Deciphering Nature from Data: An Applied Machine Learning course (and little bit of AI) .

An immersive five-day journey into the world of artificial intelligence (AI) and machine learning (ML) . This course is a blend of theoretical knowledge, intuitions and practical examples from physics , biology and other fields. Designed to deepen your understanding and application of AI and ML in your own field.

Program Overview

Day 1: Teaching machines from data

- **An Historical Overview** From the epic of Gilgamesh to Ada Lovelace, the first programmer. From ancient myths to modern AI, exploring the evolution of computational thought and its impact on contemporary technology.
- Clarify the **distinctions between AI, ML, and Deep Learning**, demystifying these terms for a clear understanding of their unique roles and interrelations.
- Introduction to supervised and unsupervised learning, illustrating the different approaches to teaching machines from data.
- Classification and regression, understanding how machines can categorize data and predict outcomes.
- Model evaluation techniques, learning how to assess the performance and accuracy of models.

Day 2: Unsupervised Machine Learning

- How to visualize multidimensional data?
- Principal Component Analysis (PCA), a cornerstone of dimensionality reduction, connections with classical mechanics, its limitations and applications.
- Understand how PCA serves as a stepping stone to more sophisticated algorithms that unveil hidden patterns in complex data sets.
- Explore the manifold hypothesis and various graph dimensionality reduction techniques, unlocking new ways to visualize and comprehend multi-dimensional data.
- Introduction to embeddings and their role in simplifying complex data structures for better analysis and visualization.
- Discuss clustering algorithms and their significance in grouping data without predefined labels, showcasing their utility in diverse fields like physics and biology.
- Examples to illustrate how clustering helps in discovering natural groupings and patterns within data.

Day 3: Do Neural Networks Dream?

- **From Perceptrons to Advanced Neural Networks**

    - Journey through the development of neural networks, starting from the first artificial neuron to sophisticated modern architectures.
    - The universal approximation theorem, highlighting the capabilities and theoretical limits of neural networks.
- **Evaluation and Validation of Models**
    - Cover the essentials of model evaluation in the context of supervised learning, emphasizing the importance of accuracy and reliability.
    - Introduction to cross-validation methods, offering insights into techniques for assessing the generalizability of neural network models.
- **Diverse Architectures of Neural Networks**
    - Explore various types of neural networks, understanding their unique structures and functionalities.
    - Provide a glimpse into how different neural network architectures are suited to specific tasks.

Day 4: How do Neural Network "think"?

- **Learning Mechanisms of Neural Networks**
    - Examine how neural networks learn, with a layer-by-layer analysis of their structure and function using the embedding techniques from Day 2.
    - Discuss the concept of learning in the context of neural networks, demystifying how they adapt and improve over time.
- **Neural Networks and Differential Equations**
    - Explore the recent connection found between neural networks and differential equations, particularly focusing on neural ordinary differential equations (ODEs).
    - Discuss the implications of this connection for scientific research and practical applications, bridging the gap between traditional mathematical models and modern AI techniques.
- **Scientific Machine Learning**
    - Introduction to the field of scientific machine learning, no more black boxes.
    - Differentiable programming.
    - How neural networks can complement and enhance traditional scientific models, offering new perspectives and solutions to complex problems.

Day 5: The Raise of the Transformers

- **The Transformative Role of Neural Networks in Language**
  - The evolutions of neural networks on Natural Language Processing (NLP), highlighting the advancements brought about by Transformer architectures.
  - The role of dimensionality reduction techniques in NLP, facilitating the processing and analysis of linguistic data and how "logic" emerges.
  - The emergence of Large Language Models, (technologies like ChatGPT) and their significance in reshaping the landscape of communication, information processing and science.

This course is designed to be a non formal introduction to AI and ML, suitable for both beginners and those seeking to deepen their understanding through practical examples and applications across various scientific domains. You'll leave not only with theoretical insights and intuitions but practical knowledge, equipped with Python and Julia code snippets for hands-on experimentation.
Among the examples of applications of ML in science that will be shown. a few are extracted from these works where the instructor was involved.

- Nuñez, Matias. "Exploring materials band structure space with unsupervised machine learning." *Computational Materials Science* 158 (2019): 117–1
- Nuñez, Matias, Weht, Ruben, & Nunez-Regueiro, Manuel. "Searching for electronically two-dimensional metals in high-throughput ab initio databases." *Computational Materials Science* (2020).
- Barber, Jesse R., Rubin, Juliette J., ..., Nuñez, Matias, Kawahara, Akito Y., et al.. "Anti-bat ultrasound production in moths is globally and phylogenetically widespread" , Proceedings of the National Academy of Sciences (PNAS) (2022).
- Nuñez, Matías, Barreiro, Nadia L., Barrio, Rafael A., & Rackauckas, Christopher. "Forecasting virus outbreaks with social media data via neural ordinary differential equations." *Scientific Reports* volume 13, Article number: 10870 (2023).
- Cornaglia, Pablo S., Nuñez, Matias, & Garcia, D. J. "Unveiling exotic magnetic phases in Fibonacci quasicrystals through machine learning." *Phys. Rev. B* 108,

144429 (2023).

About the instructor**:

Dr. Matias Nuñez is a researcher at the Consejo Nacional de Investigaciones Cientificas y Tecnologicas (CONICET) in Argentina, holding a Ph.D. in Physics from North Carolina State University, USA, and a M.S. from the infamous Instituto Balseiro, in Bariloche, Argentina. He is deeply involved in applied science at the Centro Atomico Bariloche and at the Institute of Biodiversity and Environment Research (INIBIOMA). His research interests are diverse, covering electronic structure calculations, material science, complex systems, and the application of machine learning in biology and physics. Dr. Nuñez is at the forefront of innovative projects, leading a multidisciplinary team under Fundación Manuel Sadosky to address real-world challenges using AI technologies, and merging researchers with the private sector to solve specific problems. He has established collaborations with companies such as Neufitech and URBAN inc, focusing on utilizing AI and machine learning to enhance communication abilities (link to news article) and analyze urban patterns from images for social simulations. Dr. Nuñez is collaborating with the group led by Dr. Aurora Hernández-Machado at the University of Barcelona, focusing on augmenting their fluid dynamics calculations through the application of machine learning techniques. Through his work, Dr. Nuñez effectively bridges the gap between theoretical research and practical applications, contributing to advancements in various scientific domains.

When he is not working, Dr. Nuñez is probably playing in Nature.