# HIGH PERFORMANCE RESEARCH COMPUTING

## Micro-credentials in Research Computing

09/30/2022

High Performance
Research Computing
DIVISION OF RESEARCH

# Outline

- Overview of Microcredentials
- Details about Specific Courses
- Demonstrations of Online Course Elements

# Overview of Microcredentials

# Background

- The High Performance Research Computing Group has many years of experience teaching computer skills.
  - Short courses
  - Workshops
  - Summer Camps
  - 1-on-1 User Support
- We are excited to announce that we are ready to take our expertise to the next level.

# Short Courses

- Short courses provide small-scale learning opportunities targeting specific skills.
- Short courses fill gaps in coursework for traditionally non-computing degree programs.
- Online, asynchronous courses developed with support from Texas A&M Engineering Studio for Advanced Instruction and Learning (eSAIL).

TEXAS A&M UNIVERSITY
Engineering Studio for
Advanced Instruction & Learning

# Research Skills

- Exercises and topics designed for researchers
  - E.g., graduate students
- Coding skills for specific disciplines and purposes
- Training in standard workflows and common practices
  - Especially useful for High Performance Computing

*Not just another generic tutorial!*

# Microcredentials

- Microcredentials are rewards for completion of small-scale learning goals, recognized by academia and industry.
- Supported by Texas A&M Engineering Experiment Station Education Generations (TEES EDGE)
- This program is part of the professional and continuing education credit system.
  - Outside the university course credit system

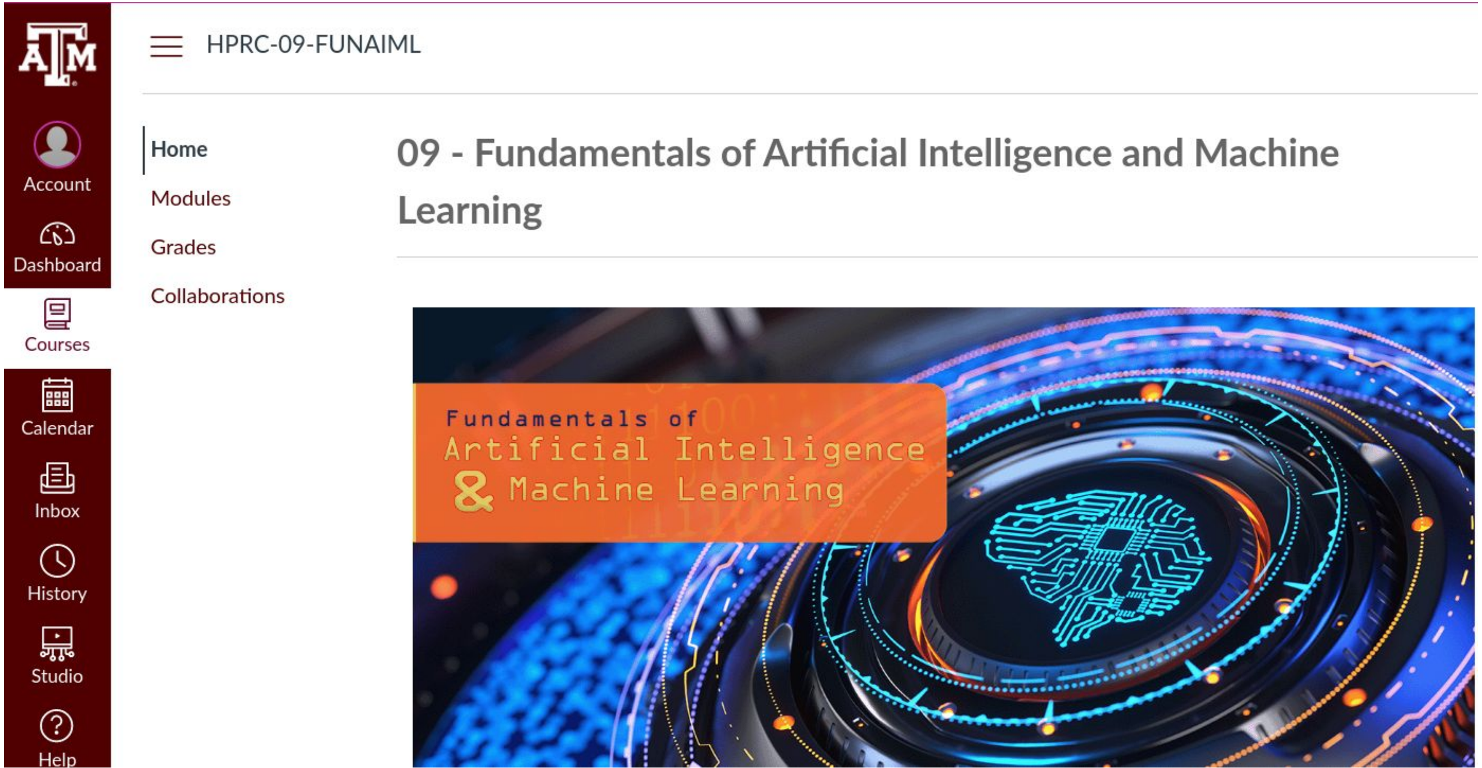
TEES EDGE
Professional Education

# Audience

- This program will eventually be publicly available
  - Currently: only TAMU members, by invitation

*We invite you to help us test our courses!*

# Canvas Learning Management System

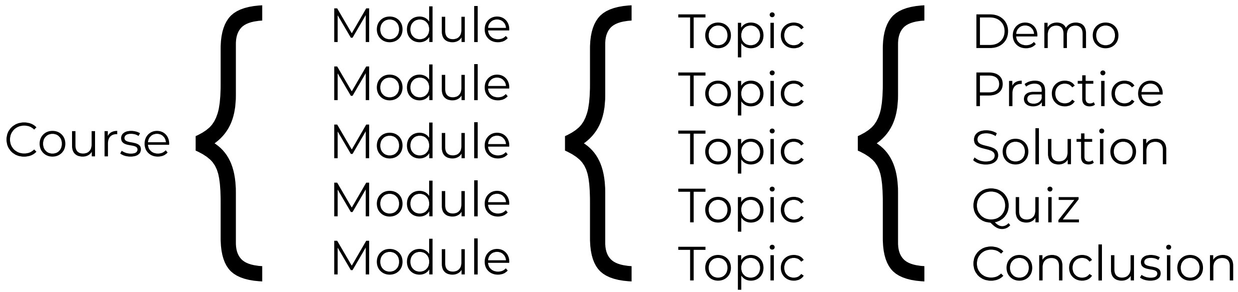


HPRC-09-FUNAIML

09 - Fundamentals of Artificial Intelligence and Machine Learning

# Online Course Structure

Online Courses are organized hierarchically.



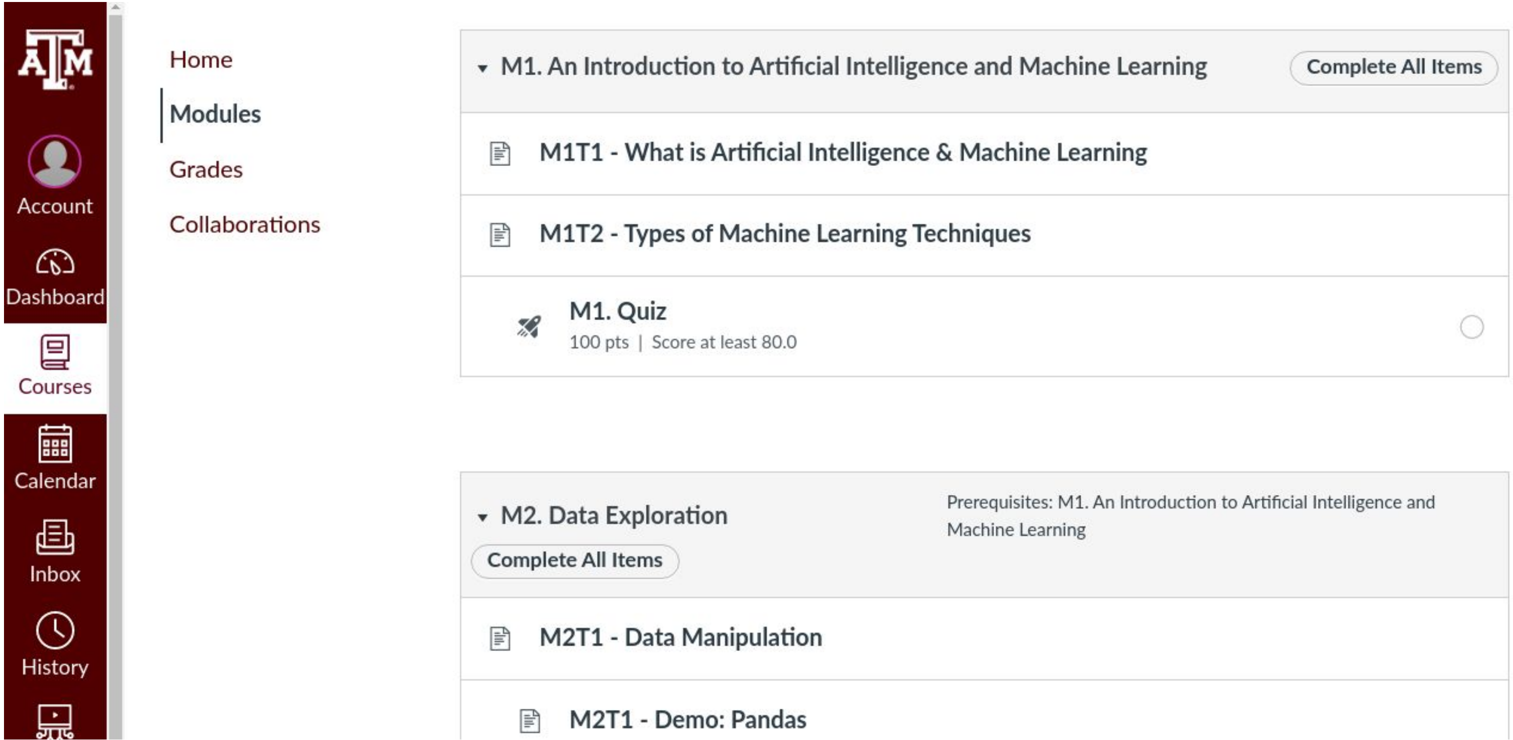
Course

Module
Module
Module
Module
Module

Topic
Topic
Topic
Topic
Topic

Demo
Practice
Solution
Quiz
Conclusion

# Example Course Hierarchy



▾ M1. An Introduction to Artificial Intelligence and Machine Learning — Complete All Items

- M1T1 - What is Artificial Intelligence & Machine Learning
- M1T2 - Types of Machine Learning Techniques
- M1. Quiz — 100 pts | Score at least 80.0 ○

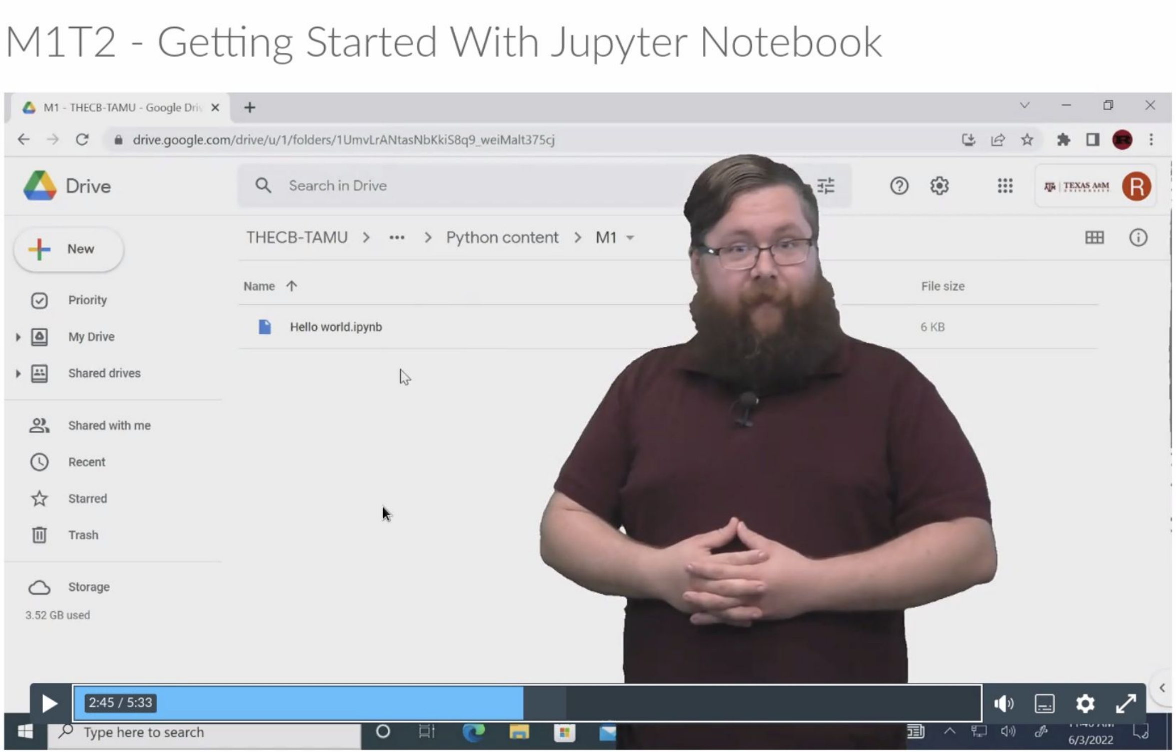
▾ M2. Data Exploration — Complete All Items — Prerequisites: M1. An Introduction to Artificial Intelligence and Machine Learning

- M2T1 - Data Manipulation
- M2T1 - Demo: Pandas

# Demo, Practice, Solution

- Each Topic has a cadence of course materials
  - Demo (a video lecture) 5-10 minutes
  - Practice 10-20 minutes
  - Solution (a video lecture) 5-10 minutes
- The student stays maximally engaged with minimal wait between activities.

# Example Demo Video



M1T2 - Getting Started With Jupyter Notebook

# Quizzes for Completion

- Each module has at least one quiz.
  - “about 5” questions selected at random from a pool of questions.
  - Retries are allowed, but the questions will vary.
- Passing the module quiz is required to proceed to the next module.
- Some courses also have a final quiz.
- Passing all quizzes (≥ 80%) is required to earn your micro-certificate.

# Table of Courses (1/2)

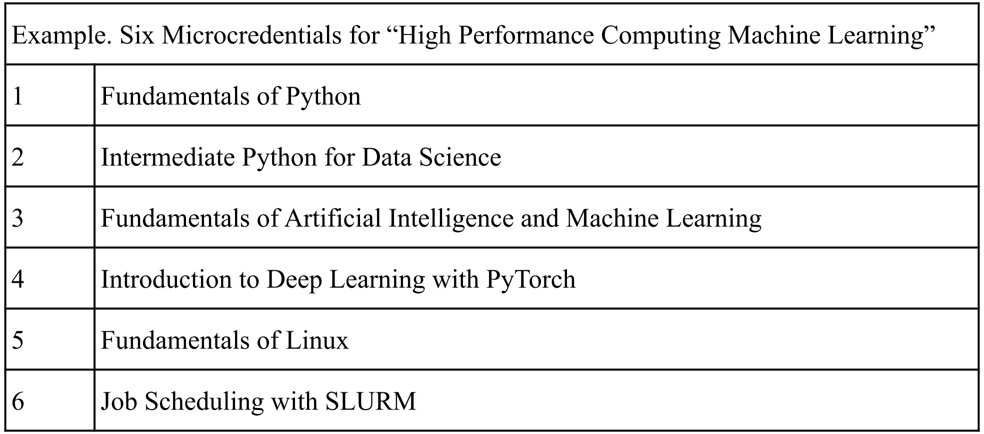
| Theme | Course Title | CIP CODE(s) | Duration | Delivery Mode |
|---|---|---|---|---|
| Cybersecurity | Fundamentals of Cybersecurity | 11.1003 | 0.3 PDU | Asynchronous |
| Coding | Fundamentals of Python | 11.0201 | 1 PDU | Both |
| | Intermediate Python for Data Science | 11.0202, 30.71 | 1 PDU | Both |
| | Advanced Python for Data Science | 11.0202, 30.71 | 0.5 PDU | Both |
| | Fundamentals R Programming | 11.0201 | 1 PDU | Both |
| | Intermediate R Programming | 11.0202 | 1 PDU | Both |
| | GPU Programming with CUDA | 30.3001 | 0.3 PDU | Live |
| AI/ML | Fundamentals of Artificial Intelligence and Machine Learning | 11.0102 | 0.3 PDU | Both |
| | Introduction to Deep Learning with TensorFlow | 11.0804, 11.0202 | 0.3 PDU | Both |
| | Introduction to Deep Learning with PyTorch | 11.0804, 11.0202 | 0.3 PDU | Both |
| | Using Scikit-Learn for Artificial Intelligence and Machine Learning | 11.0804, 11.0104, 11.0202 | 0.3 PDU | Both |

# Table of Courses (2/2)

| Theme | Course Title | CIP CODE(s) | Duration | Delivery Mode |
|---|---|---|---|---|
| Bioinformatics | RNA-seq and Differential Expression | 11.0104, 11.0401, 26.1103 | 0.3 PDU | Both |
| | Short Variant Discovery | 11.0104, 11.0401, 26.1103 | 0.3 PDU | Both |
| | Metagenomics | 11.0104, 11.0401, 26.1103 | 0.3 PDU | Both |
| | ChIP-seq | 11.0104, 11.0401, 26.1103 | 0.3 PDU | Both |
| Linux | Fundamentals of Linux | 11.0201 | 0.3 PDU | Both |
| | Linux for Administrators | 11.1006, 11.1001 | 0.3 PDU | Live |
| Cloud Computing | Job Scheduling with SLURM | 11.0103 | 0.3 PDU | Live |
| | Containers and Orchestration | 11.0103 | 0.3 PDU | Live |
| | Introduction to Cloud and Cluster Computing | 11.0103 | 0.3 PDU | Live |
| | Parallel Computing Using OpenMP | 11.0201 | 0.3 PDU | Asynchronous |
| | Parallel Computing Using MPI | 11.0201 | 0.3 PDU | Asynchronous |

# Stackable Courses

- Some short courses have prerequisites
- Stack microcredentials to build your own program



| Example. Six Microcredentials for "High Performance Computing Machine Learning" | |
|---|---|
| 1 | Fundamentals of Python |
| 2 | Intermediate Python for Data Science |
| 3 | Fundamentals of Artificial Intelligence and Machine Learning |
| 4 | Introduction to Deep Learning with PyTorch |
| 5 | Fundamentals of Linux |
| 6 | Job Scheduling with SLURM |

# Details about Specific Courses

# Cybersecurity

One course:

- Fundamentals of Cybersecurity

# Fundamentals of Cybersecurity

- This course covers fundamental concepts in cybersecurity

- M1 - Introduction and Security Trends
    - The security problem
    - Threats to security
    - Attributes of actors
    - Security trends
    - Targets and attacks
    - Approaches to cybersecurity

# Fundamentals of Cybersecurity

- M2 - General Security Concepts
  - Security basics
  - Security tenets
  - Security approaches
  - Security principes
  - Security models

- M3 - The Role of People in Security
  - Social engineering
  - Poor security practices
  - People as a security tool

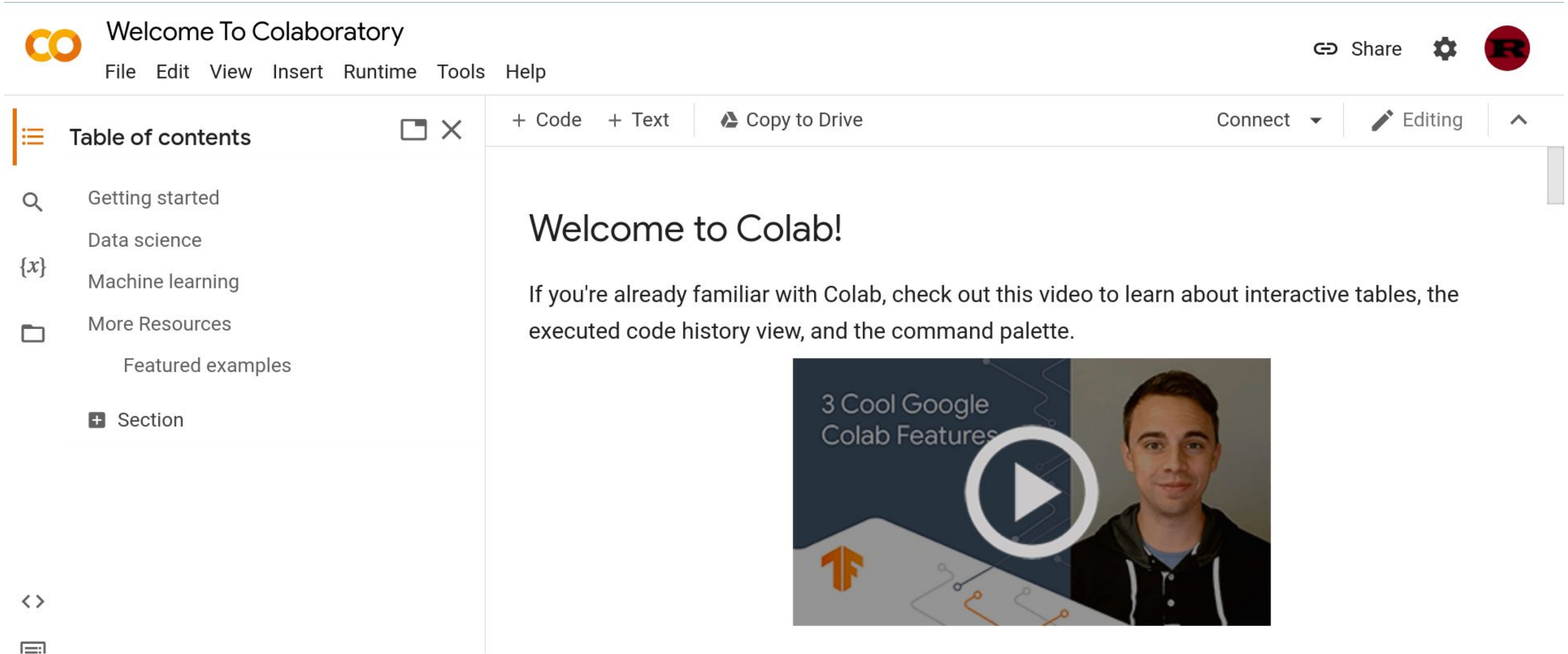
# Fundamentals of Cybersecurity

- M4 - Types of Attacks and Malicious Software
    - Avenues of Attack
    - Malware
    - Attacking Computer Systems
    - Advanced Persistent Threats
    - Tools
    - Auditing

# Python Programming

- Three courses:
  - Fundamentals of Python
  - Intermediate Python for Data Science
  - Advanced Python for Data Science
- Each course is a *prerequisite* for the next.
- Learning takes place using the Google Colab integrated development environment.
- Topics and exercises are selected to be relevant for scientific research applications.

# Google Colaboratory



Welcome to Colab!

If you're already familiar with Colab, check out this video to learn about interactive tables, the executed code history view, and the command palette.

# Fundamentals of Python

- 10 hours
- This course covers the most important core components of Python programming at the introductory level.
- Students will learn fundamental programming concepts such as variables, data structures, flow control, and object-oriented programming.

# Fundamentals of Python

- Using Google Colaboratory
- Variables
- Data Types
- User Input
- Operations
- Control structures
- Errors and Files
- Lists
- Dictionaries
- Classes
- Modules

# Intermediate Python for Data Science

- 10 hours
- This course covers a selection of scientific programming tools commonly used in Python programming at the intermediate level.
- Students will learn research techniques such as manipulating and visualizing data, exploring functions, modeling, and retrieving data from the internet.
- *Prerequisite: Fundamentals of Python*

# Intermediate Python for Data Science

- Arrays with NumPy
- Plotting with Matplotlib
- Mathematics with SciPy
- Data Tools with Pandas
- Web Scraping

# Advanced Python for Data Science

- 3 hours
- This course covers a selection of scientific programming tools commonly used in Python programming at the advanced level.
- Students will learn research techniques such as handling multidimensional data, and parallelization.
- *Prerequisite: Intermediate Python for Data Science*

# Advanced Python for Data Science

- Arrays with Xarray
- Parallelization with Dask

# Artificial Intelligence and Machine Learning

- Four courses:
  - Fundamentals of Artificial Intelligence and Machine Learning
  - Using Scikit-Learn for Artificial Intelligence and Machine Learning
  - Introduction to Deep Learning with TensorFlow
  - Introduction to Deep Learning with PyTorch
- The four courses are *independent* of each other.
- *Recommended* prerequisite: Intermediate Python
- Learning takes place using the Google Colab integrated development environment.

# Fundamentals of Artificial Intelligence and Machine Learning

- Introduction to AI/ML
    - What is AI/ML and their Relationship
        - AI and ML Description
        - Relationships
    - Terminology
        - Data Formats
        - Types of Data
            - Labeled Data
            - Unlabeled Data
        - What is training?
        - What is testing?
        - Common types of Learning

# Fundamentals of Artificial Intelligence and Machine Learning

  - Types of ML techniques
    - Supervised learning
      - Regression
      - Classification
    - Unsupervised learning
      - Clustering
- Data Exploration
  - Data Manipulation with Pandas
    - Demo
    - Practice
  - Data Visualization with Matplotlib
    - Demo
    - Practice

# Fundamentals of Artificial Intelligence and Machine Learning

- Application of ML techniques
  - Demo 1: Predict House Prices
  - Practice 1: Linear Regression
  - Demo 2: Classify Handwritten Digits
  - Practice 2: Classification
  - Demo 3: Build a Clustering Model
  - Practice 3: Clustering
- Final Assessment

# Using SciKit-learn for Artificial Intelligence and Machine Learning

- Introduction to ML Algorithms
    - Linear Regression
        - Guided Practice
    - Logistic Regression
        - Guided Practice
    - Support Vector Machine
        - Guided Practice
    - K-Means Clustering
        - Guided Practice

# Introduction to Deep Learning with TensorFlow

- Overview of AI/ML/DL
  - What is Deep Learning and Its Advantages
  - Learning Principle of DL
  - Convolution
  - Pooling
  - Convolutional Neural Network (CNN)
- TensorFlow
  - TensorFlow Introduction
  - TensorFlow Keras API
  - Demo 1: Get Started with TensorFlow
  - Demo 2: Classify Handwritten Digits with TensorFlow

# Introduction to Deep Learning with PyTorch

- Overview of AI/ML/DL
  - What is Deep Learning and Its Advantages
  - Learning Principle of DL
  - Convolution
  - Pooling
  - Convolutional Neural Network (CNN)
- PyTorch
  - PyTorch Introduction
  - Major Components
  - Demo 1: Get Started with PyTorch
  - Demo 2: Classify Fashion MNIST with PyTorch

# R Programming

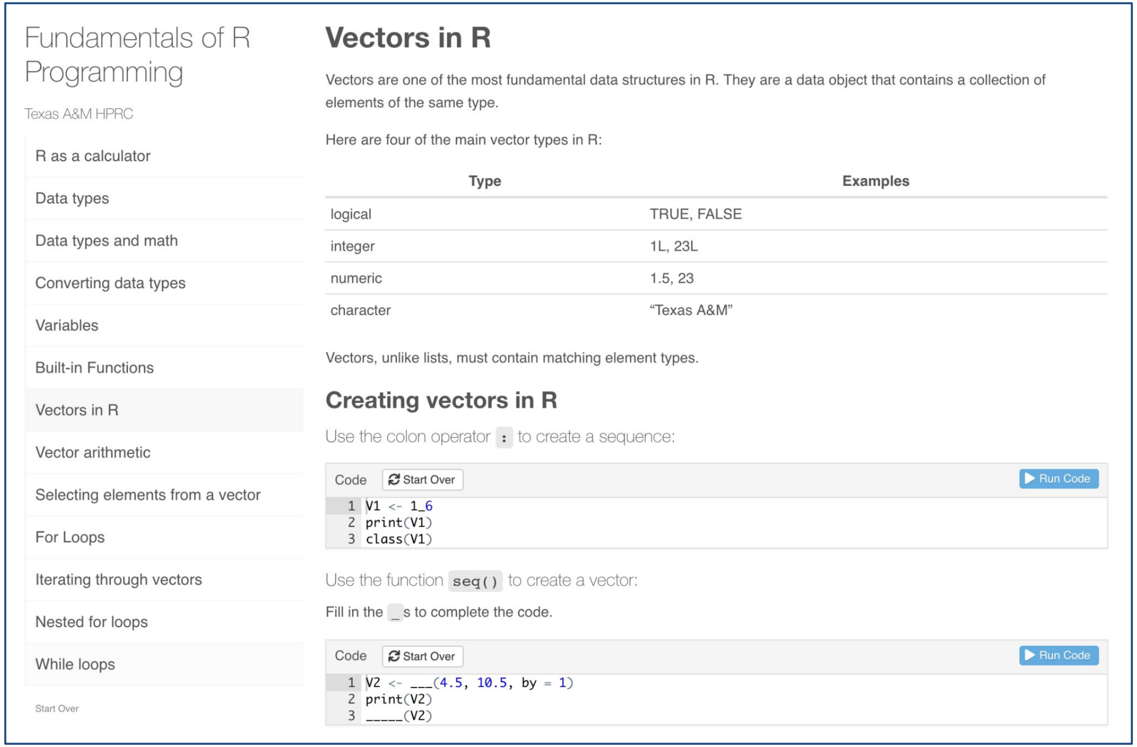
- Two courses:

1. Fundamentals of R Programming
2. Intermediate R Programming

- The first is a *prerequisite* for the second.

# Fundamentals of R Programming

- 6 hours
- RStudio
- Topics Covered:
  - Data types
  - Variables
  - Built-in Functions
  - Vectors
  - Loops



Fundamentals of R Programming

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- R as a calculator
- Data types
- Data types and math
- Converting data types
- Variables
- Built-in Functions
- Vectors in R
- Vector arithmetic
- Selecting elements from a vector
- For Loops
- Iterating through vectors
- Nested for loops
- While loops

Start Over

## Vectors in R

Vectors are one of the most fundamental data structures in R. They are a data object that contains a collection of elements of the same type.

Here are four of the main vector types in R:

| Type | Examples |
|---|---|
| logical | TRUE, FALSE |
| integer | 1L, 23L |
| numeric | 1.5, 23 |
| character | “Texas A&M” |

Vectors, unlike lists, must contain matching element types.

### Creating vectors in R

Use the colon operator `:` to create a sequence:

```
V1 <- 1_6
print(V1)
class(V1)
```

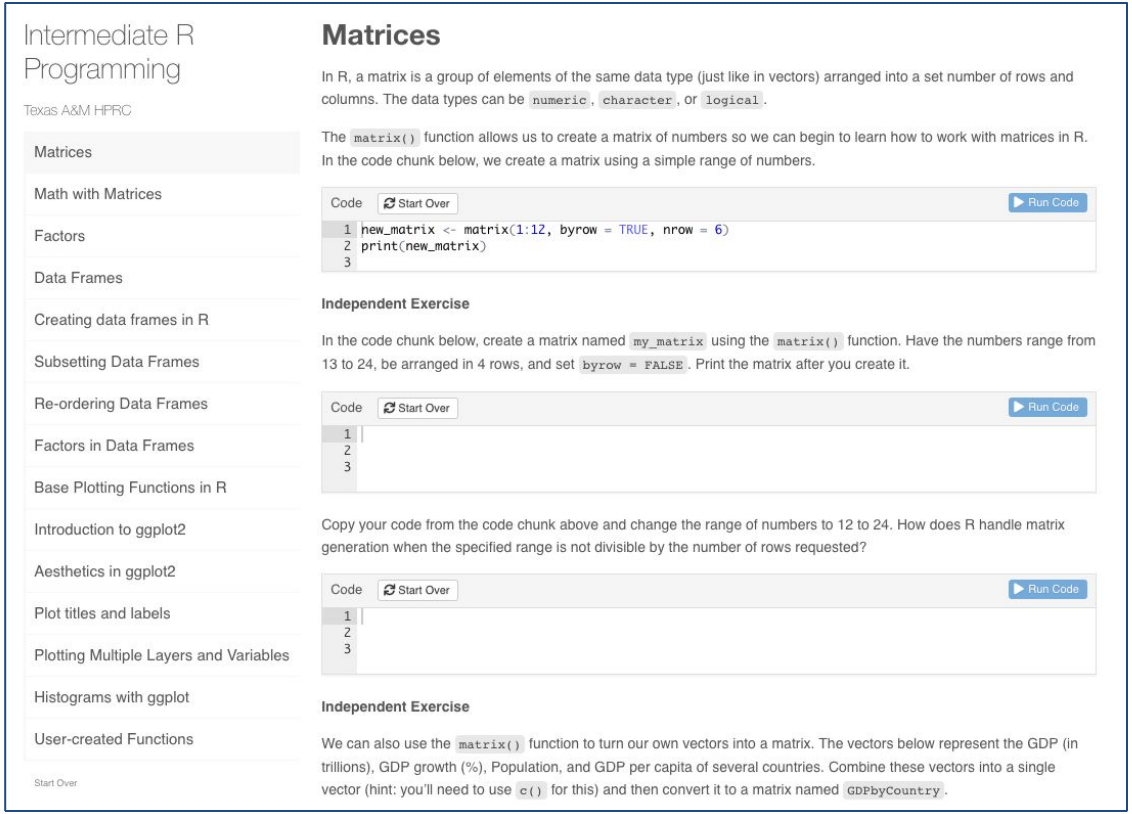
Use the function `seq()` to create a vector:

Fill in the `_`s to complete the code.

```
V2 <- ___(4.5, 10.5, by = 1)
print(V2)
_____(V2)
```

# Intermediate R Programming

- 6 hours
- RStudio
- Topics Covered:
    - Matrices
    - Factors
    - Data frames
    - Base plotting
    - ggplot2
    - User-created functions



## Matrices

In R, a matrix is a group of elements of the same data type (just like in vectors) arranged into a set number of rows and columns. The data types can be `numeric`, `character`, or `logical`.

The `matrix()` function allows us to create a matrix of numbers so we can begin to learn how to work with matrices in R. In the code chunk below, we create a matrix using a simple range of numbers.

```r
new_matrix <- matrix(1:12, byrow = TRUE, nrow = 6)
print(new_matrix)
```

**Independent Exercise**

In the code chunk below, create a matrix named `my_matrix` using the `matrix()` function. Have the numbers range from 13 to 24, be arranged in 4 rows, and set `byrow = FALSE`. Print the matrix after you create it.

Copy your code from the code chunk above and change the range of numbers to 12 to 24. How does R handle matrix generation when the specified range is not divisible by the number of rows requested?

**Independent Exercise**

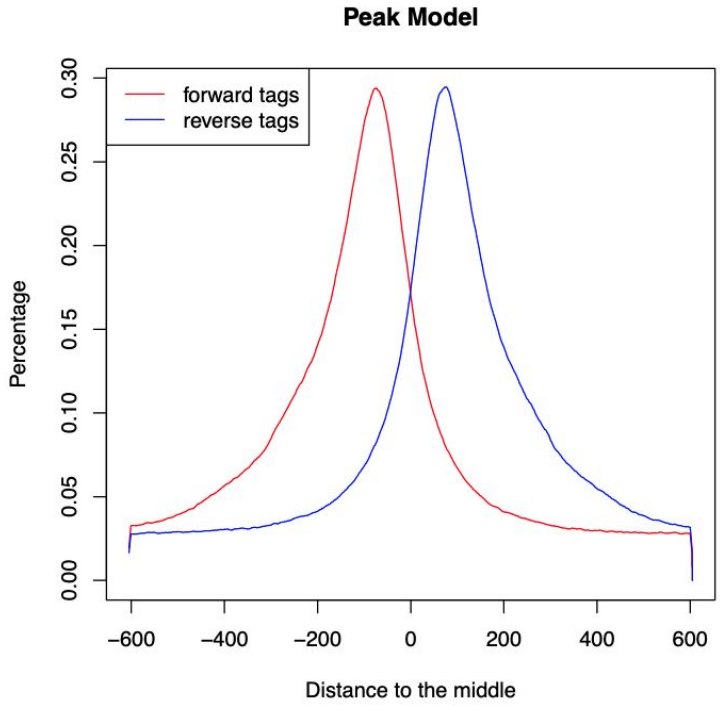
We can also use the `matrix()` function to turn our own vectors into a matrix. The vectors below represent the GDP (in trillions), GDP growth (%), Population, and GDP per capita of several countries. Combine these vectors into a single vector (hint: you'll need to use `c()` for this) and then convert it to a matrix named `GDPbyCountry`.

# Biology Applications

- Four courses:
  - Introduction to ChIP-seq
  - Short Variant Discovery
  - Introduction to Metagenomics
  - RNA-seq and Differential Expression
- These four courses are *independent* of each other

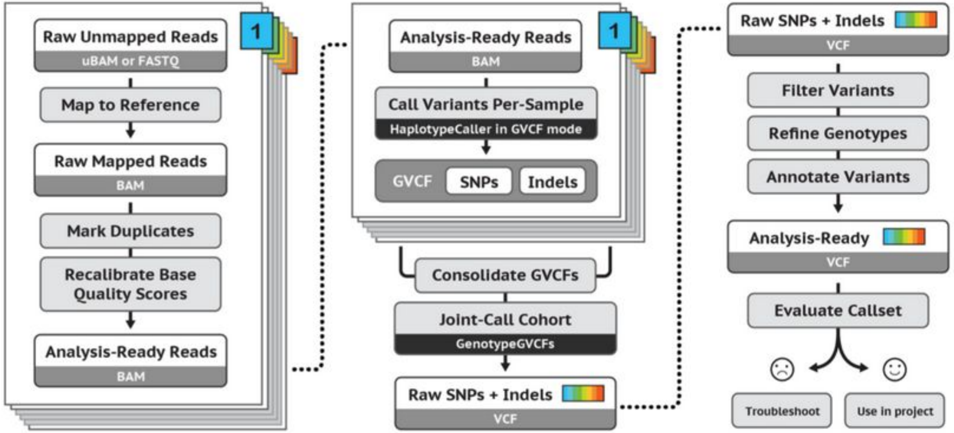
# Introduction to ChIP-seq

- 3 hours
- ChIP-seq experiment overview
- Commonly used software
- Bioinformatics on the Grace Cluster
- Full ChIP-seq pipeline
  - Library QC and Trimming
  - Read mapping
  - ChIP-QC
  - Peak calling



# Short Variant Discovery

- 5 hours
- Commonly used software
- Bioinformatics on the Grace cluster
- Step-by-step through GATK
  - Library QC and Trimming
  - Alignment and processing
  - Per-sample variant calling
  - Cohort sample calling
  - Variant filtering



https://gatk.broadinstitute.org/hc/en-us/articles/360035535932-Germline-short-variant-discovery-SNPs-Indels-

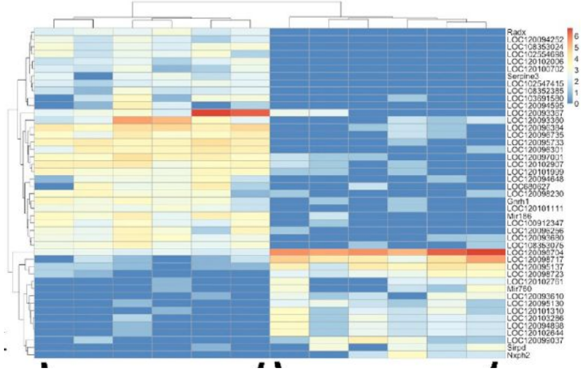
# Introduction to Metagenomics

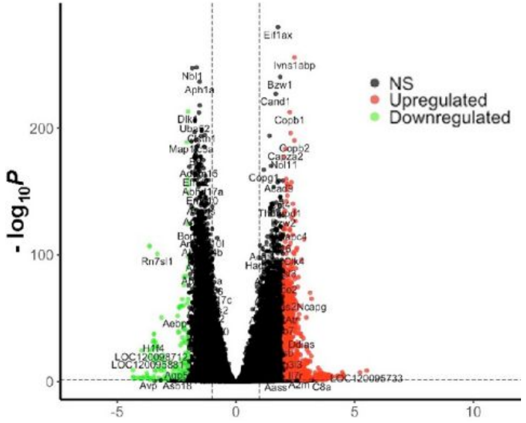
- 3 hours
- Metagenomics sequencing strategies
- Commonly used software
- Full pipeline for marker gene analysis (16s) with QIIME2
  - QIIME2 terminology/format
  - Importing data
  - Denoising and filtering
  - Diversity analyses
  - Taxonomic classification

https://qiime2.org/

# RNA-seq and Differential Expression

- 4 hours
- Discuss commonly used RNA-seq software
- Experimental Design
- Full Differential Expression Pipeline
  - Illumina library processing
  - Short-read mapping
  - Count generation
  - Differential expression analysis in R
  - Data visualization in R





Orzabol et al. 2022

# Demonstrations of Online Course Elements

*time permitting*

# Acknowledgements

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