



diiP Summer School

2024

Introduction AI for Research

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- My name is Yvonne Becherini
- I am an Astroparticle Physicist
- I work at University of Paris Cité, <u>Laboratoire Astroparticule et Cosmologie &</u> <u>Data Intelligence Institute of Paris</u>
- My principal interests are
 - Astroparticle Physics
 - Gamma-Ray & Neutrino Astronomy
 - Extragalactic sources
- I develop Data Analysis methods with Machine Learning
- I give two courses: Applied Data Analytics and Advanced Applied Data Analytics on Zoom.



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Applied Data Analytics

Monday	Tuesday	Wednesday	Thursday	Friday
09/10/23	10/10/23	11/10/23	12/10/23	13/10/23
10h00-11h20 Introduction Objective of the course	10h00-11h20 Classic supervised Learning	10h00-11h20 Classic Supervised Learning Regression	10h00-11h20 Neural Networks	10h00-11h20 Unsupervised Learning & Generative Models
11h20-11h30	11h20-11h30	11h20-11h30	11h20-11h30	11h20-11h30
Break and	Break and	Break and	Break and	Break and
Poll 🥗	Poll 🥗	Poll 🥗	Poll 🥗	Poll 🥗
11h30-13h00 Data preparation	11h30-13h00 Classic supervised Classification	11h30-13h00 Notebooks	11h30-13h00 Deep Learning	11h30-13h00 Students present their data analysis challenges

Advanced Applied Data Analytics

Monday	Tuesday	Wednesday	Thursday	Friday
22/01/24	23/01/24	24/01/24	25/01/24	26/01/24
10h00-11h20 Introduction Objective of the course (Review of some basic topics)	10h00-11h20 Visualization of the latent space Variational Autoencoders	10h00-11h20 Graph Neural Networks	10h00-11h20 Bayesian Deep Learning	10h00-11h20 Self-supervised Learning
11h20-11h30	11h20-11h30	11h20-11h30	11h20-11h30	11h20-11h30
Break and	Break and	Break and	Break and	Break and
Poll 🥗	Poll 🥗	Poll 🥗	Poll 🥗	Poll 🥗
11h30-13h00 Generative Adversarial Networks	11h30-13h00 Transformers	11h30-13h00 Graph Embedding Methods	11h30-13h00 Bayesian Deep Learning	11h30-13h00 Self-supervised Learning

Monday	Tuesday	Wednesday	Thursday	Friday
	Supervised Learning	Knowledge-guided Data Science	Anomaly detection for Time Series	Generative Adversarial Networks
	Al in Medicine/Biology		Al in Industry	Al in Particle Physics
Large Language Models	Representation Learning	High-Dimensional Vector Similarity Search	Graph Neural Networks	
Social Dinner		Bateau Mouche		

... and now the Summer School!

The goal is to understand:

- → The mechanisms of generation of energy in the Universe
- → The creation and propagation of energetic particles in the Universe: gamma-rays, neutrinos, protons
- → The nature of Dark Matter



Methods used:

- Observation of phenomena through ultra-precise and ultra-sensitive particle detectors
- → The analysis of the data acquired is often complex for one main reason: the signal searched is tiny, compared to a huge amount of background

Very High Energy Gamma Ray Astronomy Experiments

- Observations are made:
 - With <u>Imaging Atmospheric Cherenkov</u> <u>Telescopes</u> detecting the Cherenkov light generated in the atmosphere by the passage of highly relativistic charged particles
 - <u>Wide field of view detector arrays</u>: Surface detectors catching the particles in the atmospheric showers
- Gamma rays from astrophysical sources are rare, and at the same time we receive a huge amount of background events from cosmic rays (very similar)
- The amount of data generated can be huge: several TB per month



After data are calibrated, we need to perform the reconstruction of the kinematics of the gamma ray: incoming direction and energy

This can be done with algorithms or using ML regression

Regression is a method allowing to estimate the value of a variable associated with the signal (or the background).

With the help of simulations and data analysis, we can infer what the values expected for a particular event are

When we run the reconstruction algorithms, we run them on all data, i.e. on all gamma ray signal and all proton background events.

Then everything is passed to the next step, the suppression of the background



Extract a rare "signal" in the presence of a large amount of noise, which is equivalent to finding a needle in a haystack

Need to develop powerful methods to extract these rare events.

For most problems, after having cleaned properly the data, the answer is

• Event classification through user-defined features

But if you wish to achieve a better classification performance in difficult analysis regions, better to switch to Deep Learning

 \rightarrow Y. Becherini et al., Astroparticle Physics (2011) \rightarrow M. Senniappan, Y. Becherini et al, JINST (2021)

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The HESS telescope array is located in Namibia and is a 5-tel array of Imaging Atmospheric Cherenkov Telescopes detecting the Cherenkov light created in the atmosphere by the passage of highly relativistic charged particles.

One of the most crucial steps in the analysis of data, is the suppression of the cosmic ray background to extract the "signal" of gamma-rays.









Gamma/Proton classification in H.E.S.S. data

• Supervised feature-based ML

Experimental Image

Camera Display

Simulated Gamma-Ray

Real Hadron

- Classification of gamma-rays and protons using a set of user-defined input variables
- The algorithm performing the separation is the Boosted Decision Trees method.



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BDT response

<u>"A new analysis strategy for detection of faint</u> gamma-ray sources with Imaging Atmospheric Cherenkov Telescopes", Astroparticle Physics, (2011)

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BDT response

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Camera Display



- The final response of the algorithm to an independent set of data (test data) allows defining an analysis cut before looking at the real data.
- The final analysis cut can be based on a desired gamma-ray efficiency. Example: if I say I will cut at 0.4 on the right plot, I will have 95% of gamma-rays and a contamination of less than 1% of protons.
- When the analysis cuts are frozen, you are allowed to look at the real data.



The Active Galactic Nucleus Centaurus A



2008: discovery with a detection significance of 5σ with standard analyses (no ML)



2016: Re-analysis of data using supervised ML 9.8σ!

Appearance of a second source in the field of view!



A clear gain in the detectability of gamma-ray emitting sources

Current contributions to the field through the diiP Chair





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Key Points

• LLMs are advanced models trained on massive text data to understand and generate human language.

Today

- They are used in applications such as chatbots, automated content creation, and language translation.
- Examples include GPT-4 and BERT, both of which have shown impressive capabilities in language processing tasks.
- Key concepts include transformers and attention mechanisms, which allow for efficient processing of long-range dependencies in text.

Today

LLMs can automatically summarize large volumes of text, highlighting key points concisely.

This helps researchers quickly understand the core of the research, saving time and aiding in relevance assessment. LLMs like GPT can be integrated into Electronic Health Record (EHR) systems to help doctors generate comprehensive patient notes during consultations, reducing the time spent on paperwork.

Legal professionals use LLMs for efficient document review and legal research. E-commerce leverages LLMs for product descriptions and customer interactions.

Finance sectors simplify financial reporting and customer support with LLMs.

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Education can benefit from intelligent tutoring systems and educational content generation using LLMs.

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Tuesday _____ dij

"Train on Labeled Data to Make Accurate Predictions"



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Supervised learning utilizes **labeled data**, where each example is paired with an output label.

It is used for both classification tasks

(e.g., image recognition) and **regression** tasks (e.g., predicting house

Common algorithms include **linear** regression, logistic regression, support vector machines, and neural networks.



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The data is typically split into **training**, validation, and test sets to evaluate

model performance.

Overfitting occurs when a model learns
the training data too well, capturing
noise instead of the underlying pattern.



Tuesday



"Discover underlying patterns and features in data for various machine learning tasks"



NLP Applications

Includes tasks like translation and sentiment analysis.

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Word Embeddings

Used in NLP to represent words in dense vector spaces, capturing semantic meanings.



Computer Vision Applications

Includes tasks like object detection and image classification.

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Feature Discovery

Trains models to automatically discover features from raw data.



Autoencoders

Learn efficient codings of input

data by compressing and

reconstructing it.



Reduced Need for Manual Engineering

Reduces the need for manual

feature engineering.

Wednesday



"Integrate domain-specific knowledge into data science for improved accuracy and better interpretability"

Uses techniques like **rule-based systems** and

hybrid models for better decision-making processes.

Applied in fields such as healthcare and

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environmental science to leverage specific domain expertise.



science to enhance model performance and interpretability.

Integrates domain knowledge into data



Enhances data-driven insights with expert knowledge for more accurate and reliable

outcomes.

Facilitates better understanding of data

 patterns and trends through domain-specific knowledge.

Wednesday



"Find Similarities Fast in Complex Data with High-Dimensional Vector Search"

Techniques like Approximate Nearest Neighbors (ANN) help in finding similar vectors in high-dimensional spaces.

Locality-Sensitive Hashing (LSH) is used to hash input items so that similar items map to the same buckets with high probability.

Applications include recommendation systems where user preferences are matched with similar items, and image retrieval systems that find images with similar features.

Key concepts include vector spaces, where data points are represented as vectors, and similarity metrics, which measure how alike two vectors are.



"Identify unexpected patterns and outliers in time series"

Anomaly detection in time series identifies unusual patterns that deviate from expected behavior.

Methods include statistical models (e.g., ARIMA), machine learning models (e.g., isolation forest), and deep learning models (e.g., LSTM).

Applications include financial fraud detection, where unusual transactions are flagged, and equipment failure prediction, where abnormal sensor readings indicate potential issues.

Key concepts involve understanding time series data, seasonality (regular patterns), and trend analysis (long-term movement).

Thursday _____

GNNs are neural networks designed to work with graph-structured data, capturing relationships between nodes and edges. Techniques include Graph Convolutional Networks (GCNs) which apply convolution operations on graphs, and Graph Attention Networks (GATs) that use attention mechanisms.

Applications include social network analysis, where GNNs help to understand user interactions, and drug discovery, where they model molecular structures. Key concepts include nodes (entities), edges (relationships between entities), and graph embedding (vector representation of nodes in a graph).



Friday



GANs consist of two neural networks, a generator and a discriminator, that compete against each other.

Applications include image generation, data augmentation, and style transfer.

The generator creates fake data samples, while the discriminator tries to distinguish between real and fake samples.

Key concepts involve adversarial training, where the generator and discriminator are trained simultaneously.

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Training Process

Involves techniques like backpropagation for error correction and gradient descent for optimizing the model. Key for model accuracy.

Convolutional Networks

data, such as images. Utilize

Specialized for processing grid-like

convolutional layers to detect features.

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Feedforward Networks

Simplest type, where connections do not form cycles. Used in applications like image and speech recognition.

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Recurrent Networks

Designed for sequential data, like time series or text. They have loops to maintain memory of previous inputs.



Neural Networks

Basic types include feedforward, convolutional, and recurrent neural networks, each suited for different tasks.

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Regularization Techniques

Methods like dropout and batch normalization help prevent overfitting and improve model generalization.



The latent space is an abstract multidimensional space that encodes a meaningful internal representation of externally observed events Samples that are similar "in the external world" are positioned close to each other in the latent space.

🔬 Latent space

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In the feature extraction phase, the model has captured the important patterns of the input that are needed for the image classification task.

In the latent space, images that depict the same object have very close representations.

Generally, the distance of the vectors in the latent space corresponds to the semantic similarity of the raw images.

The green points correspond to the latent vector of each image extracted from the last layer of the model.

We observe that vectors of the same animals are closer to the latent space.

Therefore, it is easier for the model to classify the input images using these feature vectors instead of the raw pixel values.



But ... difficult to interpret the latent space meaning

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Normalization

Scaling data to a standard range to improve the performance of machine learning algorithms.

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Transformation

Converting data into a suitable format or structure for analysis.

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Cleaning

Removing or correcting errors and inconsistencies in the data to ensure quality.

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Exploratory Data Analysis (EDA)

Using statistical summaries and visualization techniques to understand data patterns and distributions.

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Data Preprocessing

Involves cleaning, normalization, and transformation of raw data to prepare it for analysis.

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Model Evaluation

Assessing model performance using metrics like accuracy, precision, recall, and cross-validation.



