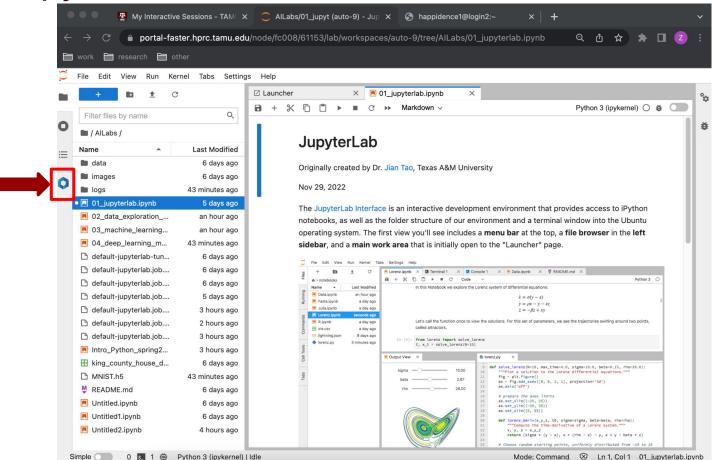
13

### Connect to JupyterLab

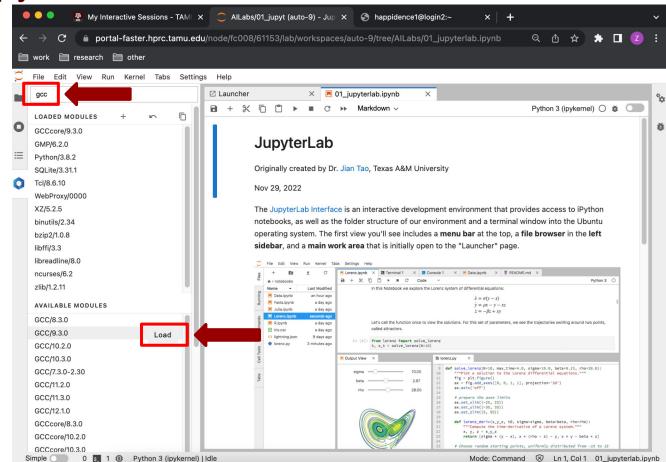


14

### JupyterLab Lmod Extension



### JupyterLab Lmod Extension



16

# **Exercise: Load Required Modules**

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

Note: numpy and matplotlib have already been in the

Scipy-bundle/2020.03-Python-3.8.2 module.

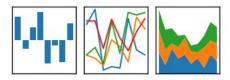
### **Test loaded modules**

•		<b>₽</b> №	ly Intera	active Se	essions - <sup>-</sup>	TAMU >	< C	AIL	abs/	01_ju	pyt (au	to-9) -	Jup X	ę	🗿 happi	dence1	l@logi	n2:~		×	+						`	-
÷		C 🔒	porta	l-faster	.hprc.ta	mu.ed	<b>u</b> /nod	e/fc0	08/	6115	3/lab/\	vorks	paces/	auto	-9/tree/	AlLab	s/01_	jupyte	erlab.i	pynb		Q	ᠿ	☆	<b>*</b> [	Z		
<b>E</b>	work	🗎 resea	rch 🖻	ather																								
	WORK																											
$\bigcirc$	File	Edit View	Run	Kernel	Tabs	Setting	gs He	elp					_															
	) H	- 10	<u>*</u>	C			⊠L	aunch	er			×	<b>0</b> 1_	jupyte	erlab.ipyr	nb	٠										1	å
	Filto	r files by na	mo			Q	8	+	Ж	Ū	۵ ۲		C 🕨		arkdown							-			))) 🖸			
0			me			~									or the '													ĕ
-	<b>I</b> / A	ILabs /						Sometimes, a content cell will get switched to editing mode. Pressing SI to a readable form.									nitt+	Enter	WIII	switch	it back		1					
≣	Name		•		Last Mod	dified			· ·	oare	auabie	ionn.																
	🖿 da				6 day	-			Т	ry ex	ecuting	the s	imple p	int st	tatement	t in the	cell b	elow.										
	in 🖿				6 day			T 1	. #	Hig	hlight	thi	coll	and	click [	Shift.	Ento	r1 to	execu	to								
	lo	•			an hou										Labs!")		FEITLE	1 10	execu	Le								
		l_jupyterlab			2 minute																							
		2_data_expl			an hou			[]			t nump		de belo	W														
		3_machine_l			an hou																							
		4_deep_lear			an hou	-																						
		efault-jupyte			6 day				Ē																	1		
		efault-jupyte			6 day					Clic	k here	to se	ee solu	tion														
		efault-jupyte			6 day	-			L																	1		
		efault-jupyte efault-jupyte			5 day 4 hour																						ч	
		efault-jupyte			2 hour			[]			t pand		de belo	w/														
		efault-jupyte	-		3 hour				"		cc you																	
		tro_Python_			3 hour																							
		ng_county_l			6 day	-			Ē																	1		
		NIST.h5			an hou					Clic	k here	e to se	ee solu	tion														
	_	EADME.md			6 day				L																	1		
		ntitled.ipynb			6 day																							
		ntitled1.ipyn			6 day	-		[ ]			t matp		ib de belo															
	_	ntitled2.ipyn			5 hour				+	WII	ce you		ie belo															
s	imple (	0	s_ 1 =	i⊉ Pytl	hon 3 (ipy	kernel)	Idle												Mod	de: Com	nmand	$\otimes$	Ln 1,	Col 1	01_jup	yterlab.	ipynl	b

# Lab II. Data Exploration



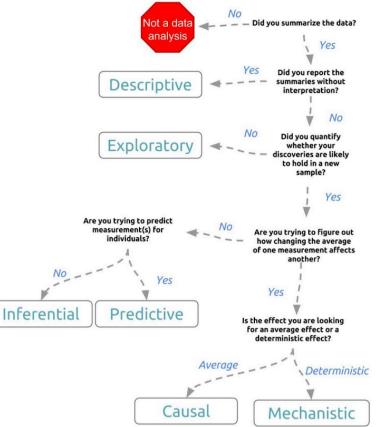




# **Types of Data Science Problems**

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

e.g., experimental science)



Credit: Jeff Leek - The Elements of Data Analytic Style

# **Data Structures**

Pandas has two data structures that are descriptive and

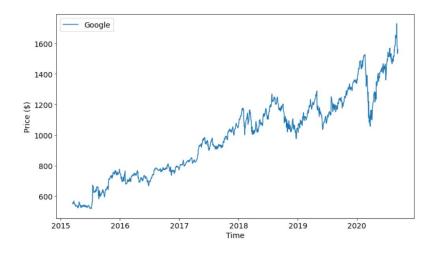
optimized for data with different dimensions.

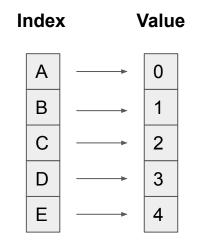
- Series: 1D labeled array
- **DataFrame:** General 2D labeled, size-mutable tabular

structure with potentially heterogeneously-typed columns

# **Series in pandas**

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

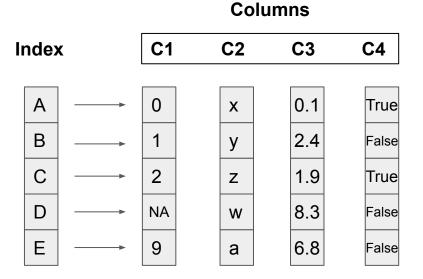




# **DataFrame in pandas**

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

A	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	20150225T0	180000	2	1	770	10000	1
2487200875	20141209T0	604000	4	3	1960	5000	1
1954400510	20150218T0	510000	3	2	1680	8080	1
7237550310	20140512T0	1.23E+06	4	4.5	5420	101930	1
1321400060	20140627T0	257500	3	2.25	1715	6819	2
2008000270	20150115T0	291850	3	1.5	1060	9711	1
2414600126	20150415T0	229500	3	1	1780	7470	1



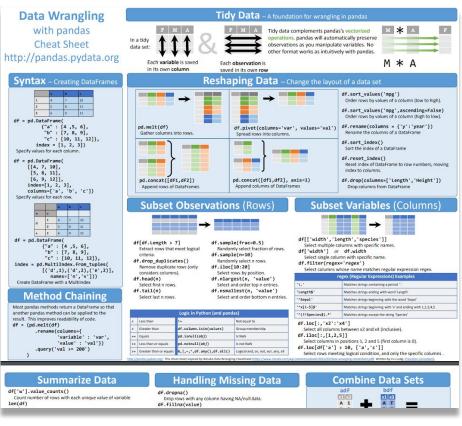
# **Pandas Learning Objectives**

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

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



# **Pandas Cheat Sheet**



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

# **Key Plotting Concepts in Matplotlib**

#### Matplotlib: Figure

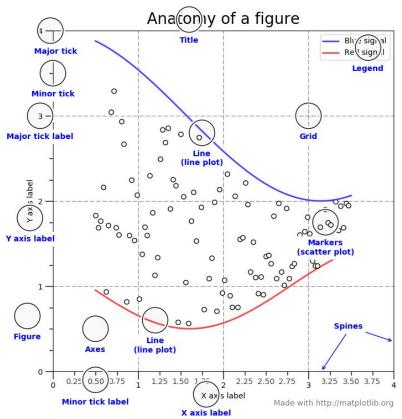
Figure is the object that keeps the whole image output. Adjustable parameters include:

- 1. Image size (set\_size\_inches())
- 2. Whether to use tight\_layout (set\_tight\_layout())

#### Matplotlib: Axes

Axes object represents the pair of axis that contain a single plot (x-axis and y-axis). The Axes object also has more adjustable parameters:

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



(Credit: matplotlib.org)

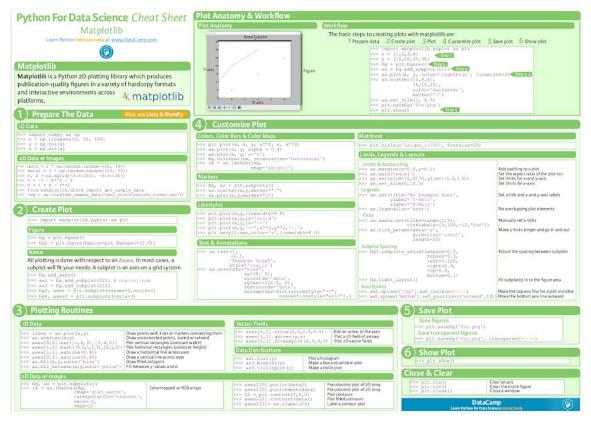
# **Matplotlib Learning Objectives**

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

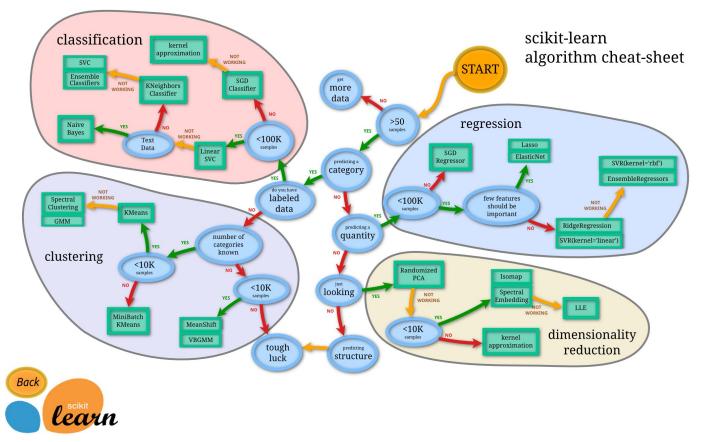


# **Matplotlib Cheat Sheet**



https://s3.amazonaws.com/assets.datacamp.com/blog\_assets/Python\_Matplotlib\_Cheat\_Sheet.pdf

# Lab III. Machine Learning



# **Main Features of scikit-learn**



Classification Regression		Clustering	Dimension Reduction	Model Selection	Preprocessing
Identifying category of an object	Predicting a attribute for an object	Grouping similar objects into sets	Reducing the number of dimensions	Selecting models with parameter search	Preprocessing data to prepare for modeling
Applications: Spam detection, image recognition. Algorithms: SVM, nearest neighbors, random forest, and more	<b>Applications</b> : Drug response, Stock prices. <b>Algorithms</b> : SVR, nearest neighbors, random forest, and more	<b>Applications:</b> Customer segmentation, Grouping experiment outcomes <b>Algorithms:</b> k-Means, spectral clustering, mean-shift, and more	<b>Applications:</b> Visualization, Increased efficiency <b>Algorithms:</b> k-Means, feature selection, non-negative matrix factorization, and more	<b>Applications:</b> Improved accuracy via parameter tuning <b>Algorithms:</b> grid search, cross validation, metrics, and more	<b>Applications:</b> Transforming input data such as text for use with machine learning algorithms. <b>Algorithms:</b> preprocessing, feature extraction, and more
		$\hat{O}$		69999 5 5 8 9 8	

Credit: icons are from The Noun Project under Creative Commons Licenses

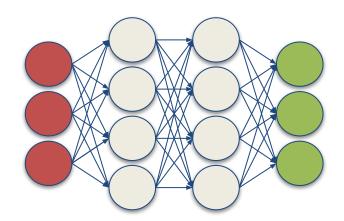
# Lab IV. Deep Learning

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

#### Animation of Neutron Networks

by Grant Sanderson https://www.3blue1brown.com/

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

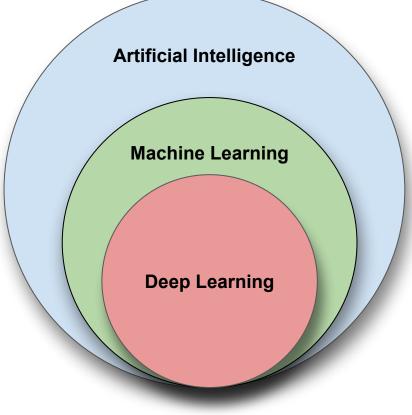






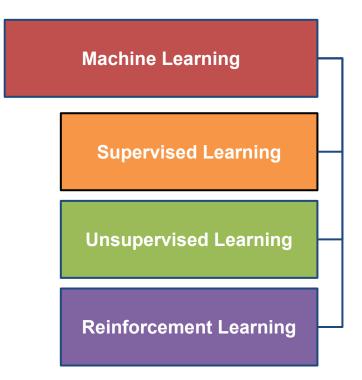
# Relationship of AI, ML, and DL

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

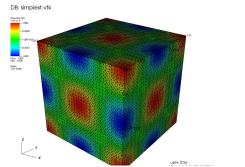


# **Types of ML Algorithms**

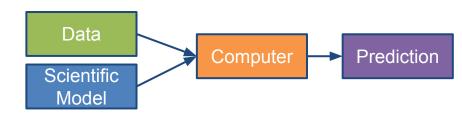
- Supervised Learning
  - trained with labeled data; including regression and classification problems
- Unsupervised Learning
  - trained with unlabeled data; clustering and association rule learning problems.
- Reinforcement Learning
  - no training data; stochastic
     Markov decision process; robotics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



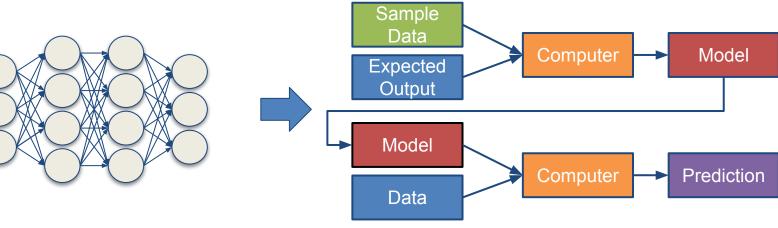
# **Machine Learning**



#### **Traditional Modeling**



#### Machine Learning (Supervised Learning)



# **Inputs and Outputs**

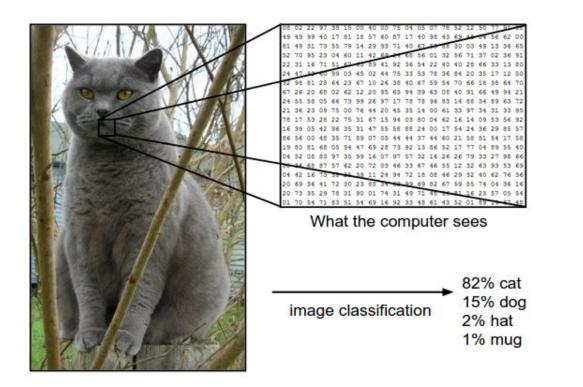
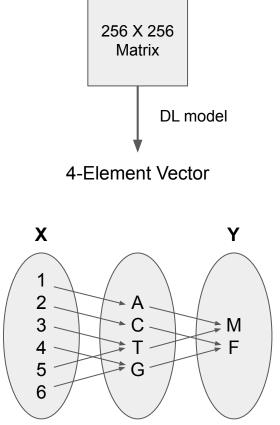
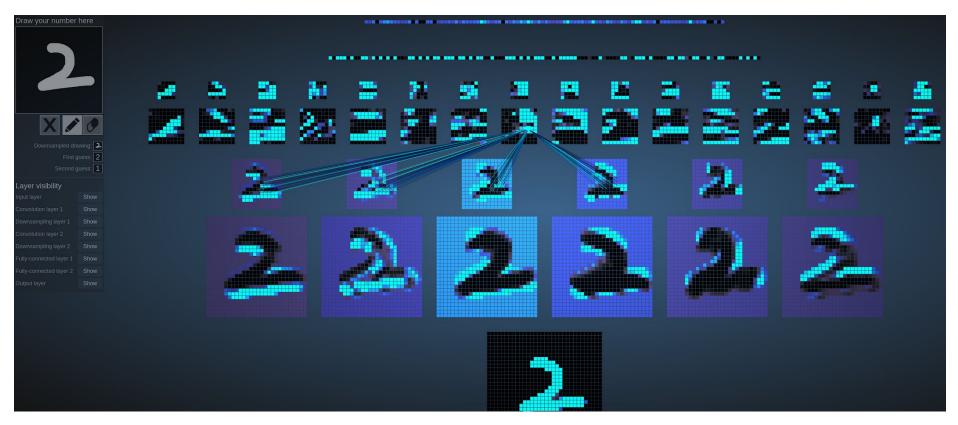


Image from the Stanford CS231 Course



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

### **MNIST - CNN Visualization**



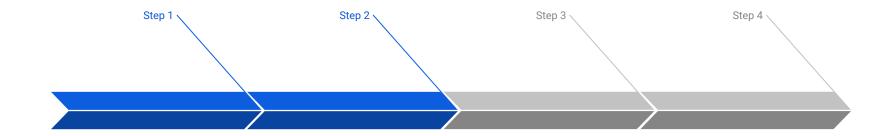
(Image Credit: <u>http://scs.ryerson.ca/~aharley/vis/</u>)

# **CNN Explainer**



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

## **Machine Learning Workflow with Keras**



#### Prepare Train Data

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

#### **Define Model**

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

#### **Training Configuration**

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

#### **Train Model**

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