

Machine Learning and AI for Scientists Tutorial (MAST) Series

December 8, 2021

Welcome to the MAST Beginner Tutorials!

- The beginner series is designed for people with little experience in machine learning and Python.
- During the talks, please use chat for your questions.
- Please keep your microphone muted.
- At the end of the talk, we welcome verbal questions/discussion

MONDAY, 6 DECEMBER	
12:00 PM → 2:00 PM	Basic Python, including installation and usage
WEDNESDAY, 8 DECEMBER	
12:00 PM → 2:00 PM	Basic NumPy (numerical Python), including usage and best practices
FRIDAY, 10 DECEMBER	
12:00 PM → 2:00 PM	Introduction to Machine Learning
MONDAY, 13 DECEMBER	
12:00 PM → 2:00 PM	Introduction to automatic gradient-enabled tensors using PyTorch, and your first neural networks
WEDNESDAY, 15 DECEMBER	
12:00 PM → 2:00 PM	A first use case: convolutional neural networks for image classification

What is MAST?

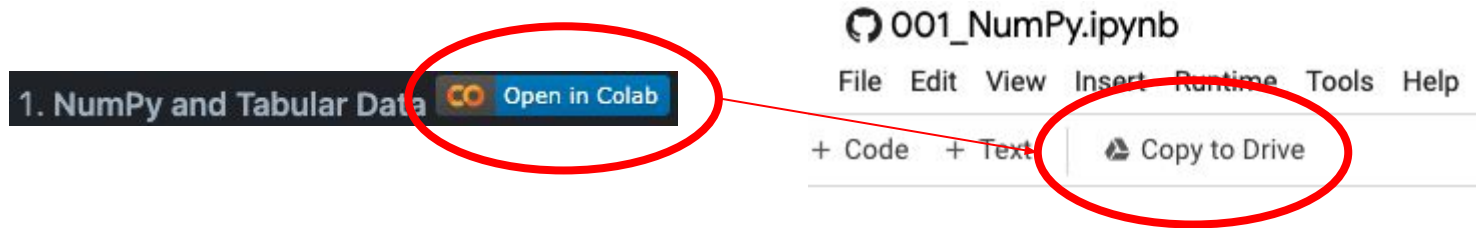
- **Machine learning and AI for Scientists Tutorials**
 - December 6-15: beginner series
 - Up next (Early 2022): intermediate series
 - Later (June 2022): Nvidia AI bootcamp (advanced series)
- Part of the Center for Computing Sciences Education and Support (CCSES) led by Nick D'Imperio at the Computational Science Initiative (CSI)
 - Goal: leveraging BNL AI/ML expertise for collaborations and education within BNL and external parties
- Also part of the lab-wide AI/ML Working Group

Goals of the beginner series

- You will perhaps start thinking about Python differently than you might have before: e.g., best practices in Python and how they apply to data science and machine learning.
- You will learn what machine learning *is*, and the types of problems it can be applied to.
- You'll understand the basics of the PyTorch automatic gradient (auto-grad) engine.
- Finally, you will see and understand a classic example: using convolutional neural networks to classify images.

Resources

- Tutorial notebooks can be found on Github
 - <https://github.com/x94carbone/AIML-tutorials> (see **master** branch)
- You can use Google Colab to open the notebooks directly



- Please use Slack for any questions, comments or discussion after the presentations
- Future resources: “office hours” for ML/AI consulting and collaborations (still developing)

Today's speaker: Matt Carbone



- PhD in chemical physics, Columbia University, 2021
- Assistant Computational Scientist, Machine Learning and Computations Group at CSI
- Focus on AI/ML techniques as applied to spectroscopy, and theoretical condensed matter