

# **Institut Pascal**

## **Learning to Discover**

### **19th-29th April 2022**



Dealing with Uncertainties workshop introduction

# Program



- 19-20 : Representation Workshop
- 21-22 : Dealing with uncertainties workshop
- 25-26 : Generators workshop
- 27-29 : final conference
  
- Each workshop : ~55 on-site participants + ~75 remote
- Final conference : 110 on-site + 80 remote

# Thursday



<b>08:55 → 12:30</b>		<b>Dealing with Uncertainties workshop: Thursday morning</b>	
		Convener: Yann COADOU (CPPM, Aix-Marseille Université, CNRS/IN2P3)	
<b>09:00</b>		<b>Workshop introduction</b>	🕒 15m
<b>09:15</b>		<b>Dealing with statistical and systematical uncertainties in High Energy Physics</b>	🕒 1h 30m
		Speaker: Nicolas Berger (LAPP Annecy)	
<b>10:45</b>		<b>Coffee break</b>	🕒 15m
<b>11:00</b>		<b>MAPIE - Model Agnostic Prediction Interval Estimator : a sk-learn contrib</b>	🕒 1h 30m
		Speakers: Nicolas Brunel (Quantmetry), Thomas Morzadec (quantmetry), Vianney Taquet (Quantmetry), Vincent Blot (quantmetry)	
<b>12:30 → 14:00</b>		<b>Lunch at the cafeteria</b>	🕒 1h 30m
<b>14:00 → 19:00</b>		<b>Dealing with Uncertainties workshop: Thursday afternoon</b>	
<b>14:00</b>		<b>Breakout sessions</b>	🕒 1h 30m
<b>15:30</b>		<b>Coffee break</b>	🕒 30m
<b>16:00</b>		<b>Breakout sessions</b>	🕒 1h 30m

# Friday



09:00 → 12:30 **Dealing with Uncertainties workshop: Friday morning**



Convener: Anja Butter (ITP Heidelberg)

09:00 **Uncertainties in Deep Learning**

🕒 1h 30m



Deep learning algorithms, based on deep neural networks, have been deployed for numerous applications over the past few years, especially in the fields of image processing and natural language processing. Their relevance are now studied for scientific applications, for instance, as new methods to solve inverse problems or as surrogate models to accelerate computations in complex simulations. In this framework, it is necessary to be able to provide a quantification of the uncertainty on the outputs given by these methods. However, in their conventional form, deep neural networks are used as deterministic algorithms and they do not raise uncertainty estimations on their predictions. Recent works are developed to address this problematic and the scientific literature provides some technics to model and estimate these uncertainties.

In this talk, we present a general overview of the state-of-the-art on this topic. We firstly introduce the notions and definitions for uncertainties and their origins in the case of machine learning predictions. Then, we present the main techniques that exist in the literature to quantify these uncertainties for deep neural networks and their possible limitations. Finally, we provide some elements to establish a methodology in order to validate and calibrate the uncertainties given by these methods.

**Speaker:** Geoffrey Daniel (CEA)

10:30

coffee break

🕒 30m

11:00 **Breakout sessions**

🕒 1h 30m



12:30 → 14:00 **Lunch at cafeteria**

🕒 1h 30m



14:00 → 19:00 **Dealing with Uncertainties workshop: Friday afternoon**



14:00 **Simulation-based inference: a cautionary tale**

🕒 1h 30m



Simulation-based inference (SBI) enables approximate Bayesian inference when high-fidelity computer simulators are used to describe phenomena of interest. SBI algorithms have quickly developed and matured over the past years and are already in use across many domains of science such as particle physics, astronomy, cosmology, neuroscience or epidemiology.

Inference, however, remains only approximate, and any downstream analysis depends on the trustworthiness of the approximate posterior. In this talk, we will review the Bayesian inference methodology in the likelihood-free setting and discuss good practices to follow, including the choice of the prior, the choice of the SBI algorithm, and diagnostics that we can use to validate inference results.

**Speaker:** Gilles Louppe (University of Liège)

# Social Events



## ☐ Thursday 21th

- Lunch at the cafeteria
- Dinner 7PM at Le Gramophone (next to Orsay-Ville RER station)
  - Please fill asap the Google Form you should have received from Sabrina

## ☐ Friday 22nd

- Lunch at the cafeteria

## ☐ Thursday

- 6:30PM visit and dinner at Musée d'Orsay in Paris
- Please fill asap the (other) Google Form you should have received from Sabrina

# Spirit



- ❑ Long talks, do not hesitate to ask questions during the talk:
  - On zoom raise your hand
- ❑ Long coffee breaks
- ❑ Break-out sessions
- ❑ Un-organised spontaneous discussions

# 3rd of a series



- 15-26 Jul 2019: Real time analysis workshop
- 14-25 Oct 2019: Advanced Pattern recognition
- Learning to discover : ~~Jul 2020, Feb 2021, Feb 2022~~, **April 2022!**

# Premices



- ❑ The whole Institut Pascal (half-building) is yours
- ❑ Two amphitheatres the big 120 one and the small 70 one (we use the big for plenary for social distancing)
- ❑ 40 offices (« Learning to Discover ») pick yours (possibly shared).
  - You can write your name on the sheet outside
- ❑ Small meeting rooms, free coffee machines...
- ❑ If you need to come early morning (before 8:45) or late afternoon (after 5:30) or in the week-end, please ask Sabrina an access card



# slack



- ❑ Primary channel of communication
- ❑ 162 participants as of this morning. Make sure you're connected (ask your neighbour)

**LEARNING**

- Fils de discussion
- Tous les messages dire...
- Mentions et réactions
- Éléments enregistrés
- Slack Connect
- Plus
- Favoris
- sabrina.soccard
- Canaux
  - # general
  - # organisation
  - # outings
  - # random
  - # sci\_conference
  - # sci\_generators
  - # sci\_representation**
  - # sci\_uncertainties
  - # transports\_and\_regio...
  - + Ajouter des canaux
- Messages directs

**# sci\_representation** 10

1 élément(s) épinglé(s) + Ajouter un marque-page

Jeudi 7 avril

**David Rousseau** 23 h 35  
a rejoint #sci\_representation.

**David Rousseau** 23 h 35  
a défini la description du canal : Discussion pertaining to representation workshop

Vendredi 8 avril

**Savannah Thais** 0 h 20  
a rejoint #sci\_representation, avec 7 autres personnes.

Hier

Épinglé par vous

**David Rousseau** 23 h 18  
Live notes will be on this [google doc](#) (please do not advertise). Anyone here can edit or comment.

Visible par vous seulement

**Slackbot** 23 h 18  
D'accord ! Je vous le proposerai de nouveau la prochaine fois.

**Francois Lanusse** 23 h 35  
a rejoint #sci\_representation.

B I

Envoyer un message #sci\_representation

A, Representation Learning, David Rousseau, introduction

# Zoom



- ❑ Zoom in meeting mode (no waiting room, everyone sees every one else connection)
  - Link, meeting ID and code distributed on slack
  - Please do not advertise beyond workshop and conference
- ❑ Anyone of you can start zoom in amphi and meeting rooms : « join » room number + code
  - Do not hesitate to exercise it yourself
- ❑ 6 break out room created. Anyone can navigate between these rooms and the main.
- ❑ Zoom chat (volatile) only to be used for connection issues
- ❑ Use slack for scientific exchanges : #sci\_uncertainties for this workshop (other specific channel can be created on request)

# Live Document



- ❑ Google doc link posted in slack  
#sci\_uncertainties (please do not  
advertise beyond workshop attendees)
- ❑ Live notes
- ❑ Break-out sessions proposed themes
- ❑ Anyone can edit / comment. Feel free to  
add info. Propose break-out sessions.

# Break-out sessions



- ☐ Semi auto organised
- ☐ Theme added in google doc, you can add your own and vote
- ☐ Org committee will assign physical and zoom room
- ☐ You take it from there
- ☐ (sketchy) report Friday end of afternoon

# (not) Facebook



- ❑ List of participants on indico lists who is here or remote for which workshop and conference
- ❑ Google sheet with one page per participant shared on slack
  - Please duplicate first (dummy) page and briefly introduce yourself, recent work, interest

# Workshop summary at the final conference



- Each workshop will be summarised in 30' at the final conference
- TBA kindly volunteered for this one
  - He might ask for your inputs

# Outcome



- ❑ Work started or continued from collaboration enriched in these workshops may be published in special edition of Computing and Software for the Big Science.
- ❑ If interested, talk to one of the organiser

# Organising committee



- ❑ Sabrina Soccard, Program Manager at Institut Pascal
- ❑ Peter Battaglia, senior scientist at Google Deepmind
- ❑ Anja Butter, ITP Heidelberg : generator models and uncertainties in ML for Particle Physics
- ❑ Cécile Germain : Emeritus professor (computer science) Université Paris-Saclay, LRI-CNRS, and INRIA TAU team, organiser of the 2014 HiggsML and 2018-2019 TrackML challenge
- ❑ Tobias Golling, associate professor at Université de Genève, generative models and anomaly detection for particle physics
- ❑ Vladimir Vava Gligorov, CNRS/IN2P3 LPNHE, leader of the LHCb Real Time analysis project, organiser of the Real Time Analysis Institut Pascal Workshop
- ❑ Eilam Gross, Weizmann Institute, organiser of the Hammers and Nails 2017 and 2019 workshop
- ❑ Michael Kagan, SLAC, co-coordinator of CERN Interexperiment Machine Learning group
- ❑ Danilo Rezende, Researcher on Probabilistic Methods for Decision Making, Senior Staff Researcher and Team Lead at Google Deepmind
- ❑ David Rousseau, CNRS/IN2P3 IJCLab : former co-coordinator of ATLAS Machine Learning group, co-coordinator of the LHC Interexperiment Machine Learning Group, organiser of the 2014 Higgs Machine Learning challenge, and of the 2018-2019 TrackML challenge
- ❑ Andreas Salzburger, CERN, coordinator of the ATLAS software upgrade group, organiser of the 2018-2019 TrackML challenge and organiser of the Advanced Pattern Recognition Institut Pascal Workshop
- ❑ Savannah Thais, Princeton, representation learning for Particle Physics, AI and ethics
- ❑ Jean-Roch Vlimant, Caltech, co-coordinator of CMS Machine Learning group, organiser of the 2018-2019 TrackML challenge
- ❑ Slava Voloshynovskiy, head of Stochastic Information Processing group, Université de Genève



# Sponsors



□ Thanks to our sponsors (see indico Menu)

- Institut Pascal
- Paris Saclay Center for Data Science
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- DataIA
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