



ScHARe

Data Management and Analysis in Python

September 18, 2024

Deborah Duran, PhD • NIMHD

Luca Calzoni, MD MS PhD Cand. • NIMHD

Elif Dede Yildirim, PhD • NIMHD



SCHARe

Workshop
setup



BE A PART OF THE FUTURE
OF KNOWLEDGE GENERATION

We have registered you for ScHARe

To opt out,
email us at
schare@mail.nih.gov

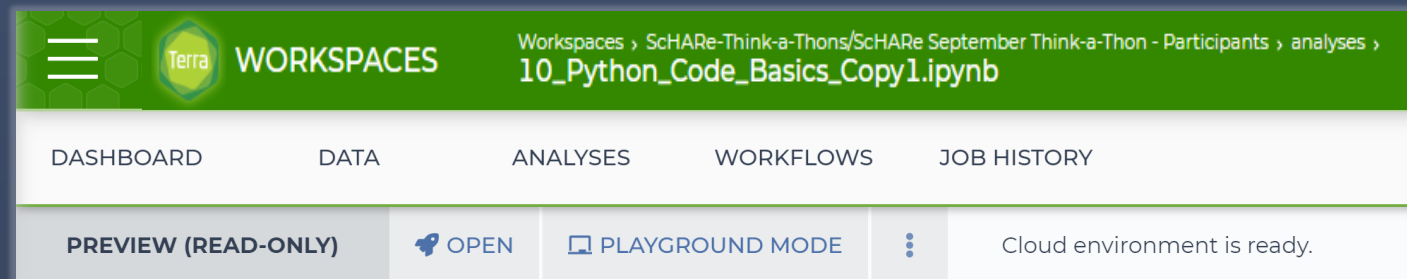
You have been:

- registered for **ScHARe**
- added to a **free temporary billing project** that will allow you to run the event materials with your instructors
- You will be active on this billing project for the duration of the Think-a-Thon. If you want to access work-in-progress after this time, you will need to set up your own billing and copy your workspaces to it

In preparation for the Think-a-Thon

Let's make sure that everyone:

- ✓ 1. has provided their Gmail address and has been registered for ScHARe
2. has created a Terra account
3. can access the tutorial we will be using today at: bit.ly/schare-python-notebooks
4. has configured their cloud environment
5. can run the tutorial in playground mode:



Please paste the address below in your browser:

bit.ly/schare-python-notebooks-2

If you have already created a Terra account and are logged in, you will see this:

bit.ly/schare-python-notebooks-2

The screenshot shows the Terra WORKSPACES interface. The top navigation bar is green and contains the Terra logo, the word 'WORKSPACES', and a breadcrumb trail: 'Workspaces > SchARE-Think-a-Thons/SchARE September Think-a-Thon - Participants > Analyses'. Below the navigation bar is a horizontal menu with tabs for 'DASHBOARD', 'DATA', 'ANALYSES' (which is selected and highlighted in green), 'WORKFLOWS', and 'JOB HISTORY'. The main content area is titled 'Your Analyses' and features a '+ Start' button and a search bar labeled 'Search analyses'. Below this is a table listing four Jupyter notebooks. Each row in the table includes a Jupyter logo, the application name 'Jupyter', the notebook name, and the last modified date 'Sep 18, 2024'. A lock icon and a three-dot menu icon are also present in the last column of each row.

Application	Name	Last Modified
Jupyter	Schare_tat_september_W-Z.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_S-Y.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_M-R.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_I-N.ipynb	Sep 18, 2024

If you have not logged in, or have not yet created a Terra account, you will see this:

bit.ly/schare-python-notebooks-2



The screenshot shows the Terra Community Workbench landing page. At the top, there is a green header with the Terra logo and the word "BETA" on the left, and a notification bell icon with a "1" on the right. The main content area features a large heading "Welcome to Terra Community Workbench" on the left. Below the heading, there is a paragraph of text: "Terra is a cloud-native platform for biomedical researchers to access data, run analysis tools, and collaborate. [Learn more about Terra.](#)" followed by another line: "If you are a new user or returning user, click log in to continue." At the bottom left, there is a blue button labeled "LOG IN". On the right side of the page, there are several hexagonal images: one showing a colorful, glowing molecular structure, and another showing a person in a lab coat and safety glasses holding a test tube.

Terra BETA

1

Welcome to Terra Community Workbench

Terra is a cloud-native platform for biomedical researchers to access data, run analysis tools, and collaborate. [Learn more about Terra.](#)

If you are a new user or returning user, click log in to continue.

LOG IN

Click on the login button:

bit.ly/schare-python-notebooks-2



Terra BETA

Welcome to Terra Community Workbench

Terra is a cloud-native platform for biomedical researchers to access data, run analysis tools, and collaborate. [Learn more about Terra.](#)


If you are a new user or returning user, click log in to continue.

LOG IN

Use the Gmail address you provided us with to log in:


terraprodb2c.b2clogin.com/terraprodb2c.onmicrosoft.com/oauth2/v2.0/authorize?response_mode=query&s...




 Sign in with Google

 Sign in with Microsoft

Use the Gmail address you provided us with to log in:

 Sign in with Google



Sign in
to continue to [Terra](#)


Email or phone


[Forgot email?](#)

To continue, Google will share your name, email address, language preference, and profile picture with Terra. Before using this app, you can review Terra's [privacy policy](#) and terms of service.


[Create account](#) [Next](#)

Input the password associated with your Gmail account:

 Sign in with Google



Hi Luca

 healthcare@|

Enter your password

Show password

To continue, Google will share your name, email address, language preference, and profile picture with Terra. Before using this app, you can review Terra's [privacy policy](#) and terms of service.

[Forgot password?](#)

If you are new to Terra, create an account now:



New User Registration

First Name *

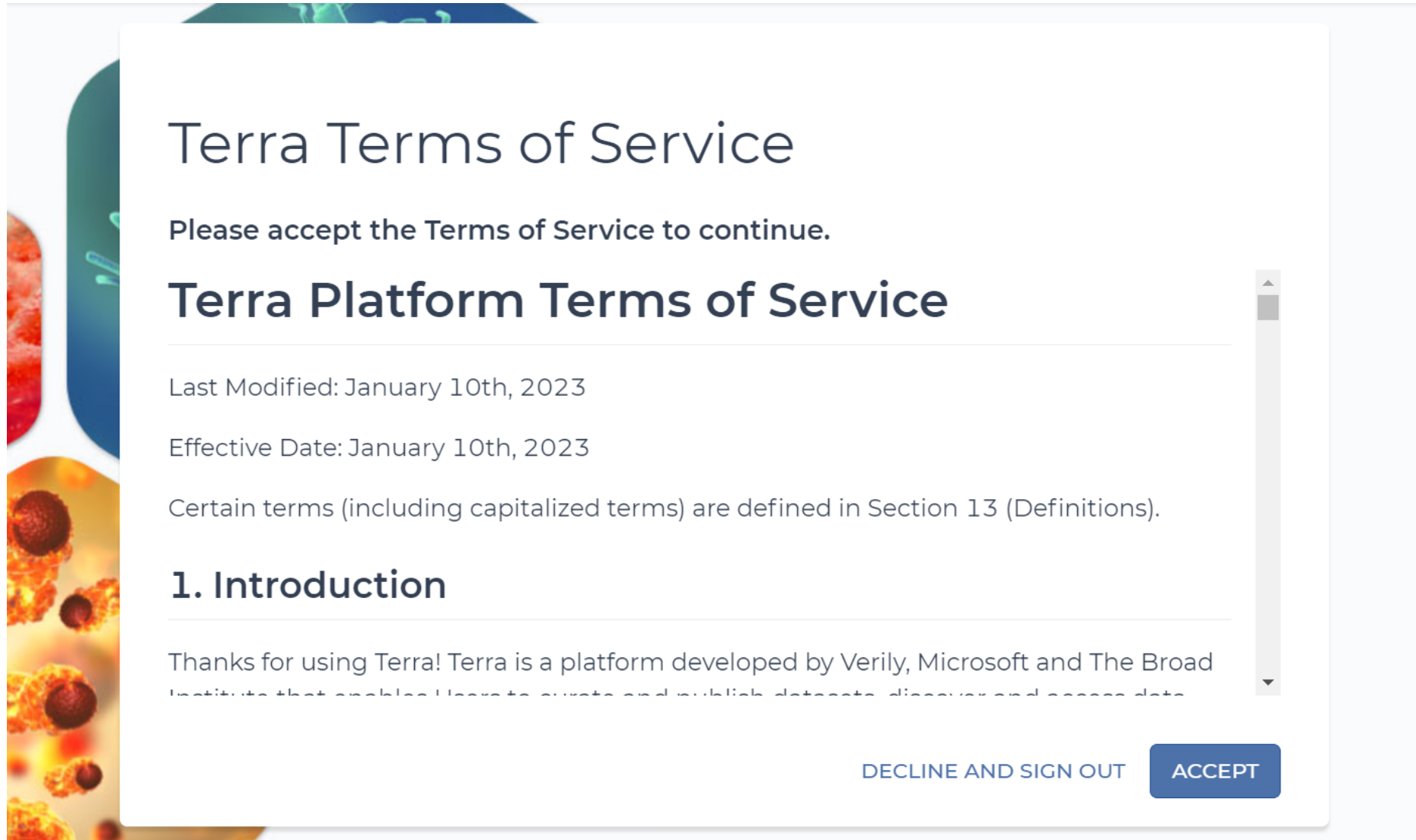
Last Name *

Contact Email for Notifications *

REGISTER

CANCEL

Accept the Terra Terms of Service:



Terra Terms of Service

Please accept the Terms of Service to continue.

Terra Platform Terms of Service

Last Modified: January 10th, 2023

Effective Date: January 10th, 2023

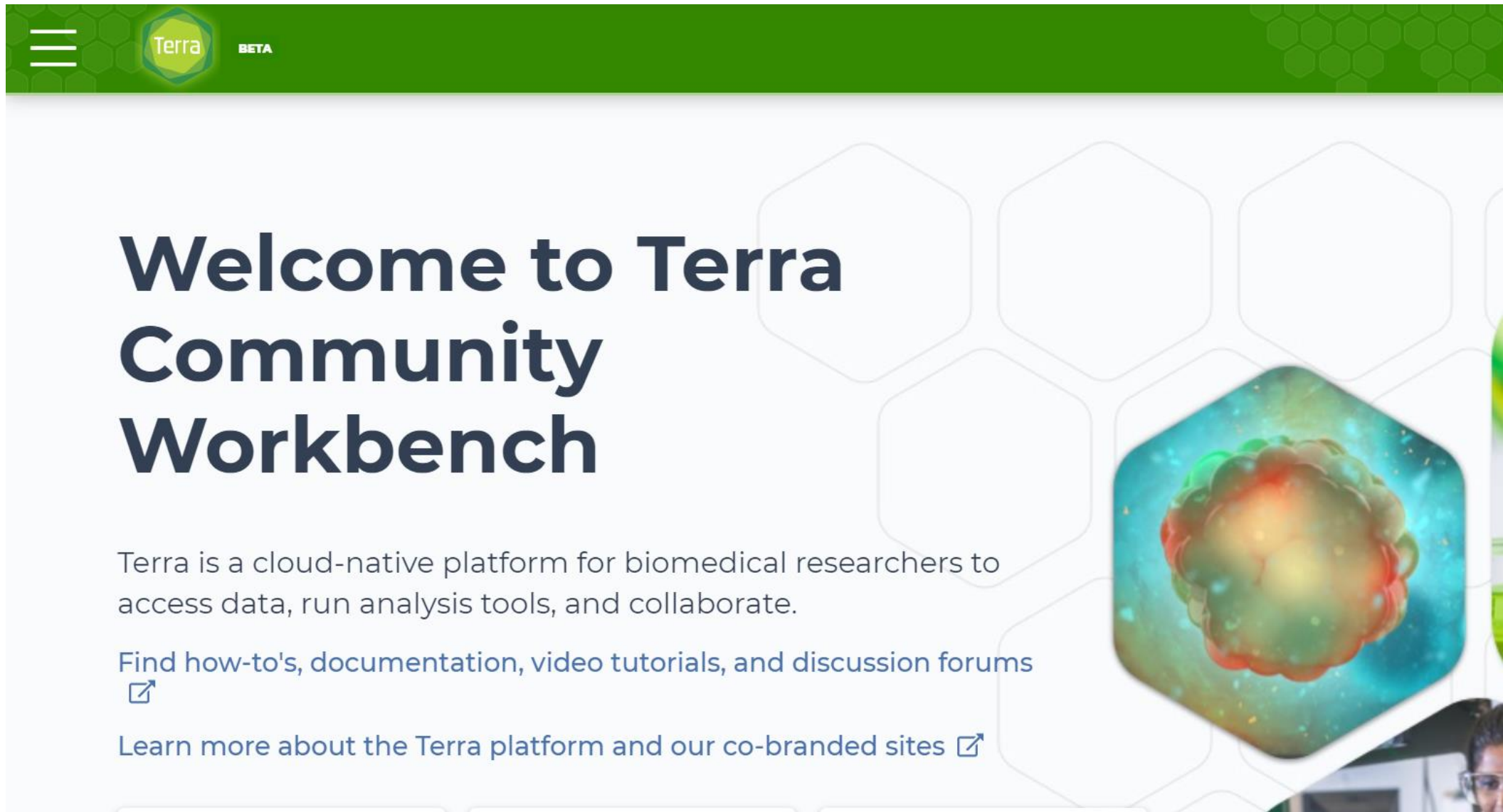
Certain terms (including capitalized terms) are defined in Section 13 (Definitions).



1. Introduction

Thanks for using Terra! Terra is a platform developed by Verily, Microsoft and The Broad Institute that enables users to create and publish datasets, discover and access data

DECLINE AND SIGN OUT ACCEPT

You will see this welcome page:



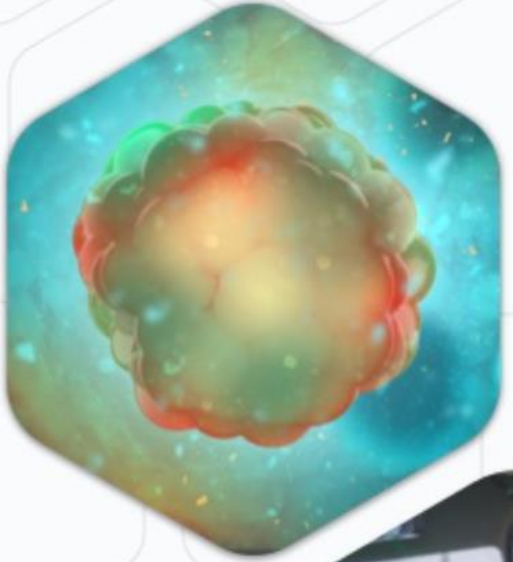
  BETA

Welcome to Terra Community Workbench

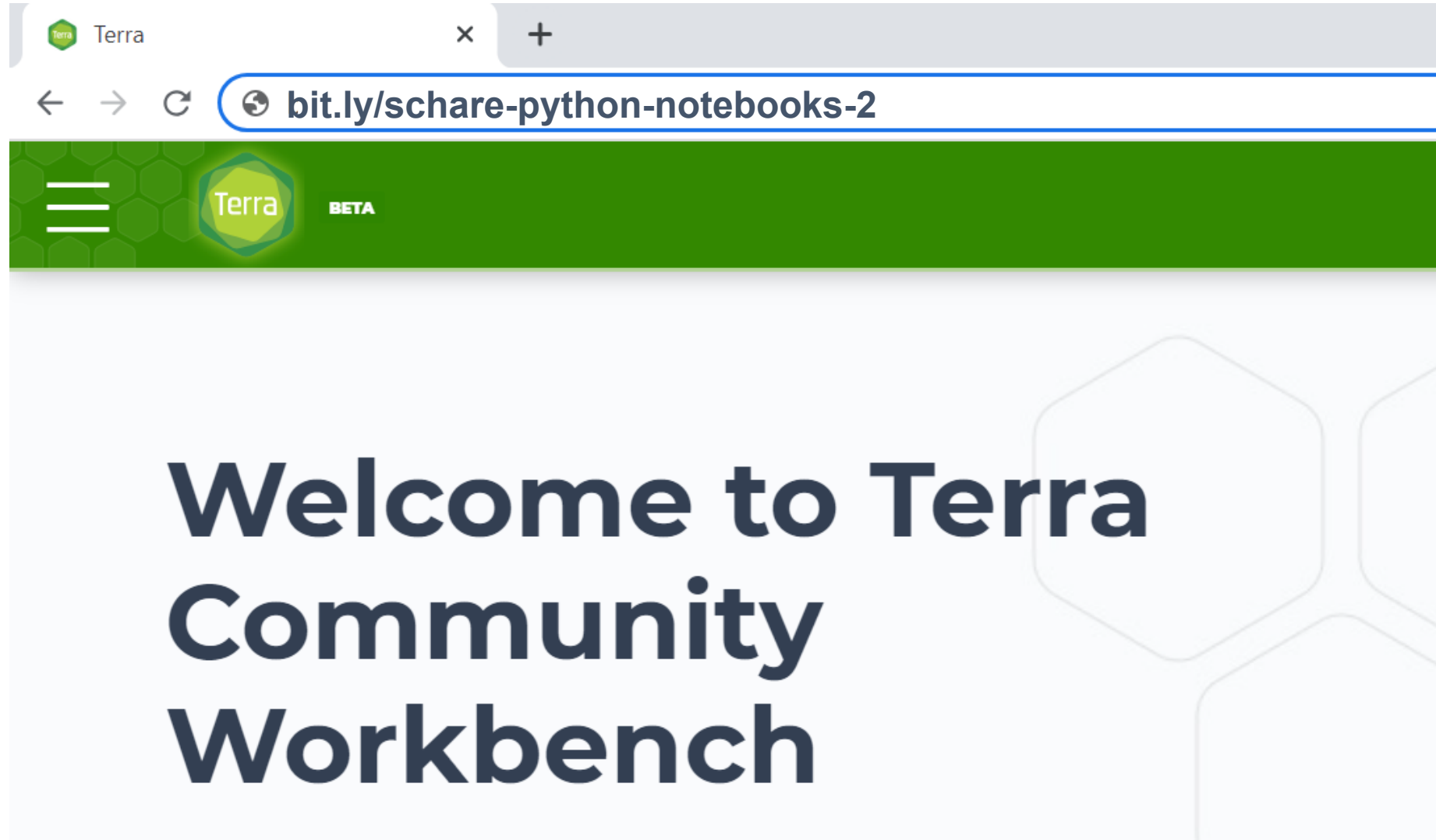
Terra is a cloud-native platform for biomedical researchers to access data, run analysis tools, and collaborate.

Find how-to's, documentation, video tutorials, and discussion forums [↗](#)

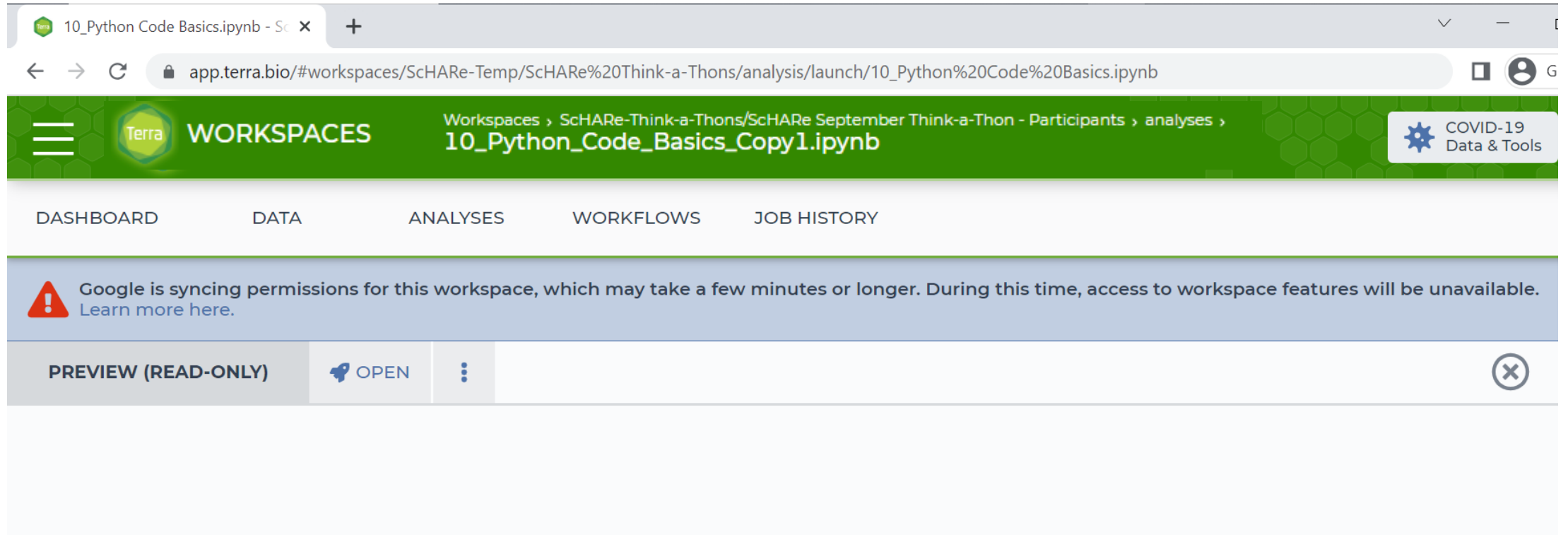
Learn more about the Terra platform and our co-branded sites [↗](#)



Paste this address in your browser: bit.ly/schare-python-notebooks-2

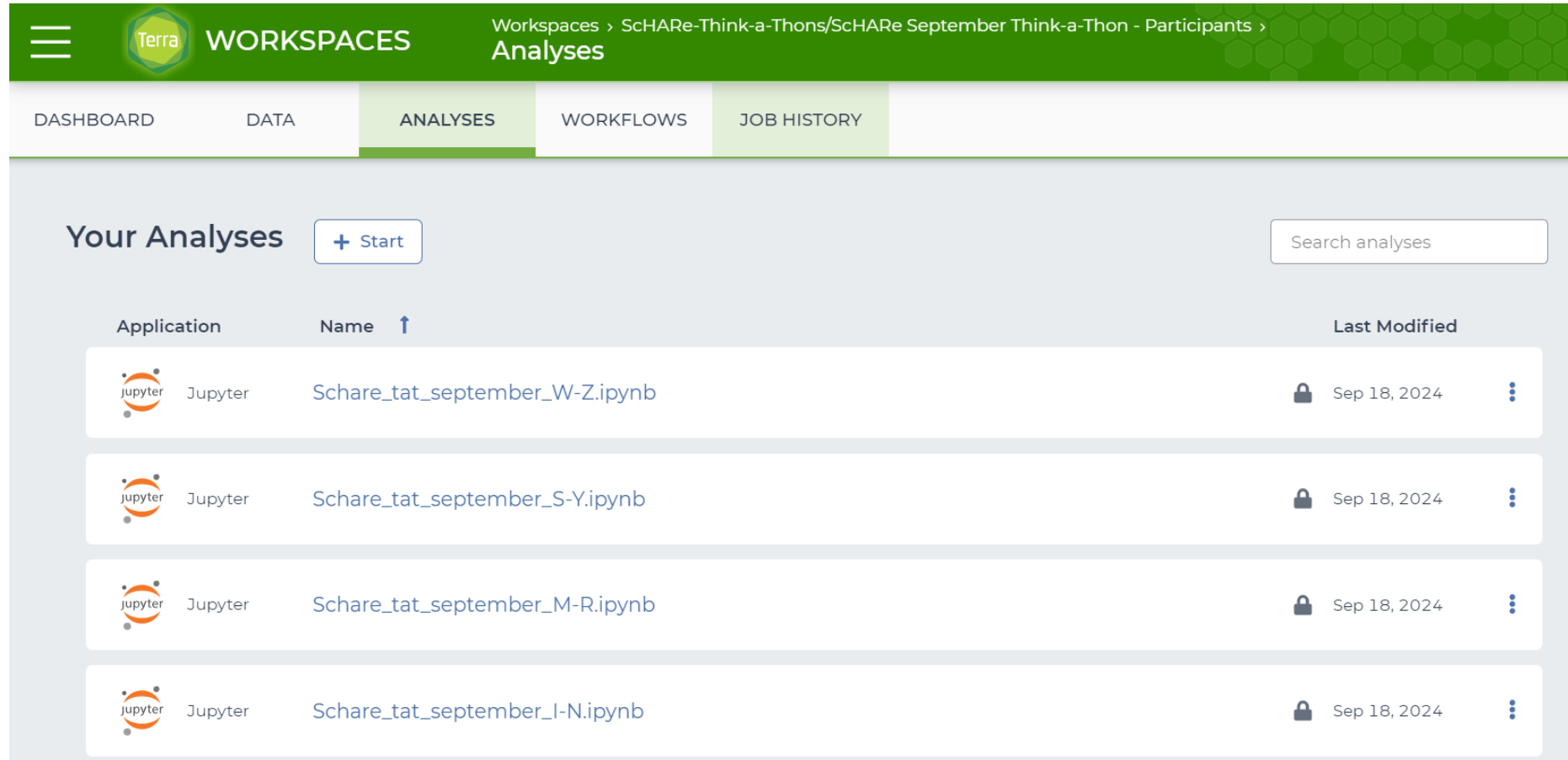


Newly registered users might see this message:



This is normal: the message should go away in a few minutes

Refreshing the page after a while, all users should see this:



The screenshot displays the Terra WORKSPACES interface. The top navigation bar is green and contains the Terra logo, the word "WORKSPACES", and a breadcrumb trail: "Workspaces > SchARE-Think-a-Thons/SchARE September Think-a-Thon - Participants > Analyses". Below this is a secondary navigation bar with tabs for "DASHBOARD", "DATA", "ANALYSES" (which is highlighted), "WORKFLOWS", and "JOB HISTORY".

The main content area is titled "Your Analyses" and includes a "+ Start" button and a search box labeled "Search analyses". Below this is a table listing four analyses, each created by "Jupyter".

Application	Name ↑	Last Modified
Jupyter	Schare_tat_september_W-Z.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_S-Y.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_M-R.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_I-N.ipynb	Sep 18, 2024

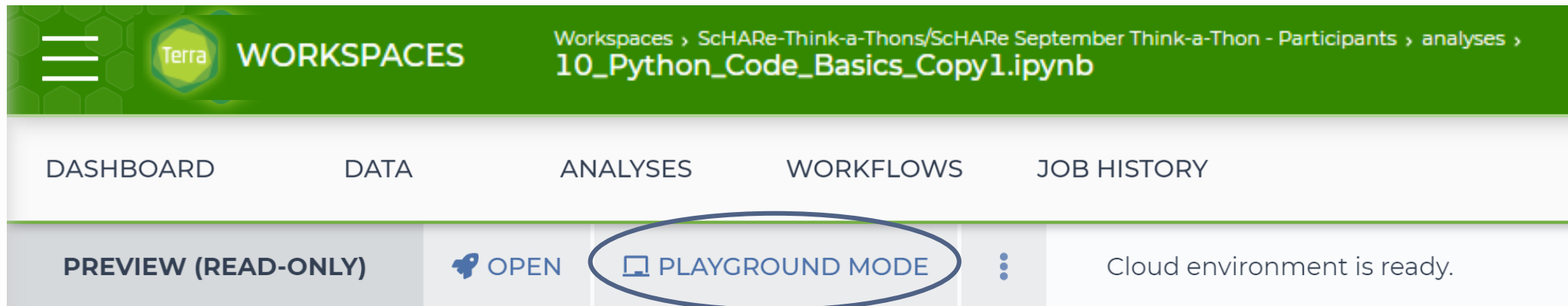
Click on the notebook containing your last name initial:

The screenshot shows the Terra WORKSPACES interface. The top navigation bar includes a menu icon, the Terra logo, and the text 'WORKSPACES'. Below this, the breadcrumb path is 'Workspaces > SchARE-Think-a-Thons/SchARE September Think-a-Thon - Participants > Analyses'. The main navigation tabs are 'DASHBOARD', 'DATA', 'ANALYSES' (which is selected), 'WORKFLOWS', and 'JOB HISTORY'. The 'Your Analyses' section features a '+ Start' button and a search box labeled 'Search analyses'. A table lists four Jupyter notebooks, each with a 'Jupyter' application icon, a name, and a 'Last Modified' date of 'Sep 18, 2024'. The notebook 'Schare_tat_september_S-Y.ipynb' is circled in blue.

Application	Name ↑	Last Modified
Jupyter	Schare_tat_september_W-Z.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_S-Y.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_M-R.ipynb	Sep 18, 2024
Jupyter	Schare_tat_september_I-N.ipynb	Sep 18, 2024

For example, if your last name starts with “S”, click on the notebook highlighted above

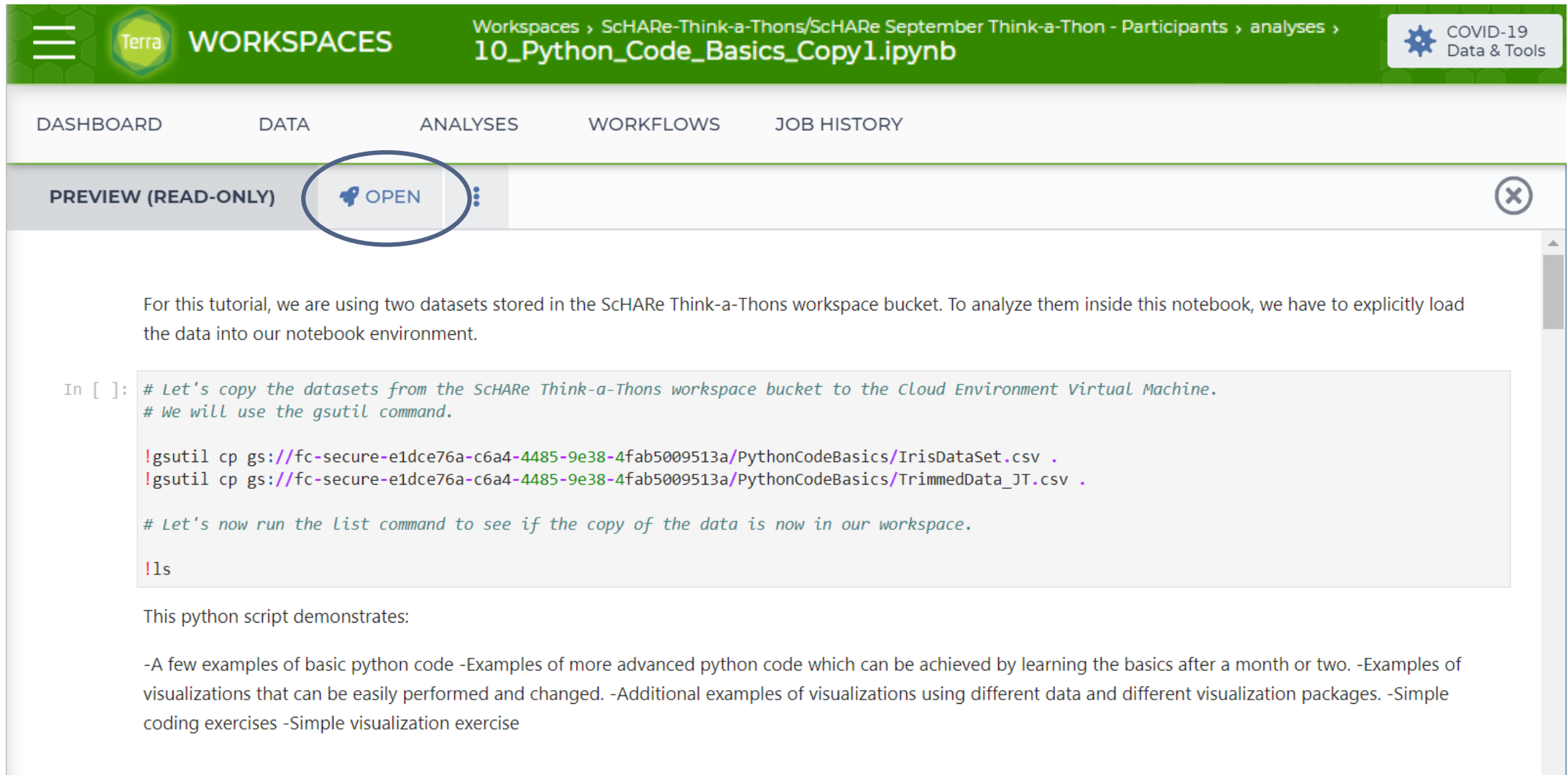
Do you see a Playground mode button?



The screenshot shows the Terra WORKSPACES interface. The top navigation bar is green and contains the Terra logo, the word "WORKSPACES", and a breadcrumb trail: "Workspaces > ScHARe-Think-a-Thons/ScHARe September Think-a-Thon - Participants > analyses > 10_Python_Code_Basics_Copy1.ipynb". Below this is a white navigation bar with tabs for "DASHBOARD", "DATA", "ANALYSES", "WORKFLOWS", and "JOB HISTORY". The main content area has a grey bar with "PREVIEW (READ-ONLY)", an "OPEN" button with a key icon, a "PLAYGROUND MODE" button with a laptop icon (circled in blue), a vertical ellipsis menu icon, and the text "Cloud environment is ready."

If yes, click on it to start your virtual computer. You are done!

If you don't see Playground mode, click on the Open button:



The screenshot shows the Terra WORKSPACES interface. The top navigation bar is green and contains the Terra logo, the word 'WORKSPACES', and the breadcrumb path: 'Workspaces > SchARE-Think-a-Thons/SchARE September Think-a-Thon - Participants > analyses > 10_Python_Code_Basics_Copy1.ipynb'. On the right of the top bar is a 'COVID-19 Data & Tools' button. Below the top bar is a navigation menu with 'DASHBOARD', 'DATA', 'ANALYSES', 'WORKFLOWS', and 'JOB HISTORY'. The main content area has a header 'PREVIEW (READ-ONLY)' and a blue 'OPEN' button with a play icon, which is circled in blue. To the right of the 'OPEN' button is a close button (X). The main content area contains a text block and a code block.

For this tutorial, we are using two datasets stored in the SchARE Think-a-Thons workspace bucket. To analyze them inside this notebook, we have to explicitly load the data into our notebook environment.

```
In [ ]: # Let's copy the datasets from the SchARE Think-a-Thons workspace bucket to the Cloud Environment Virtual Machine.
# We will use the gsutil command.

!gsutil cp gs://fc-secure-e1dce76a-c6a4-4485-9e38-4fab5009513a/PythonCodeBasics/IrisDataSet.csv .
!gsutil cp gs://fc-secure-e1dce76a-c6a4-4485-9e38-4fab5009513a/PythonCodeBasics/TrimmedData_JT.csv .

# Let's now run the list command to see if the copy of the data is now in our workspace.

!ls
```

This python script demonstrates:

- A few examples of basic python code
- Examples of more advanced python code which can be achieved by learning the basics after a month or two.
- Examples of visualizations that can be easily performed and changed.
- Additional examples of visualizations using different data and different visualization packages.
- Simple coding exercises
- Simple visualization exercise

Configure your virtual computer – accept the default values:

The screenshot shows the Terra Jupyter Cloud Environment configuration page. The browser address bar shows the URL: `app.terra.bio/#workspaces/SchARe-Temp/SchARe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb`. The page title is "10_Python Code Basics.ipynb - Sc".

The main content area is titled "Jupyter Cloud Environment" and includes a description: "A cloud environment consists of application configuration, cloud compute and persistent disk(s)."

Cost information is displayed in a table:

Running cloud compute cost	Paused cloud compute cost	Persistent disk cost
\$0.05 per hr	\$0.00 per hr	\$2.00 per month

The "Application configuration" section includes:

- A dropdown menu for the environment configuration, currently set to "Default: (GATK 4.2.4.0, Python 3.7.12, R 4.3.0)".
- Information about the environment: "What's installed on this environment?" with a "Learn more" link, and "Updated: Jun 8, 2023" and "Version: 2.2.14".
- A "Startup script" field with a "Learn more about startup scripts" link.
- A "URI" input field.

The "Cloud compute profile" section includes:

- CPU selection: "CPUs" set to "1".
- Memory selection: "Memory (GB)" set to "3.75".
- An "Enable GPUs" checkbox, which is currently unchecked, with a "BETA" label and a "Learn more about GPU cost and restrictions" link.

The "Compute type" section is partially visible at the bottom.

Click on Create below:

The screenshot shows a web browser window with the URL `app.terra.bio/#workspaces/SCHaRe-Temp/SCHaRe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb`. The page title is "10_Python Code Basics.ipynb - Sc x". The main content area is titled "Jupyter Cloud Environment" and includes a description: "A cloud environment consists of application configuration, cloud compute and persistent disk(s)."

Cost information is displayed in a light blue box:

Running cloud compute cost	Paused cloud compute cost	Persistent disk cost
\$0.05 per hr	\$0.00 per hr	\$2.00 per month

Configuration options include:

- Inactivity timeout: 30 minutes of inactivity
- Location: us-central1 (Iowa) (default)
- Persistent disk: Standard, 50 GB

A blue "CREATE" button is circled in blue at the bottom right of the configuration panel.

It will take some time...

The screenshot shows a web browser window with the URL `app.terra.bio/#workspaces/SchARe-Temp/SchARe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb`. The page header includes the Terra logo, the word "WORKSPACES", and a breadcrumb trail: "Workspaces > SchARe-Think-a-Thons/SchARe September Think-a-Thon - Participants > analyses > 10_Python_Code_Basics_Copy1.ipynb". There are also buttons for "COVID-19 Data & Tools" and a notification bell with a "2" badge. Below the header is a navigation bar with "DASHBOARD", "DATA", "ANALYSES", "WORKFLOWS", and "JOB HISTORY". A secondary bar contains "PREVIEW (READ-ONLY)", "OPEN", and "PLAYGROUND MODE". A blue oval highlights a message box that says "Creating cloud environment. You can navigate away and return in 3-5 minutes." with a close button (X) on the right.

When the system is ready, click on Playground mode:

The screenshot shows a web browser window with the URL `app.terra.bio/#workspaces/SchARe-Temp/SchARe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb`. The page header is green and contains the Terra logo, the word "BETA", and "WORKSPACES". The breadcrumb navigation shows "Workspaces > SchARe-Temp/SchARe Think-a-Thons > analyses > 10_Python Code Basics.ipynb". There is a "COVID-19 Data & Tools" button and a notification bell with a "2" badge. Below the header is a navigation bar with "DASHBOARD", "DATA", "ANALYSES", "WORKFLOWS", and "JOB HISTORY". The main content area has a "PREVIEW (READ-ONLY)" button, an "OPEN" button with a rocket icon, and a "PLAYGROUND MODE" button with a terminal icon, which is circled in blue. To the right of the "PLAYGROUND MODE" button is a status message: "Creating cloud environment. You can navigate away and return in 3-5 minutes." with a close button (X).

Click on Continue:

10_Python Code Basics.ipynb - Sc x +

app.terra.bio/#workspaces/SchARe-Temp/SchARe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb

Guest

Terra BETA WORKSPACES

Workspaces > SchARe-Temp/SchARe Think-a-Thons > analyses >

DASHBOARD DATA ANALYSE

PREVIEW (READ-ONLY) OPEN P

Playground Mode

Playground mode allows you to explore, change, and run the code, but your edits will not be saved.

To save your work, choose **Download** from the **File** menu.

Do not show again

CANCEL CONTINUE

Error Creating Cloud Environment

Details

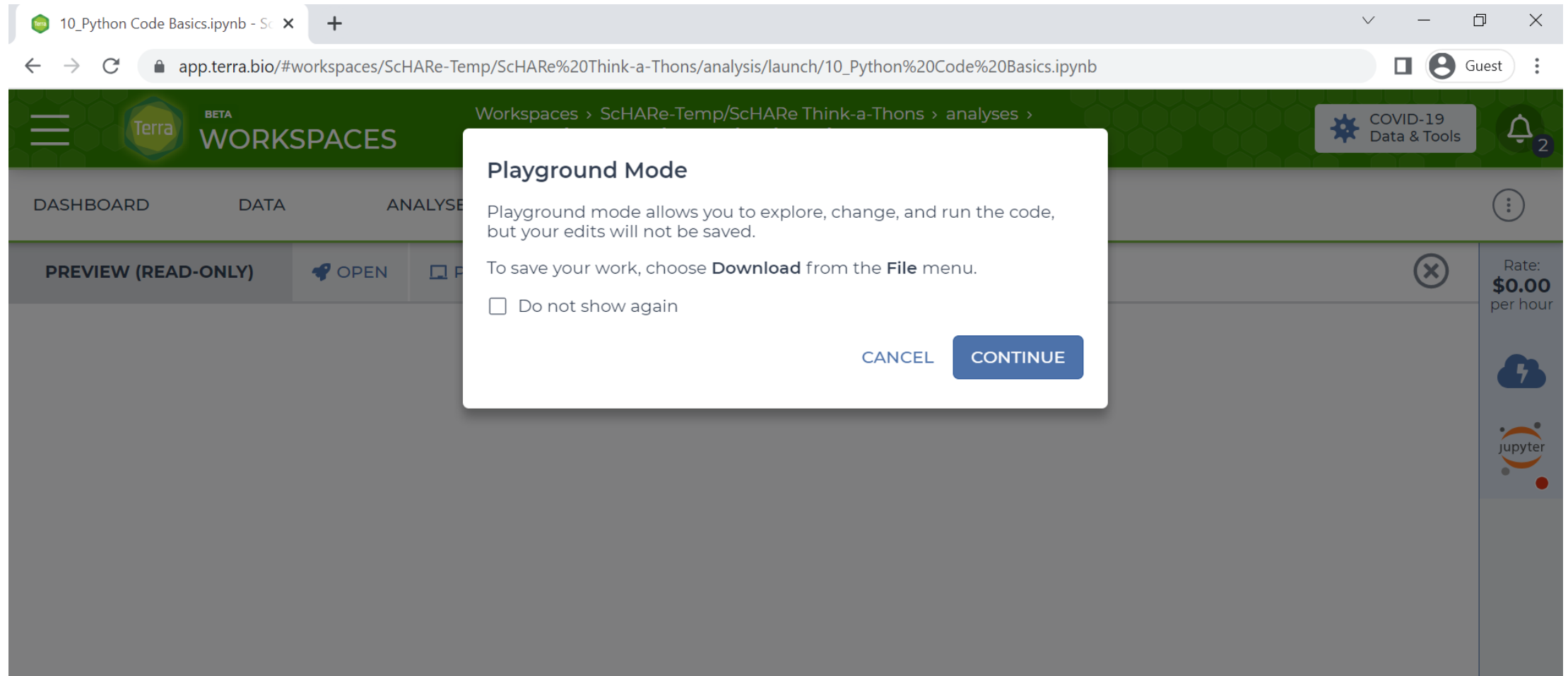
Rate: \$0.00 per hour

cloud jupyter

Note that you might encounter an error due to the large number of users – just try again in a few minutes:

The screenshot shows a web browser window with the URL `app.terra.bio/#workspaces/SCHaRe-Temp/SCHaRe%20Think-a-Thons/analysis/launch/10_Python%20Code%20Basics.ipynb`. The page displays the Terra workspace interface, including a navigation menu with 'DASHBOARD', 'DATA', and 'ANALYSES', and a 'PREVIEW (READ-ONLY)' button. A central modal dialog box is open, displaying the message 'Cloud Environment is in error state' and 'Failed to create cluster 101753 due to 5 seconds', with an 'OK' button. In the background, a notification banner reads 'Error Creating Cloud Environment' with a 'Details' link. The right sidebar shows a 'Rate: \$0.00 per hour' and a 'jupyter' logo.

If all goes well, you will see this:

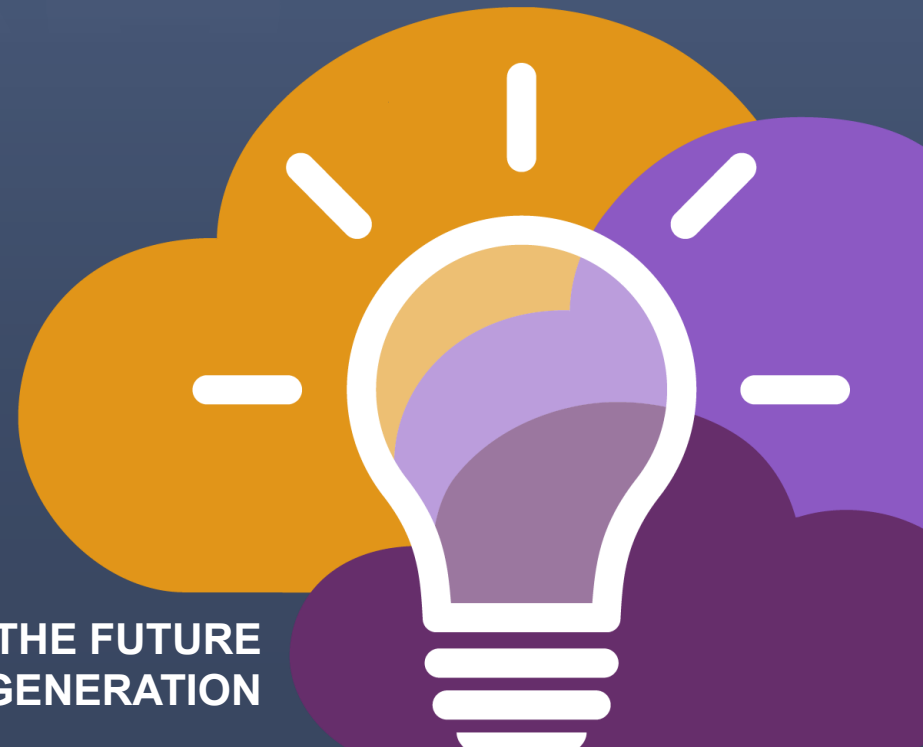


Click on Continue. You are all set!

ScHARe

Why Python?

BE A PART OF THE FUTURE
OF KNOWLEDGE GENERATION



What is Python?

Python is a **computer programming language** used in data science to:

- manipulate and analyze data and conduct statistical calculations
- create data visualizations
- build machine learning algorithms

Python's **data science libraries** are powerful. Examples include:

- **Numpy** - for linear algebra and high-level mathematical functions
- **Pandas** - for handling data structures and manipulating tables
- **SciPy** - for data science tasks like interpolation and signal processing
- **Scikit-learn** - a machine learning library that is useful for classification, regression, and clustering algorithms
- **PyBrain** - for machine learning tasks and to test and compare algorithms



Sources

www.quanhub.com/python-for-data-science/
[coursera.org](https://www.coursera.org)

What is R?

R is a **programming language** for statistical computing and graphics

It is used by data miners, bioinformaticians and statisticians for data analysis

Users have created **packages** to augment its functions

Third-party **graphical user interfaces** are also available, such as Rstudio



supports **both Python and R**

Why Python?

According to SlashData:

- there are 8.2 million Python users
- **69%** of machine learning developers and data scientists **use Python (vs. 24%** of them **using R)**

Source
stackify.com/learn-python-tutorials/

How to learn Python

How long does it take to learn Python?

It can take **2 to 5 months**, but you can write your first short program in **minutes**

Can you learn Python with no experience?

Python is the **perfect** programming language **for people without any coding experience**, as it has a simple syntax and is very accessible to beginners

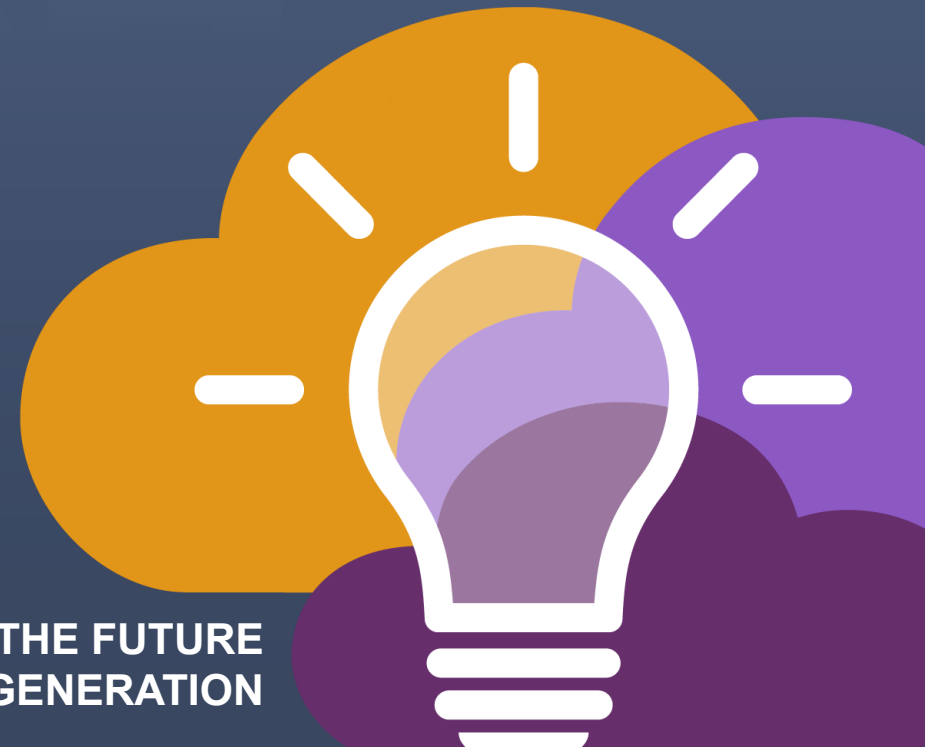
Unfamiliar terminology may be a barrier, which today's workshop will hopefully help you overcome

Links to additional **free learning resources** will be provided at the end

ScHARe

Data Management
and Analysis in
Python

BE A PART OF THE FUTURE
OF KNOWLEDGE GENERATION



ScHARe



Guest expert

Cindy Sheffield

NIH/OD/ORS



About Cindy

Cindy is **Data Services Librarian** at the NIH Library.

She began her **library career** at the Johns Hopkins Medical Institutions with a focus on Evidenced Based Medicine. She progressed within the Welch Medical Library, leaving Hopkins as the Associate Director of Education Services.

Cindy has worked at several **federal agencies** including the Department of Homeland Security, the Department of Defense, and the Department of Health and Human Services. Within DHHS she was worked for both the National Institutes of Health and the Federal Drug Administration.

Her **focus** has always been on using key resources to identify the best evidence, and then to organize and manage that evidence in a way that makes sense for users. At the NIH she works with various user groups to support literature research and data science.

She is the Outreach Librarian for the NIH Clinical Centers, Pain and Palliative Care Team, the Eunice Kennedy Shriver, National Institute of Child and Human Development, the Administration for Children and Families, and the Office of the National Coordinator for Health Information Technology.

ScHARe



Guest expert

Sarvesh Soni

NIH/NLM



About Sarvesh

Dr. Sarvesh Soni is a Research Fellow with Dr. Dina Demner-Fushman at the National Library of Medicine.

Dr. Soni has a PhD in Biomedical Informatics from The University of Texas Health Science Center at Houston (UTHealth). He researches clinical natural language processing (NLP), focusing on question answering (QA) from both structured and unstructured data present in electronic health records (EHRs).

He implemented methods to generate paraphrases of clinical questions automatically and improve EHR QA and designed systems to automatically retrieve EHR text documents and underlying exact answer spans for given clinical information needs.

ScHARe Think-a-Thon Series: An Introduction to Python for Data Science, Part 2

Cindy Sheffield, Biomedical Librarian, NIH Library

Sarvesh Soni, Research Fellow, National Library of Medicine

Introduction

- Recap from August session – 10 min
- Importance of data cleaning – 10 min
- Tools for data cleaning – 10 min
- How data impacts visualizations – 10 min
- Machine Learning primer – 10 min
- Examples of Visualizations, Data Cleaning, Machine Learning – 80 min

Attendees will be able to:

- Know how to find Python libraries to help with code functionality
- Understand the importance of data cleaning
- Know what tools are available to help with data cleaning
- Visualizations and the importance of telling an accurate story
- Understand the mechanisms behind Machine Learning

Recap from Part 1:

Slido quiz

What is a Python library?

- A collection of books about Python programming
- Answer B A collection of related modules that provide specific functionality
- A place to store Python code
- A way to access Python from the command line

Python Libraries – a collection of related modules that provide more extensive functionality and solve specific problems

Sample libraries:

Numpy

Pandas

Matplotlib

How to find libraries:

PyPI.org

GitHub

Slido quiz

Which of the following are examples of Python libraries?

- Excel, OpenRefine
- Matplotlib, Pandas, Numpy
- R, SQL
- GitHub, PyPI

Data Cleaning / Data Wrangling

Ensure:

- Data accuracy
- Data consistency
- Data quality
- Efficiency

Processes:

- Parsing (First/Last Name)
- Correcting (Typos, errors)
- Standardizing (format)
- Match (id duplicates)
- Consolidating (clean presentation)

Slido quiz

Why is clean data important?

- It allows for better decision-making and saves time
- It makes data look nice without adding any practical value
- It removes all irrelevant information from public datasets
- It ensures that data can never be incorrect

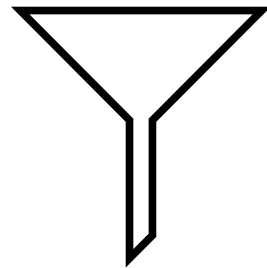
- Corrupted
- Inaccurate
- Duplicates
- Irrelevant information

Establish quality control standards:

- Account for missing values
- De-duplication / Consolidating
- Irrelevant information
- Normalize non-standard values
- Understand outliers vs. incorrect data
- Change case if needed
- Check for bad values in fields(i.e.: alpha vs. numeric, formatting, spacing)
- Ensure overall data quality

Six step process:

- *Explore*
- ***Transform***
- *Clean*
- *Enrich*
- *Validate*
- *Store*



Data Wrangling –

Mapping, merging, concatenating, or converting data, to transform the content, so it can be used for algorithmic processing and analysis.

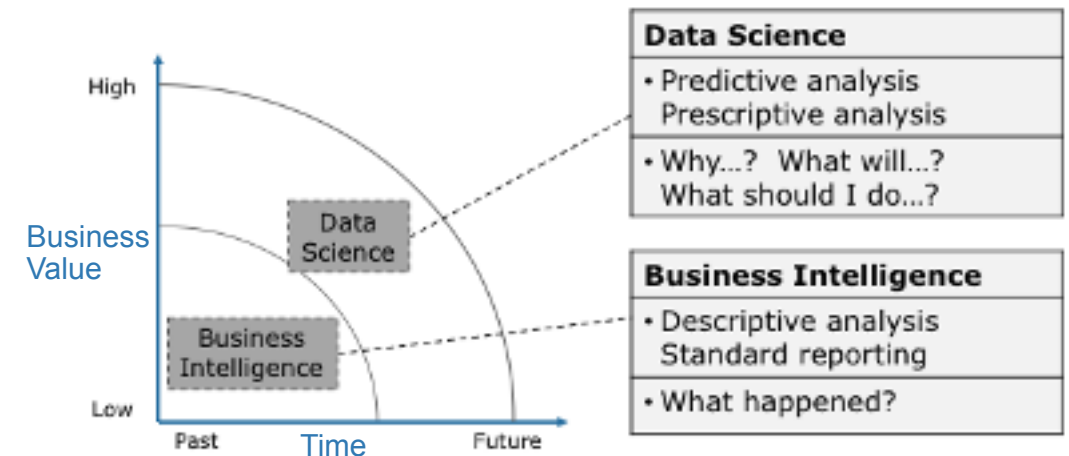
Slido quiz

Which of the following is part of the data wrangling process?

- Transforming data to prepare it for analysis
- Writing code in a programming language
- Saving data as images
- Downloading data from the internet

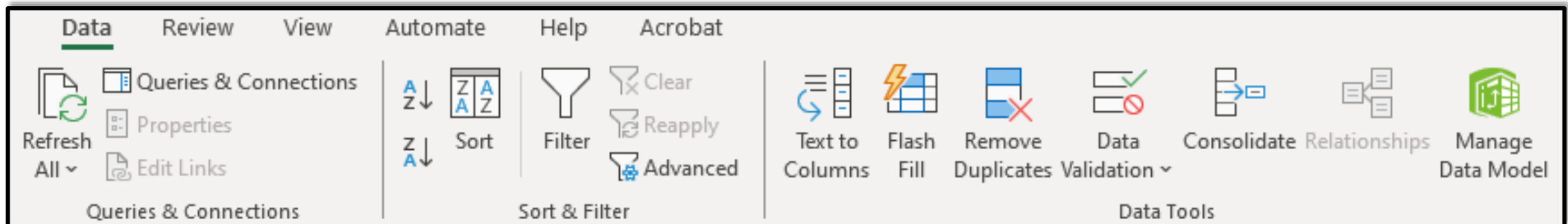
- Allows for informed decision making, and it is the precursor to artificial intelligence.
- Enhances efficiencies by saving time, effort, and resources.
- Improves satisfaction for consumers and producers
- In Public Health and Regulatory environments, it helps to maintain trust and avoid legal actions.

Business Intelligence versus Data Science



- Excel: Functions within Excel
- R: dplyr, tidyr, rrefine
- Python: Pandas, NumPy
- OpenRefine

Excel



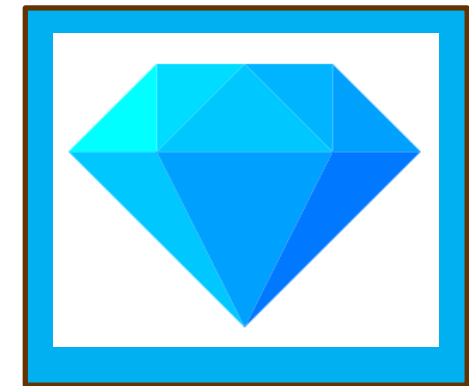
- Open Source
- Desktop application
- Data cleanup and transformation
- Faceting
- Clustering
- Reconciling

OpenRefine:

- is 'a tool for working with messy data'
- works best with data in tabular format
- can help split data into more granular parts
- can help match local data to other data sets
- can help enhance a data set with data from other sources

Tutorial: Library Carpentry: OpenRefine:

<https://librarycarpentry.org/lc-open-refine/instructor/aio.html>



Slido quiz

What is OpenRefine used for?

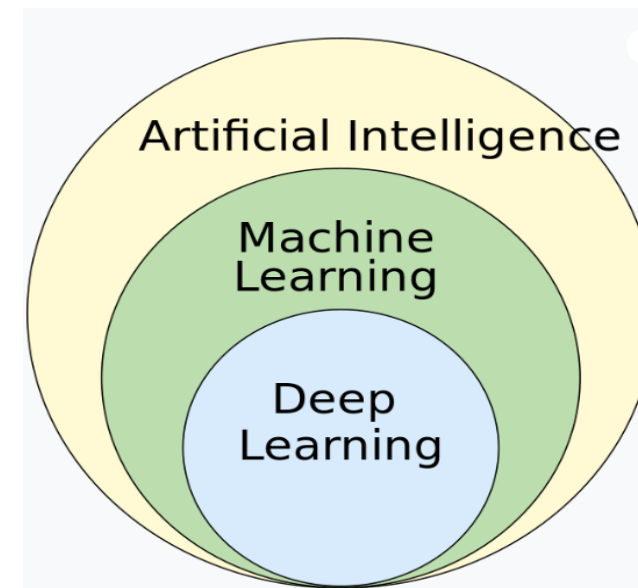
- Word processing
- Creating spreadsheets
- Data cleanup and transformation
- Developing websites

- 1. Buttrey S, Whitaker LR. *A data scientist's guide to acquiring, cleaning and managing data in R*. 1st edition ed. THEi Wiley ebooks. Wiley; 2017.
- 2. Gueta T, Carmel Y. Quantifying the value of user-level data cleaning for big data: A case study using mammal distribution models. *Ecological informatics*. 2016;34:139-145. doi:10.1016/j.ecoinf.2016.06.001
- 3. Martin N, Martinez-Millana A, Valdivieso B, Fernández-Llatas C. Interactive Data Cleaning for Process Mining: A Case Study of an Outpatient Clinic's Appointment System. Springer International Publishing; 2019:532-544. *Lecture Notes in Business Information Processing*.
- 4. Mertz D. *Cleaning data for effective data science : doing the other 80% of the work with Python, R, and command-line tools*. Packt Publishing; 2021.
- 5. Van den Broeck J, Cunningham SA, Eeckels R, Herbst K. Data cleaning: detecting, diagnosing, and editing data abnormalities. *PLoS Med*. Oct 2005;2(10):e267. doi:10.1371/journal.pmed.0020267
- 6. Walker M. *Python Data Cleaning Cookbook : Prepare Your Data for Analysis with Pandas, NumPy, Matplotlib, Scikit-Learn, and OpenAI*. Packt Publishing, Limited; 2024.
- 7. Wang X, Wang C. Time Series Data Cleaning: A Survey. *IEEE access*. 2020;8:1866-1881. doi:10.1109/ACCESS.2019.2962152

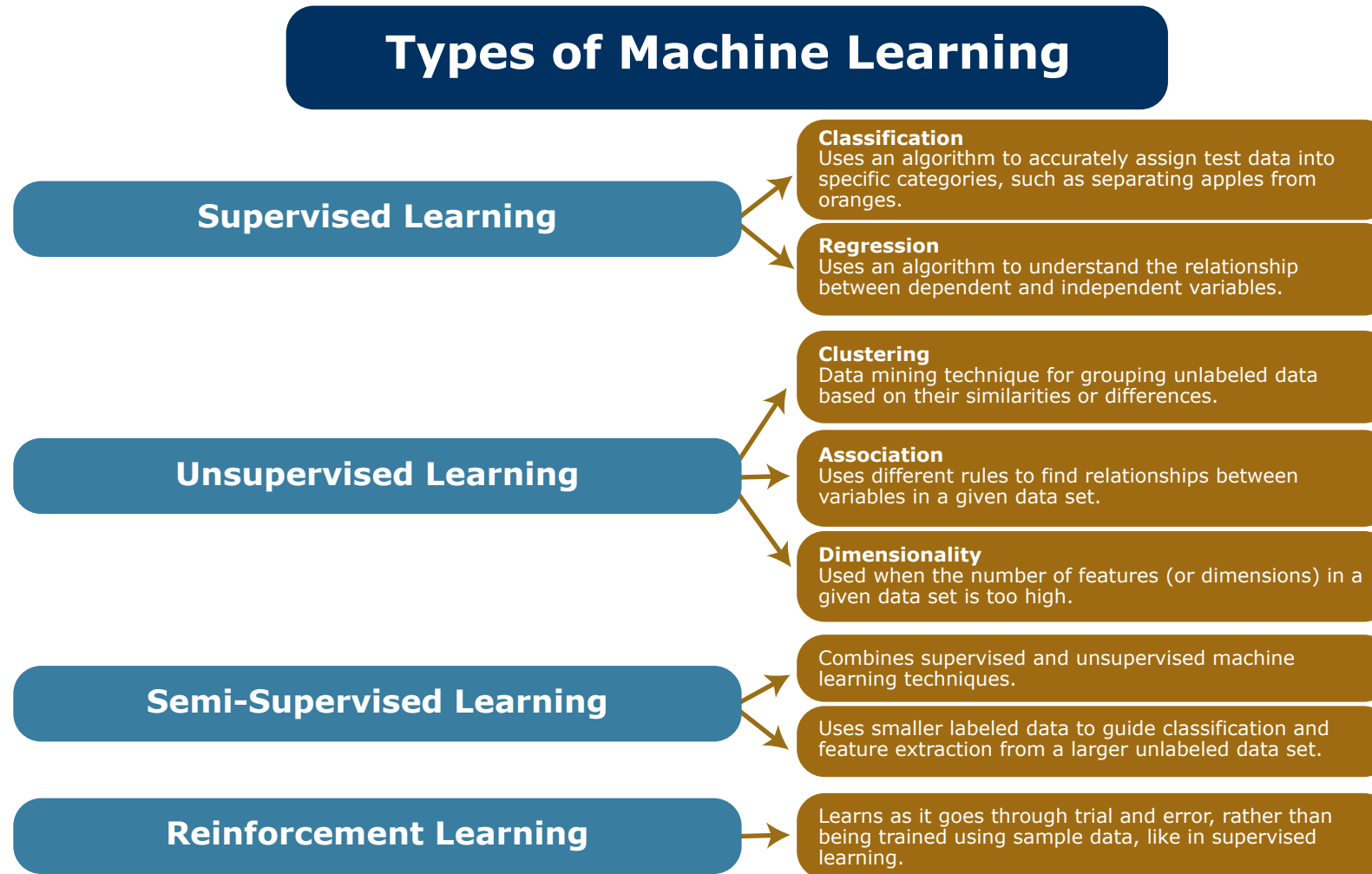
- Use to better understand data
- Prepare the data so it tells an accurate story
- Understand the data and any potential bias

Machine Learning

- Machine Learning - type of AI and CS
- Improves how software systems process and categorize data
- Focuses on the use of data and algorithms
- Imitate human learning
- Gradually improving its accuracy
- ML algorithms imitate human learning
- ML algorithms improve over time as they take large data sets



<https://bootcamp.berkeley.edu/blog/how-does-machine-learning-work/>



- Taught by example
- Training data is fed into an algorithm and teaches to categorize based on pre-set characteristics
- Algorithm can similarly sort raw data
 - Good at classifying data into pre-set categories
Example: identify spam emails or telling images apart

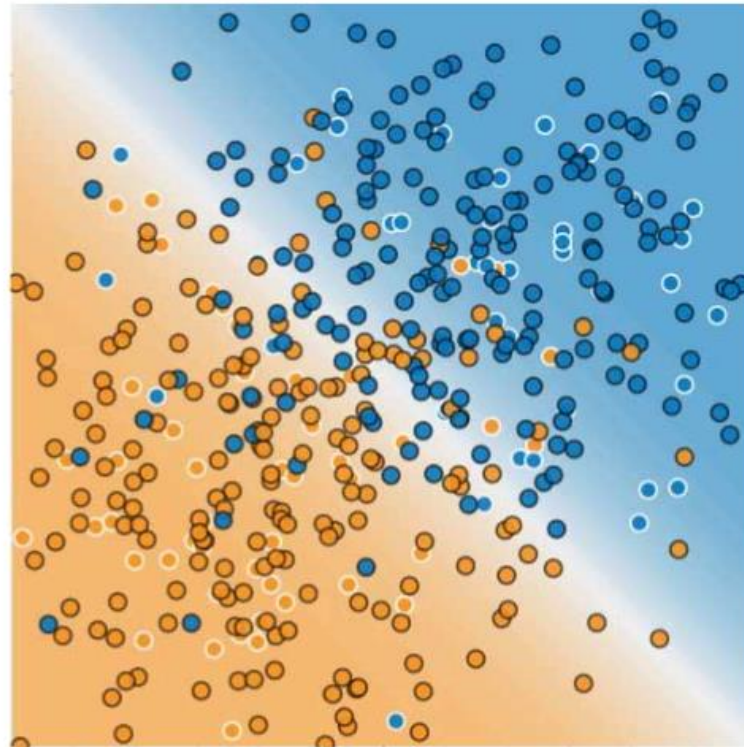
- Uses algorithms to sort unlabeled and unstructured data
- Algorithms discover data patterns without human intervention
- Good situations without clear delineations between different data categories
- Example:
 - Recommend similar types of research projects or publications

- Combines supervised and unsupervised machine learning to sort or identify data
- Involves labeling some data
- Involves rules and structure for the algorithm to use to start sorting and identifying data
- A small amount of tagged data improves an algorithm's accuracy
- Example: classify content in scanned documents: typed and handwritten

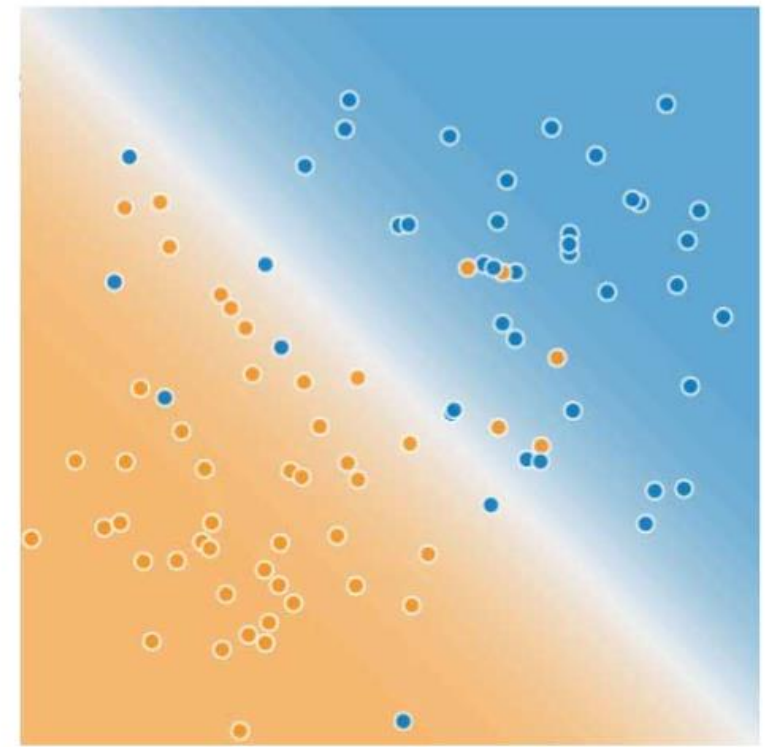
- Used for decision-making in a complex, uncertain environment
- Game-like rules system designed to maximize algorithm's score
- Programmers define rules; computer starts without guidance
- Computer learns through trial and error for optimal solutions
 - Example: used for language processing, self-driving vehicles and game-playing AIs

Training Set and Test Set

- **Training Data Set**—a subset to train a model.
- **Test data set**—a subset to test the trained model.



Training Data



Test Data

Evaluating Machine Learning Performance

		Actual (ex. Manual coding)		
		Positive	Negative	
ML model/ Algorithm Predictions	Positive	True Positive (TP)	False Positive (FP)	Positive Predictive Value
	Negative	False Negative (FN)	True Negative (TN)	Negative Predictive Value
		Sensitivity	Specificity	

- **Accuracy:** how much did the model get right; % of predictions the model or algorithm gets correct;
= $(TP + TN)/(TP+FN +FP+TN)$
- **Precision:** also called positive predictive value (PPV); the quality of the positive predictions; % of positive predictions that were correct; = $TP/TP+FP$
- **Sensitivity:** also referred to as recall; measures how well a model can detect positive instances;
= $TP/TP+FN$
- **Specificity:** measures how well the model identifies negatives instances; = $TN/TN+FP$
- **F1 score:** also used to assess accuracy of the model and it accounts for both precision and recall;
= $TP/TP + \frac{1}{2}(FP+FN)$

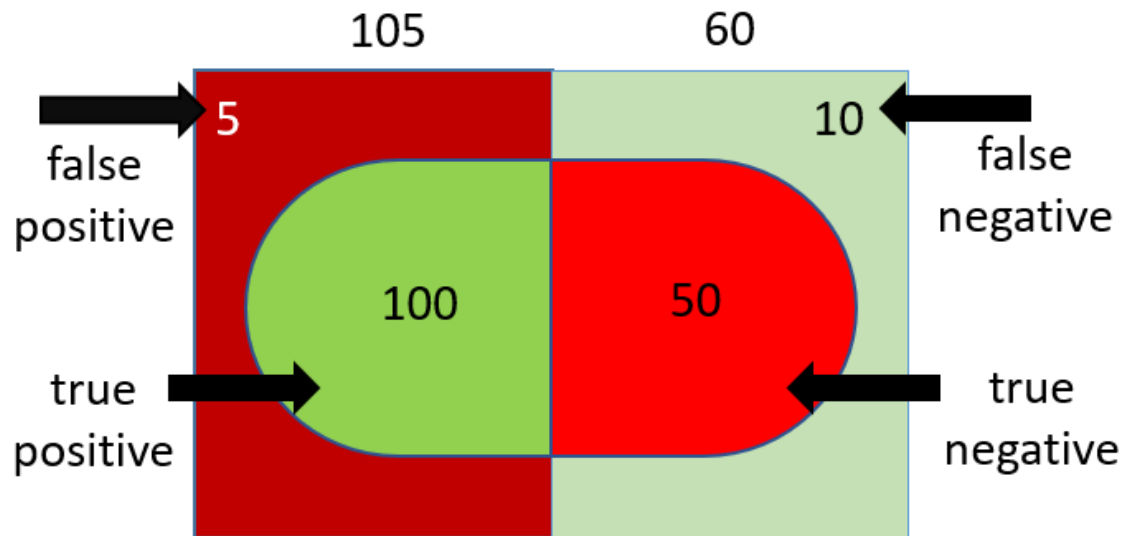
Machine Learning Performance Example

tp = AI Model found true positive = 100

fp = AI Model marked as positive; but negative = 5

tn = AI Model found true negative = 50

fn = AI Model marked as negative; but positive = 10



• **Accuracy:** how much did model get right;

$$= (tp + tn) / (tp + fn + fp + tn) = 150 / 165 = .9091$$

• **Precision:** positive predictive value (PPV);

$$= tp / tp + fp = 100 / 105 = .9523$$

• **Sensitivity:** recall; true positive instances;

$$= tp / (tp + fn) = 100 / 100 + 10 = 100 / 110 = .9091$$

• **Specificity:** negatives;

$$= tn / (tn + fp) = 50 / 50 + 5 = 50 / 55 = .9091$$

• **F1 Score:** assesses accuracy; precision and recall;

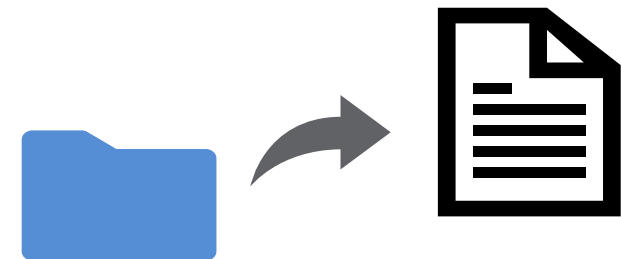
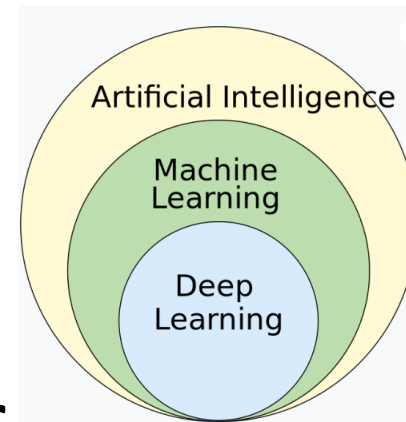
$$= 2 (precision * recall / precision + recall)$$

$$\text{Or} = TP / TP + \frac{1}{2}(FP + FN)$$

$$= 100 / 100 + .5(10 + 5)$$

$$= 100 / 107.5 = .9302$$

- Subset of Machine Learning
- Teaches computers to process data similar to human brain
- Recognize picture patterns, text, sounds and other data
- Produce insights and predictions based on data
- Use to automate tasks typically done by humans:
 - describe images
 - transcribe files into text

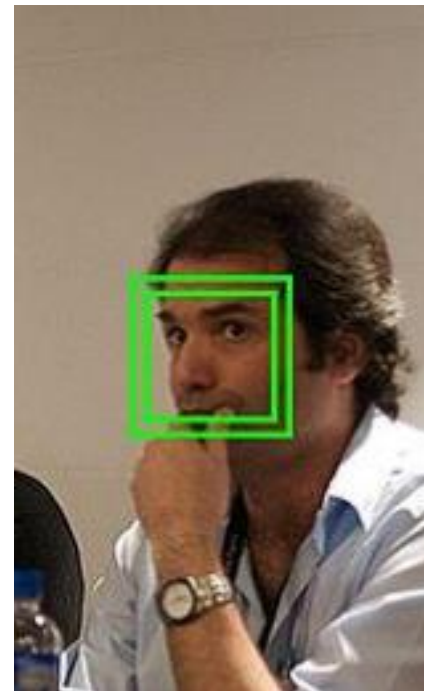


Used in everyday products:

- Digital assistants
- Voice-activated television remotes
- Fraud detection
- Automatic facial recognition

Uses of Deep learning:

- Self-driving cars
- Defense systems
- Medical image analysis
- Factories



Natural Language Processing (NLP)

- NLP is an artificial intelligence technique
- Subset of machine learning
- Allows machines to process and understand language like humans
- Uses computational linguistics combined with machine learning, deep learning and statistical modeling
- Understands intent and sentiment
- Stores information and context to strengthen future responses

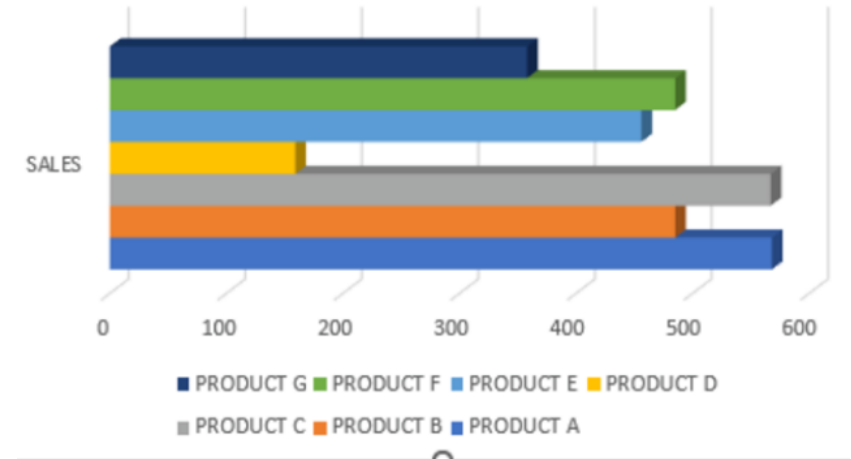


- **Text analysis and data mining**
 - helps scientists extract valuable information from vast amounts of unstructured text data
- **Automated Literature Review**
 - allows for automated literature; speeds up gathering and summarizing research
- **Semantic Search and Information Retrieval**
 - enhances search engines, enabling more relevant results
- **Language Translation**
 - enables translation between different languages

- **Knowledge Representation**
 - convert textual information into structured data
- **Sentiment Analysis**
 - understand public opinion and reactions to scientific breakthroughs or research findings.
- **Question-Answering Systems**
 - enables specific questions and receive relevant answers from large databases or scientific literature
- **Automated Report Generation**
 - generate summaries, abstracts, or reports automatically, reducing manual effort

Clinical Applications

- analyze electronic health records
- extract important medical information
- diagnosing patients
- identifying patterns in medical data



Data Interpretation and Visualization

- interpret and understand complex scientific data
- generate visualizations

