AISSAI : AI and the Uncertainty Challenge in Fundamental Physics

Summary

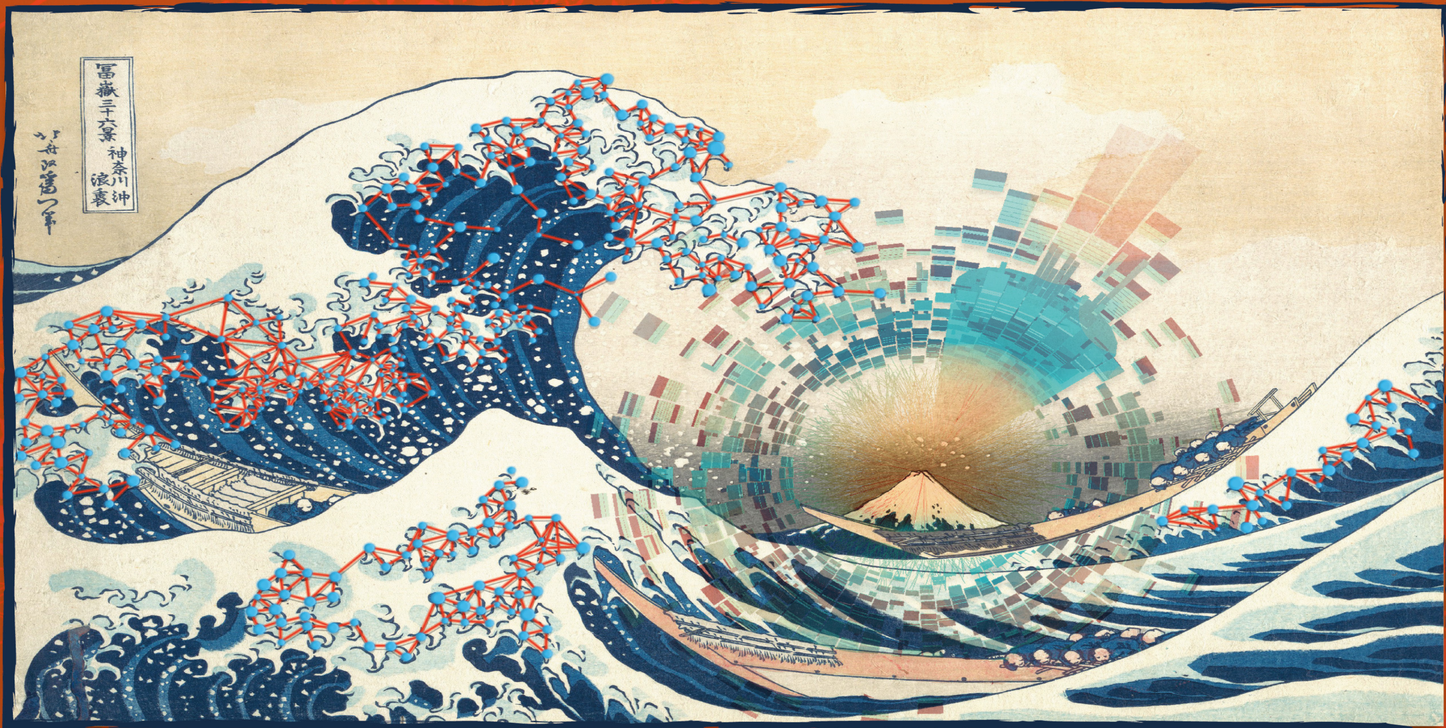
David Rousseau
(IJCLab-Orsay)

AISSAI Anomaly Detection Workshop
Clermont-Ferrand, March 2024

All slides and recordings available

ARTIFICIAL INTELLIGENCE AND THE UNCERTAINTY CHALLENGE IN FUNDAMENTAL PHYSICS

27 NOV - 1 DEC 2023



SCIENTIFIC COMMITTEE

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LAPP, USMB, CNRS

Program Manager
Vincent Folliard
AISSAI

- UNCERTAINTY QUANTIFICATION
- EXPLAINABLE/TRUSTWORTHY AI
- DATA-FRUGAL/DATA-CENTRIC AI
- SIMULATION-BASED INFERENCE, UNFOLDING,...
- ARCHITECTURES: ADVERSARIAL, BAYESIAN,...
- CONTROLLING UNCERTAINTIES IN GENERATIVE MODELS
- BENCHMARKS DATASET AND CHALLENGES

INDICO.IN2P3.FR/E/AIUPHYS2023

AISSAI
AI for science, science for AI

CNRS IN2P3 · scai · DATAIA · université PARIS-SACLAY · INSTITUT PASCAL

SCAI, PARIS AND INSTITUT PASCAL PARIS-SACLAY

Mon-Tues @ Jussieu Université Paris-Sorbonne

AISSAI

& Institut Pascal

would like to thank you
for your coming and your participation

Wed-Thu @ Institut Pascal Université Paris-Saclay

….. 25 hours of talks…

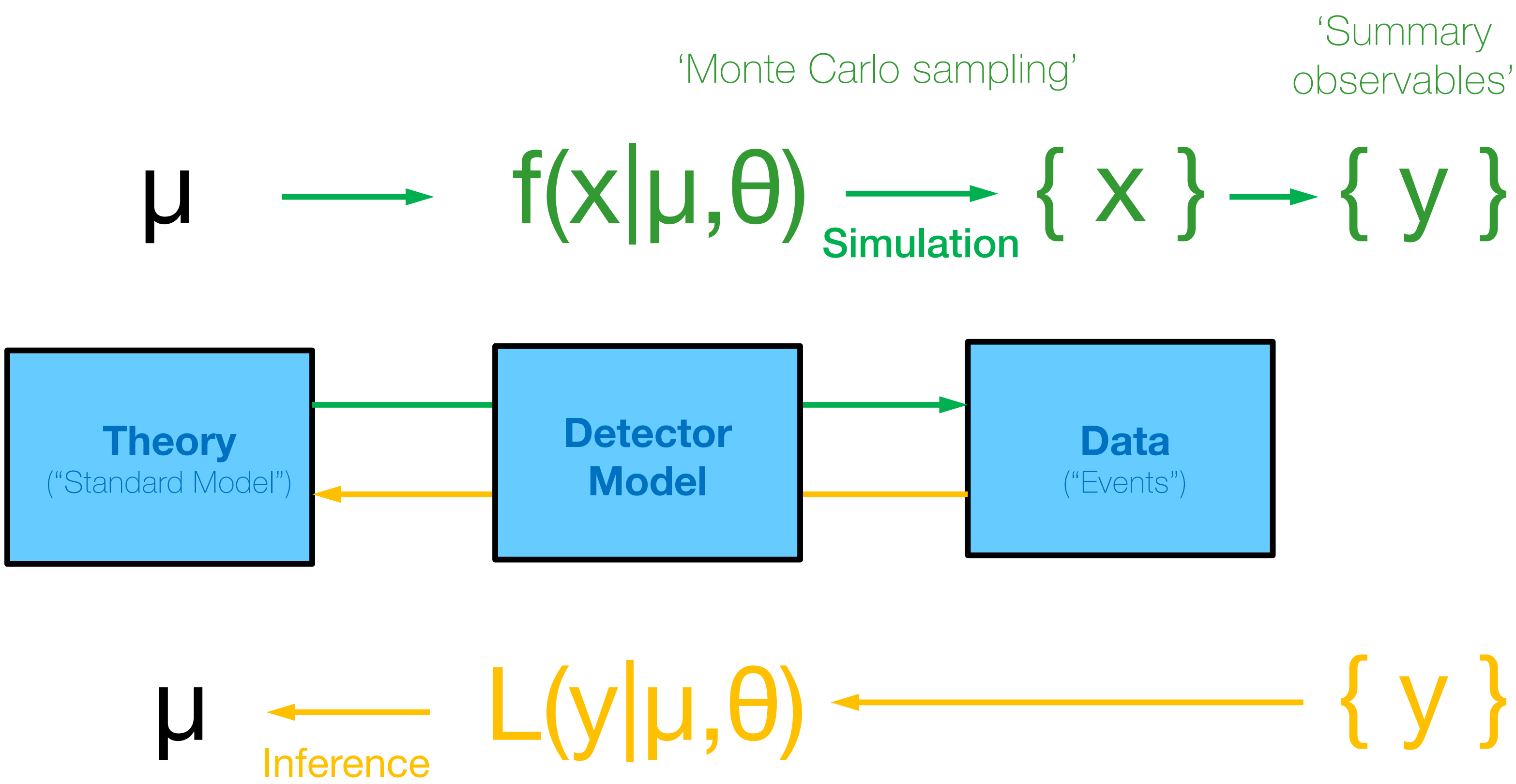
… just an invitation here…

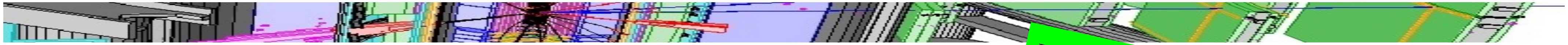
Uncertainties in HEP

Wouter Werkerke (NIKHEF)

Particle physics data analysis in a nutshell

W Werkerke





Most complex measurement ever ?

Phys.Rev.Lett. 114 (2015)191803

Combined Measurement of the Higgs Boson Mass in pp Collisions at $\sqrt{s} = 7$ and 8 TeV with the ATLAS and CMS Experiments

(ATLAS Collaboration)[†]
(CMS Collaboration)[‡]

(Received 25 March 2015; published 14 May 2015)

A measurement of the Higgs boson mass is presented based on the combined data samples of the ATLAS and CMS experiments at the CERN LHC in the $H \to \gamma\gamma$ and $H \to ZZ \to 4\ell$ decay channels. The results are obtained from a simultaneous fit to the reconstructed invariant mass peaks in the two channels and for the two experiments. The measured masses from the individual channels and the two experiments are found to be consistent among themselves. The combined measured mass of the Higgs boson is $m_H = 125.09 \pm 0.21\,(\text{stat}) \pm 0.11\,(\text{syst})$ GeV.

Systematical uncertainties: everything we don't know exactly

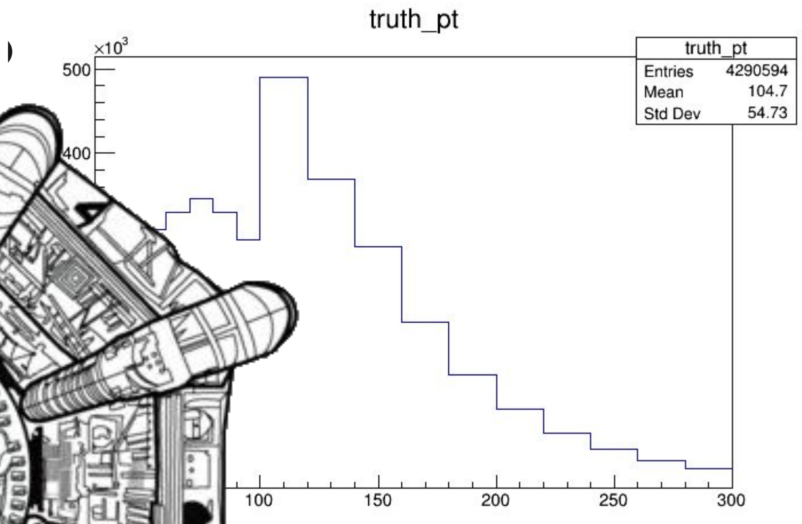
Unfolding in HEP

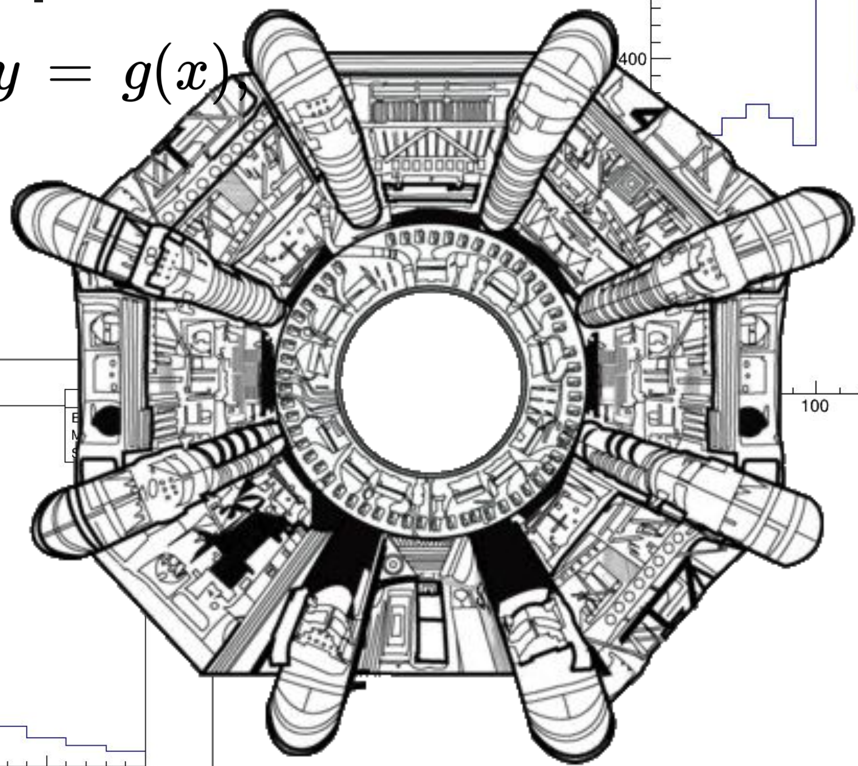
Vince Croft (NIKHEF)

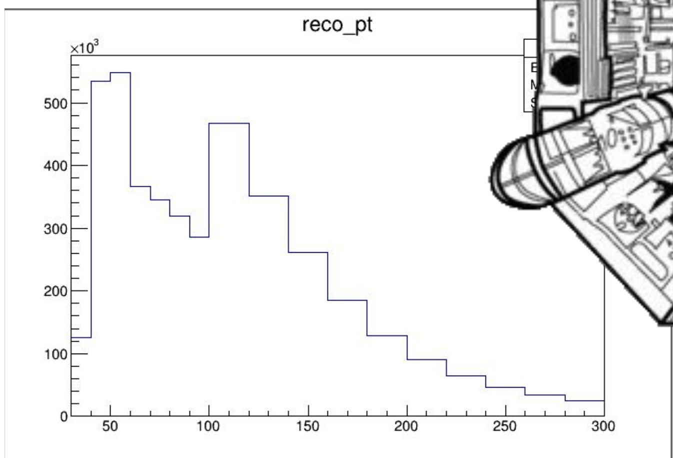
Dr. Vincent Croft Unfolding in High Energy Physics: **Artificial Intelligence and the Uncertainty Challenge in Fundamental Physics** November 30th 2023

Focus on distributions

$$\int_0^1 K(x,y)f(y)dy = g(x)$$







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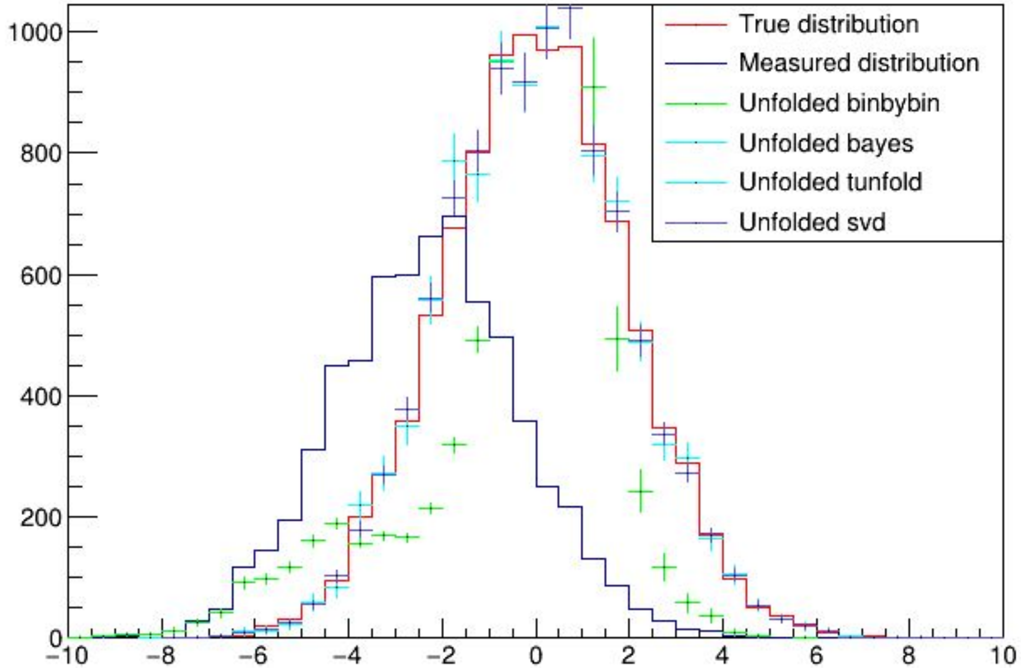
A Summary of Unfolding Methods in RooUnfold

- Common interface to multiple methods
- Each with different error propagation
- Each with different responses to distributions
- Each with different regularisation parameters.

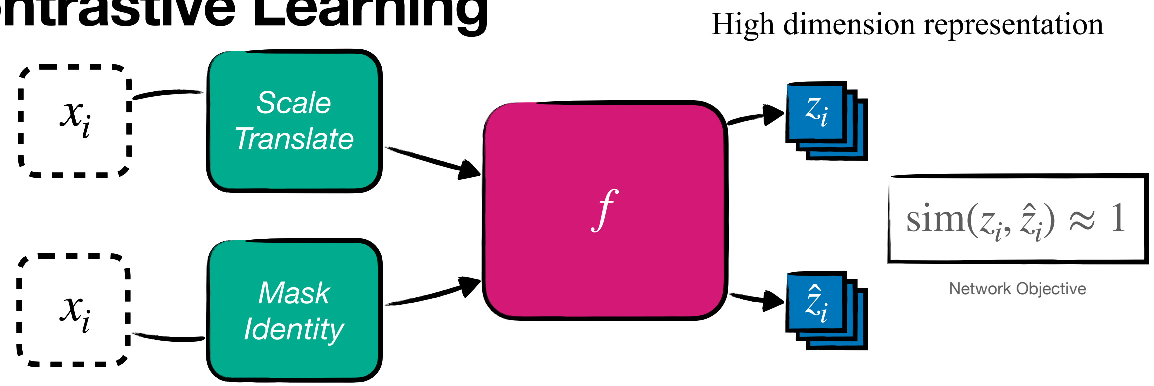
Open in SWAN



Contrastive learning for de-biasing

Radi Radev, CERN

Contrastive Learning



Pass pairs of **augmented events** through a **neural network** f to extract **vector representations.**

Representations from **same** event - **high similarity**

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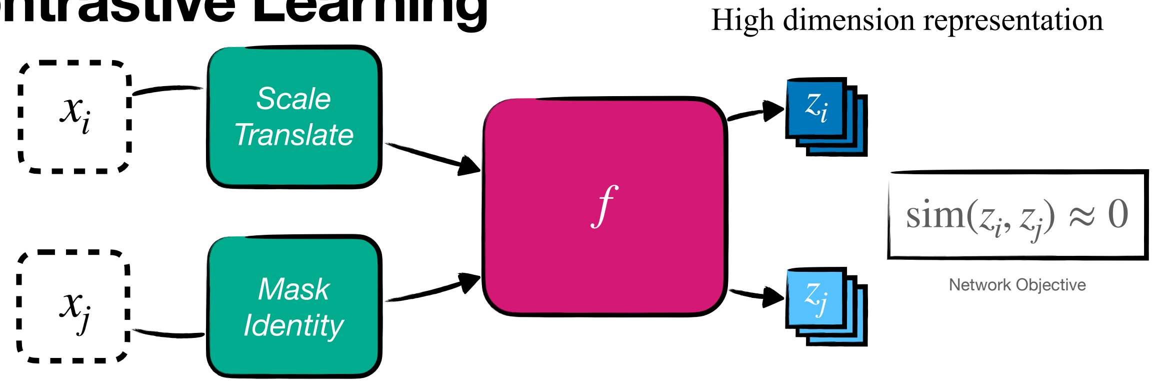
Contrastive Learning



Pass pairs of **augmented events** through a **neural network** f to extract **vector representations.**

Representations from **different** events - **low similarity**

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Application to Dune Lar TPC event reconstruction

Uncertainty Quantification in industry

Vincent Chabridon (EDF Electricité de France)

UC#1 – Safety analysis of accidental transients

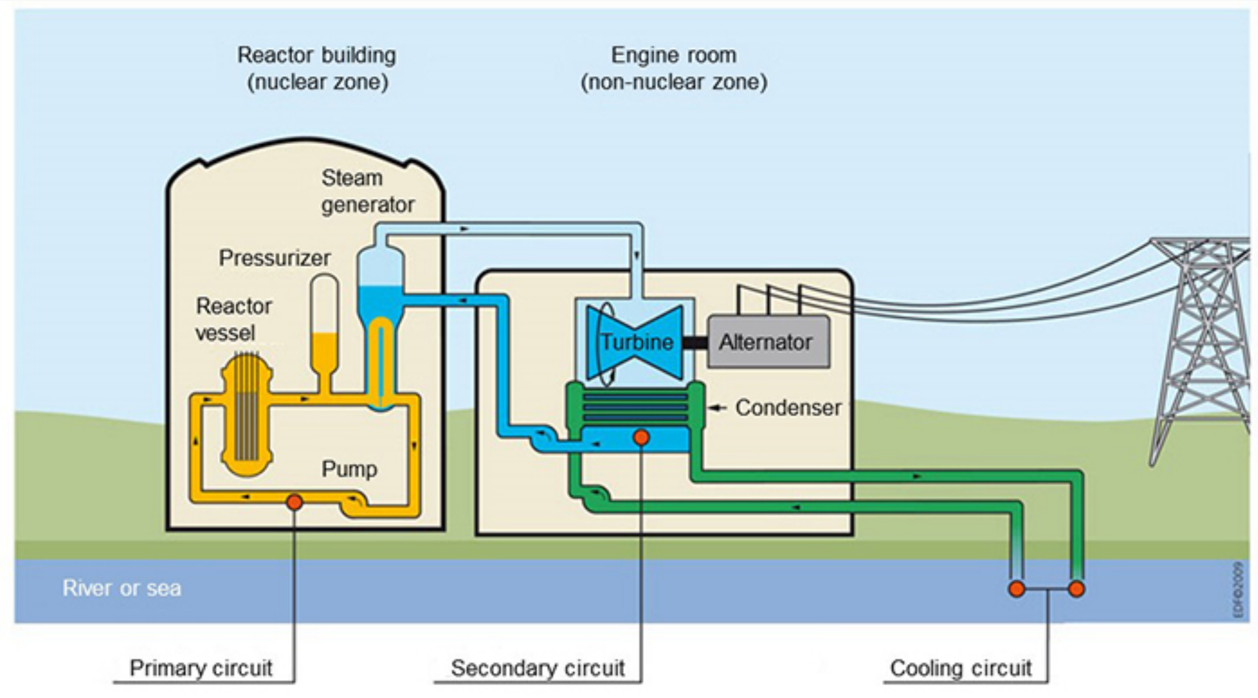
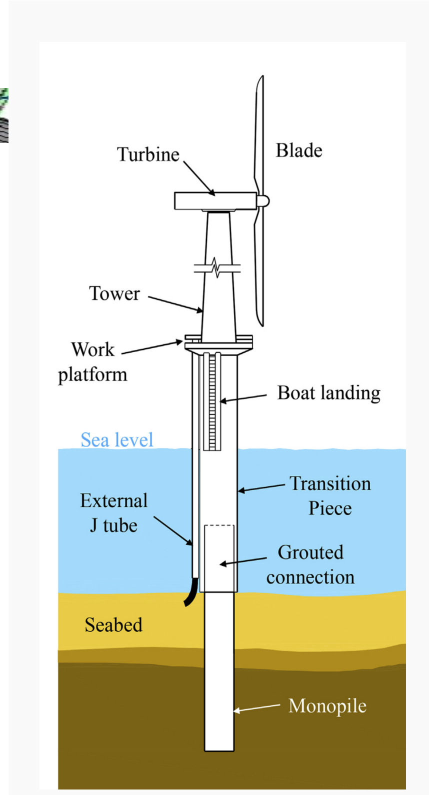


Figure 7: A typical French pressurized water reactor (source: IRSN).

☆ **The 3 safety barriers.**

➩ (#1) **cladding**, (#2) **primary circuit**, (#3) **reactor building**



- Complex/heavy simulators
- ➔Cannot brute-force explore the input parameter space
- Correlations in the input parameter space for risk evaluation

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OpenTURNS: an open-source library for UQ

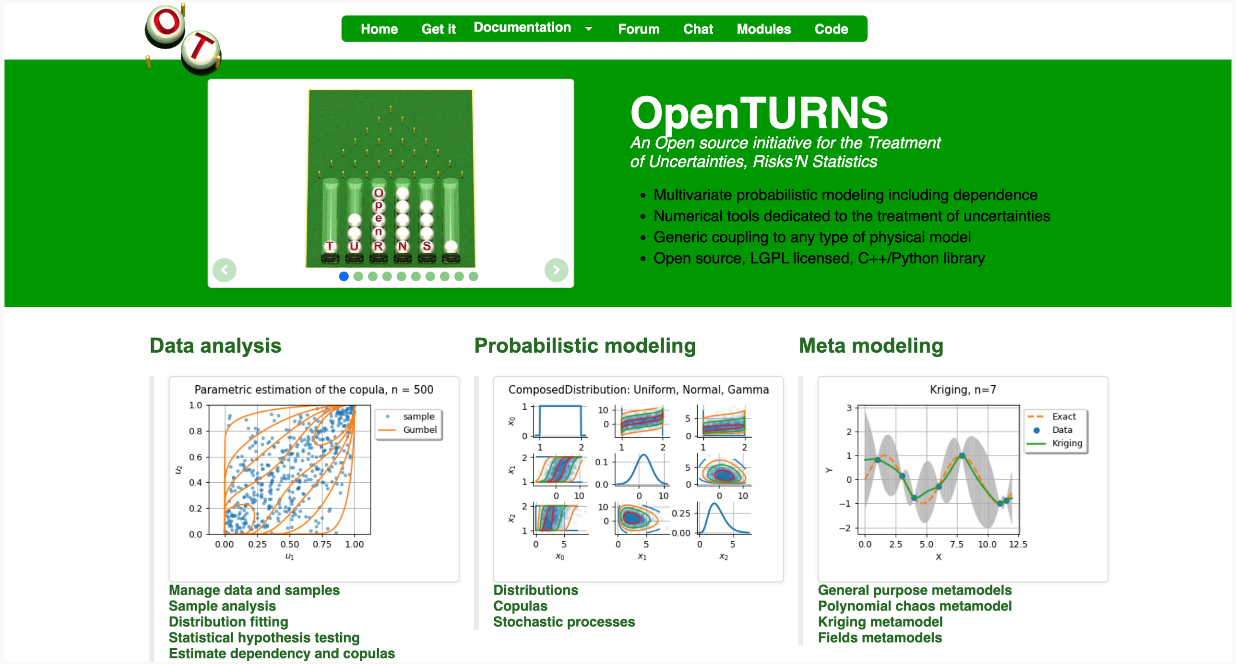

Figure 20: OpenTURNS' webpage.

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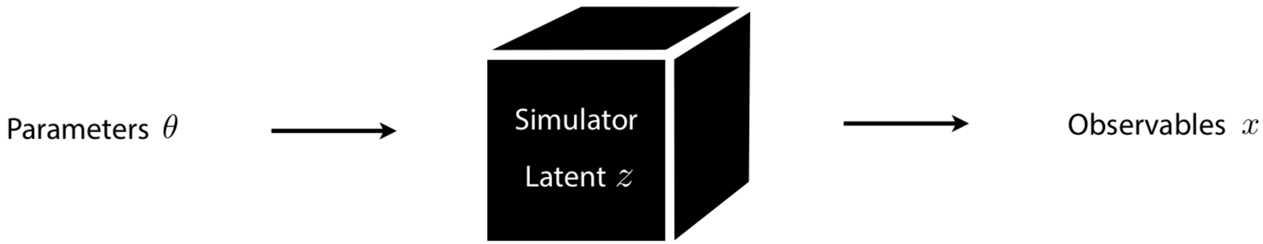
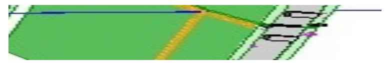
Simulation Based Inference

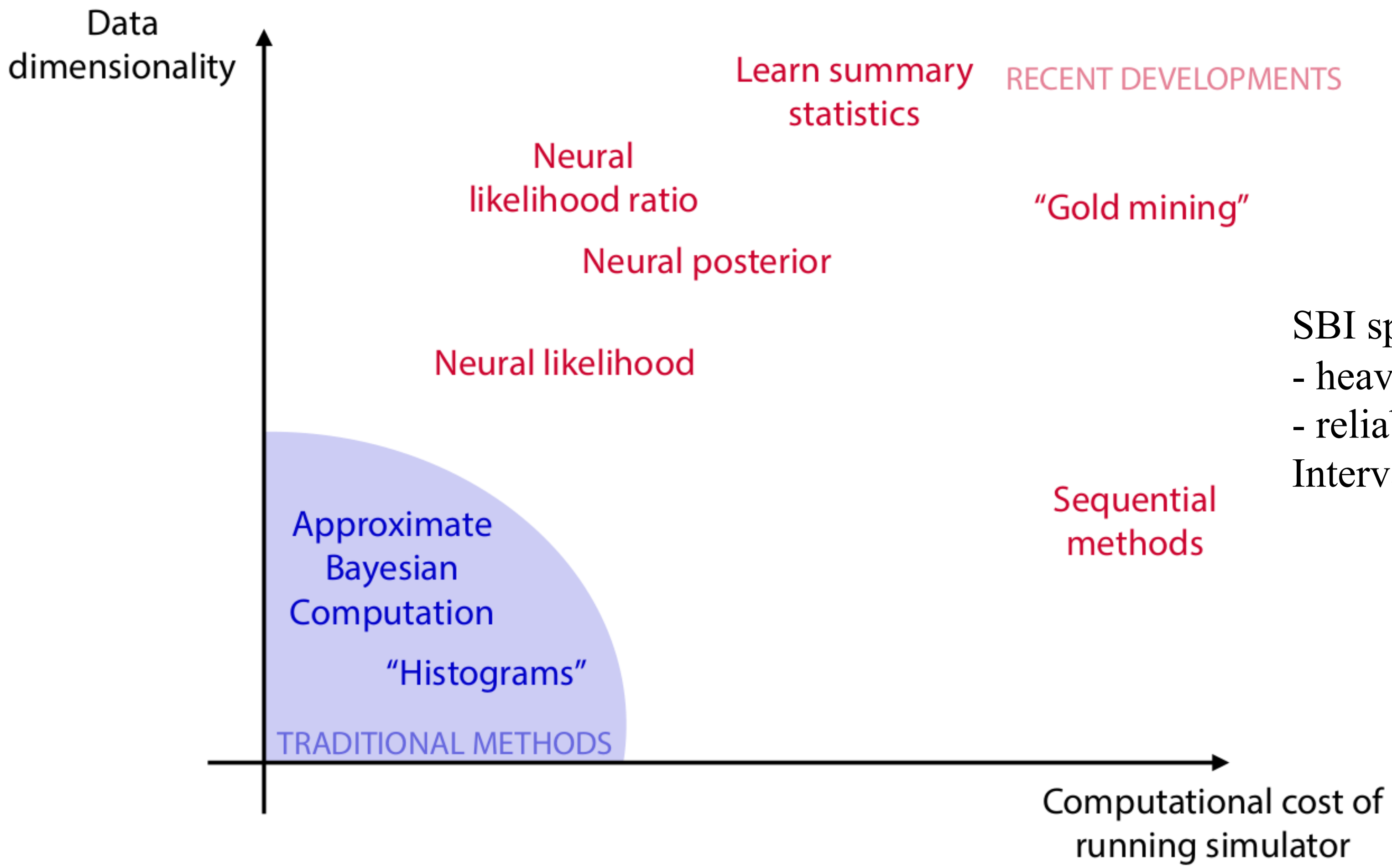
Prosper Harrison, Gilles Louppe, Michael Kuusela



Prediction:
- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x|\theta)$

Inference:
- Interactions between low-level components lead to challenging inverse problems
- Likelihood $p(x|\theta) = \int \mathrm{d}z\; p(x, z|\theta)$ is intractable





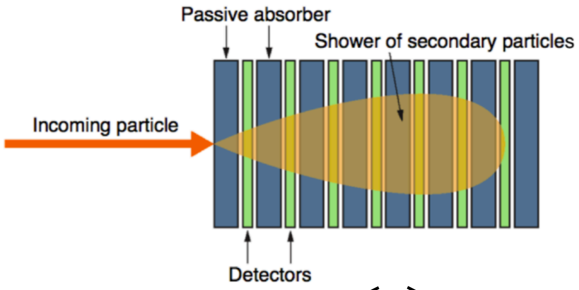
SBI specific to Fundamental Science
- heavy accurate simulators
- reliable parameter (and Confidence Interval) inference

Uncertainty in Generator Models

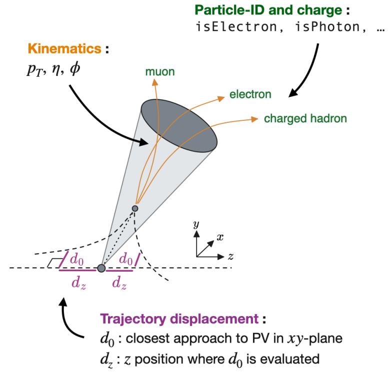
Gregor Kasieczka

Simulation targets

Calorimeter Showers

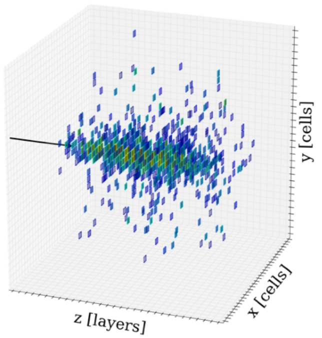


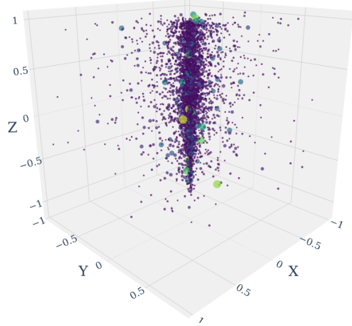
Jet Constituents



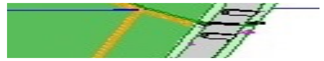
as fixed grid

as point cloud

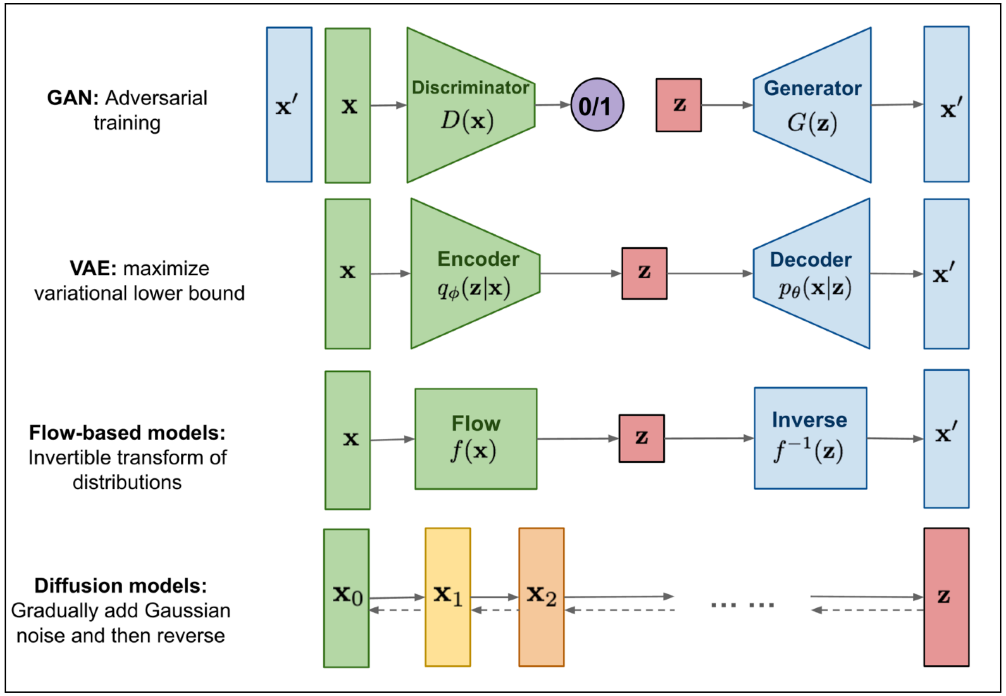




Generative Models

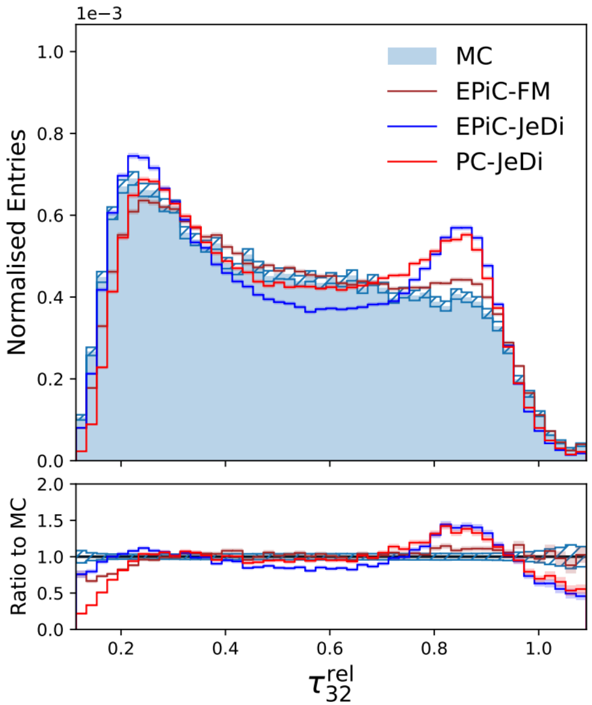


→Use generative models trained on simulation or data as efficient surrogates



Overview of generative architectures

Metrics



Wasserstein distance

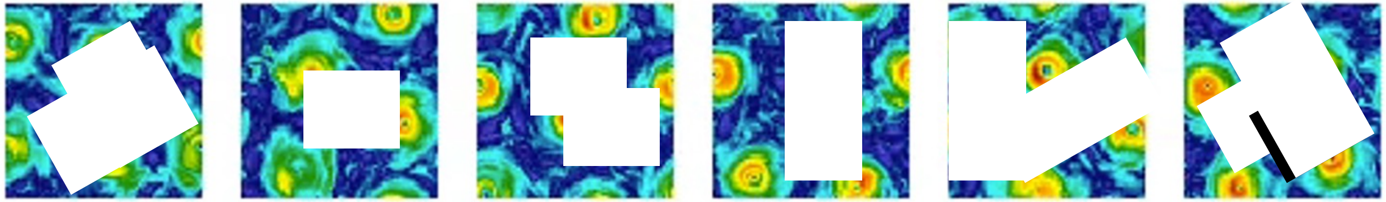
More robust, well defined also for non-overlapping distributions

Kullback-Leibler divergence

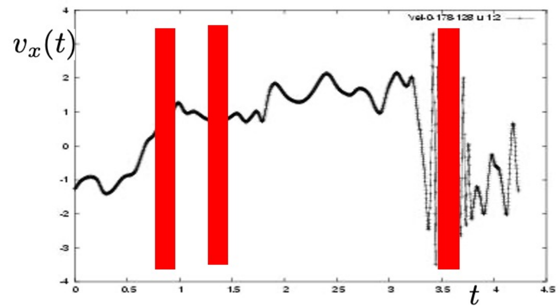
More intuitive for shape-mismodelling

But also multi-dimensional

Complex Fluids and Complex Flows Group
Dept. Physics & INFN - University of Rome 'Tor Vergata'
biferale@roma2.infn.it
https://biferale.web.roma2.infn.it/



Rotation rate? | Viscosity? | Reynolds number? | Boundary comditions? | Forcing properties? | Aspect ratio?



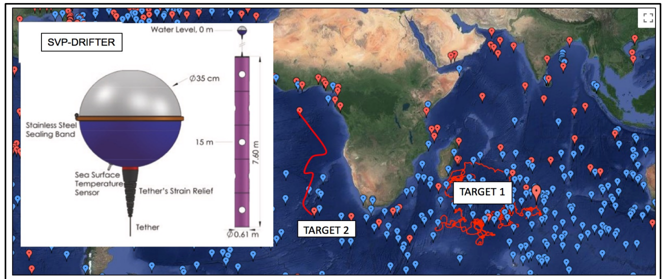


FIG. 1: INSTANTANEOS WORLDWIDE DISTRIBUTION OF DRIFTERS FROM THE GLOBAL DRIFTER MAP PROGRAM [www0]. WE HIGHLIGTHED IN RED TWO POTENTIAL TARGETS: (1) KEEP THE PROBES INSIDE A GIVEN REGION OR (2) MINIMISING THE NAVIGATION TIME AMONG TWO END-POINTS (ZERMELO PROBLEM). INSET: A SKETCH OF THE DRIFTER WITH THE LONG DROUGE AT 15M DEPTH.

Machine-learning and equations-informed tools for generation and augmentation of turbulent data.

Artificial Intelligence and the Uncertainty challenge in Fundamental Physics
Paris 2023

CREDITS: T. LI, M. BUZZICOTTI, F. BONACCORSO, S. CHEN. M. WAN

Genetics, genomics, transcriptomics, proteomics

Burak Yelmen

DNA: Deoxyribonucleic acid - **genetic information**
RNA: Ribonucleic acid - **transcribed** genetic information
Protein: Amino acid chains with 3D structure - **translated** genetic information
Gene: A sequence of DNA transcribed into a functional RNA - could be protein **coding** or **non-coding**
Genome: Entirety of DNA in an organism - 3 billion base pairs in human genome

Flow of genetic information (Central dogma)

DNA ⇄ **RNA** → **Protein** → **Structure and function**

ATGCAATGC
| | | | | | | | |
TACGTTACG

AUGCAAUGC

MQC

2

AISSAI – Orsay Nov 28-Dec 1 2023

Robustness to Uncertainties in ML Applications for Particle Physics

Tommaso Dorigo

INFN, Padova

AISSAI PhyStat workshop
Machine Learning Assisted Sampling
Application to Physics

Marylou Gabrié (Ecole Polytechnique)

Assisting sampling with surrogate generative models [12]

No data a priori, only a density of probability $\rho_*(x)$ (Bayesian posterior, Boltzamnn distribution)

▷ **Architecture strategies:** Design generative models to incorporate known symmetries to ease the learning of a surrogate $\rho_\theta \approx \rho_*$ (e.g. Lattice QCD gauge invariances)

▷ **Training strategies:**
- Variational inference (VI)
- Adaptive training to create data as you go

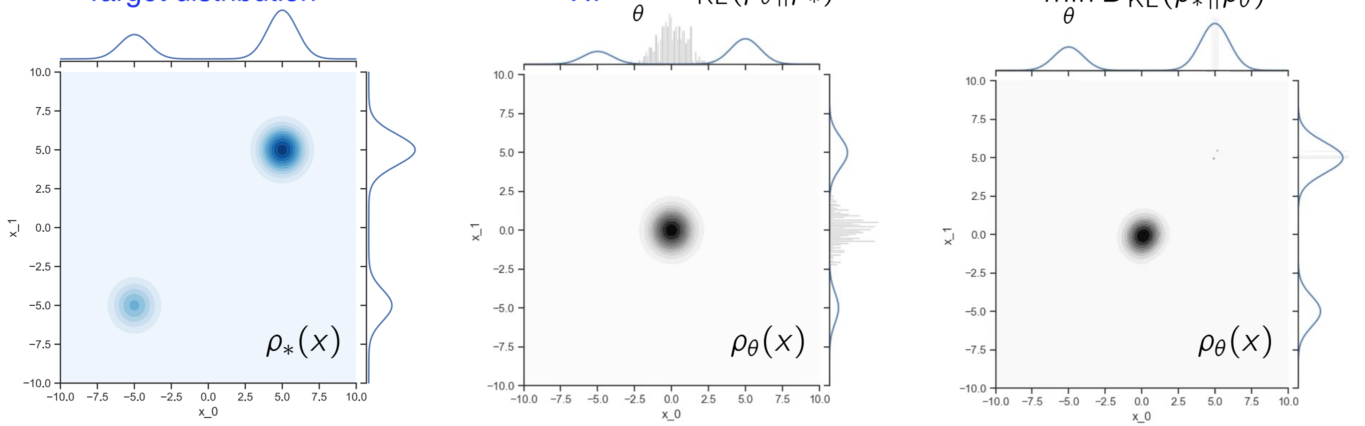
MCMC convergence garantees!

Adaptive MCMC:

Target distribution

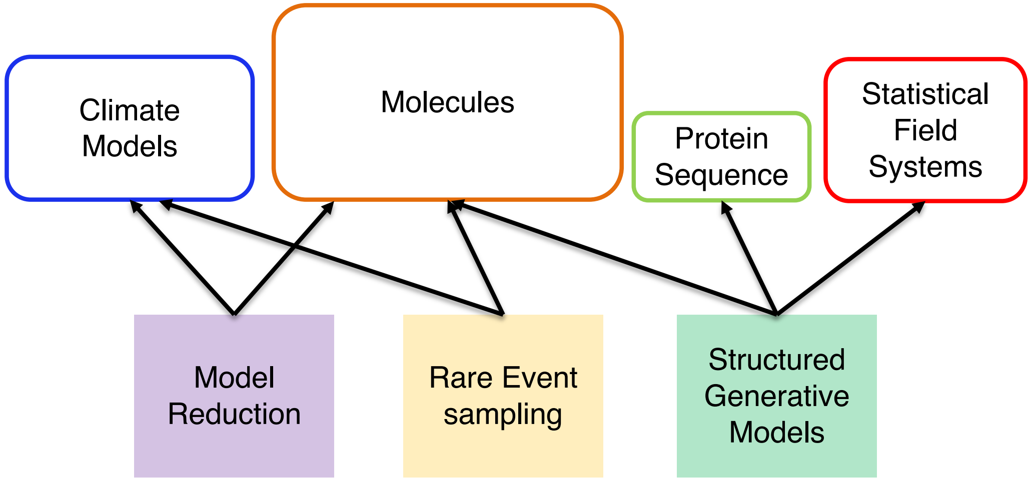
VI: $\min_\theta D_{\mathrm{KL}}(\rho_\theta \| \rho_*)$

$\min_\theta D_{\mathrm{KL}}(\rho_* \| \rho_\theta)$



Learning a well covering generative model requires minimum knowledge of modes before-hand

Conclusion: how/where has machine learning helped?



▷ Autoencoders to learn non-linear dimensionality reductions

▷ Variational principles to solve eigenvalue problems
& partial differential equations

▷ Normalized generative models to accelerate sampling

▷ Structured generative models to extract/exploit structure from data

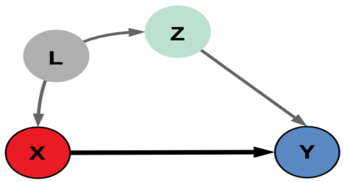
Summary of the AISSAI Causality workshop

Alessandro Leite LISN

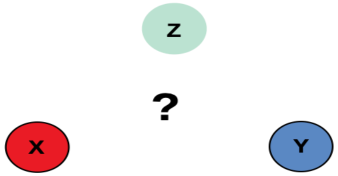
Causal inference framework

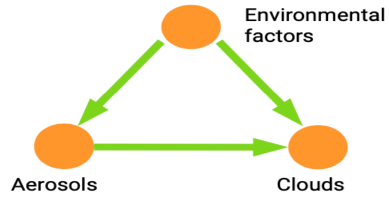
Two types of questions:

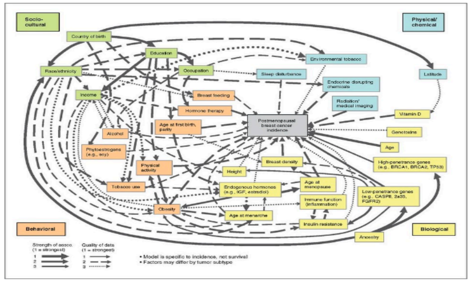
1. **Assume qualitative causal graph** to **quantify causal effects:**



2. Make **general assumptions** to **learn causal graph:**







Slide credit: *Jakob Runge*

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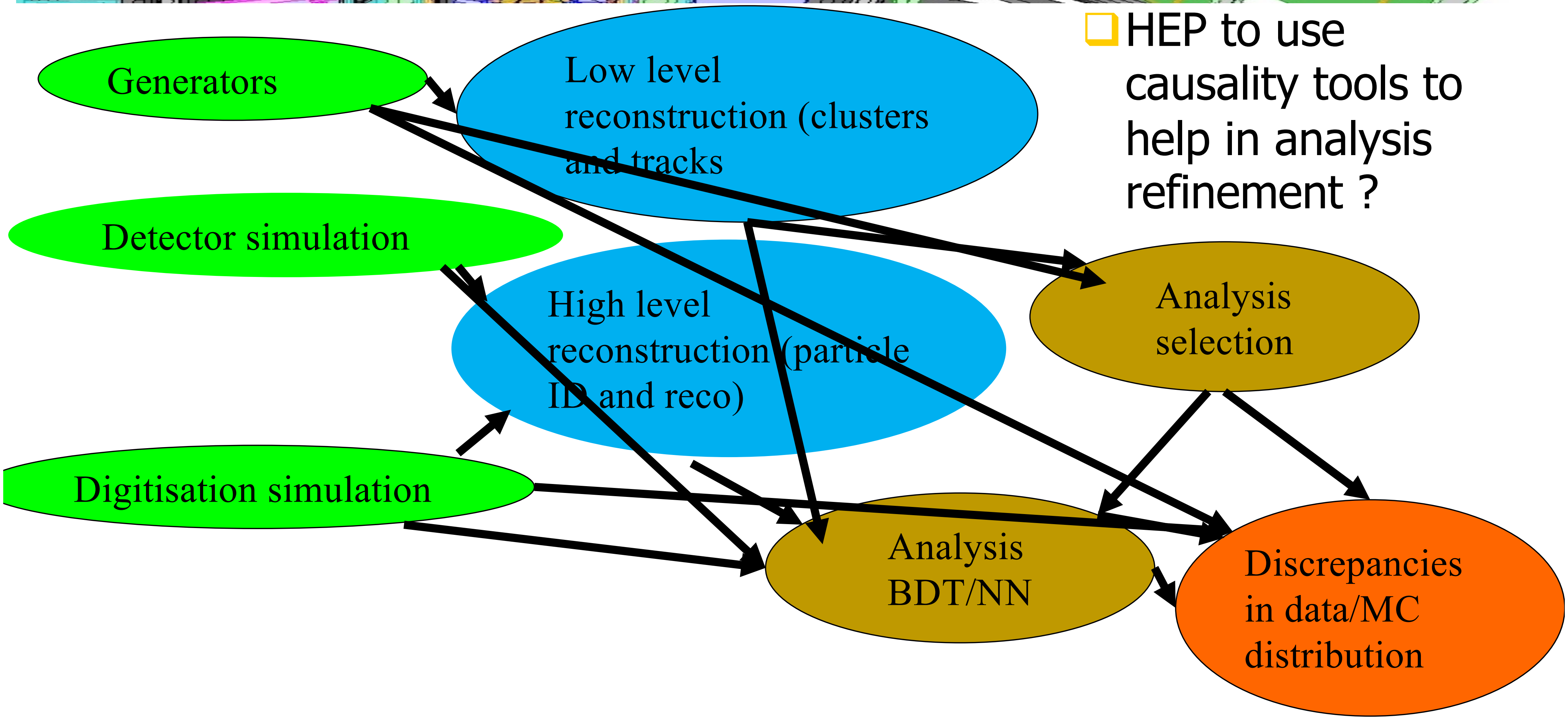
Causality in HEP



- HEP to use causality tools to help in analysis refinement ?

Fair Universe competition

Fair Universe: HiggsML Uncertainty Challenge

- Extension of previous HiggsML challenge from 2014, a classification problem for Higgs decaying to Tau leptons based on final state 3-momenta and derived quantities: l, h, MissingET, up to 2 jets
- Dataset : HiggsML 2014 data set on CERN Open Data portal

⇒new Fair Universe dataset, with following improvements

- Instead of ATLAS G4 simulation, use Pythia LO + Delphes
- Numbers of events 800.000⇒ >10 millions
- Parametrised systematics (Nuisance Parameters) :
  - Tau Energy Scale : on had Tau Pt (and correlated MET)
  - Jet Energy Scale (and correlated MET impact)
  - additional randomised Soft MEt
  - background normalisation
  - W background normalisation (a subdominant poorly constrained BKG)
- Task : given a pseudo-experiment with given signal strength, provide a Confidence Interval

Create pseudo-experiments

Test Dataset

$\{\mathbf{x}, \mathbf{w}\}$

$\{\mathbf{x}, \mathbf{w_1}\}$, w_1 = Pois (w)

$\{\mathbf{x}, \mathbf{w_2}\}$, , w_2 = Pois (w)

$\{\mathbf{x}, \mathbf{w_N}\}$, , w_N = Pois (w)

Case 1

$\{NP\} = \{NP\}_1$

$\mu = \mu_1$

Case 2

$\{NP\} = \{NP\}_2$

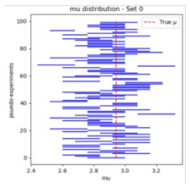
$\mu = \mu_2$

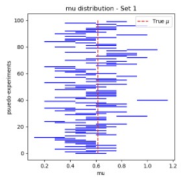
…

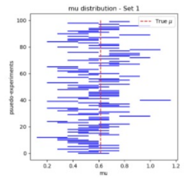
Case N

$\{NP\} = \{NP\}_N$

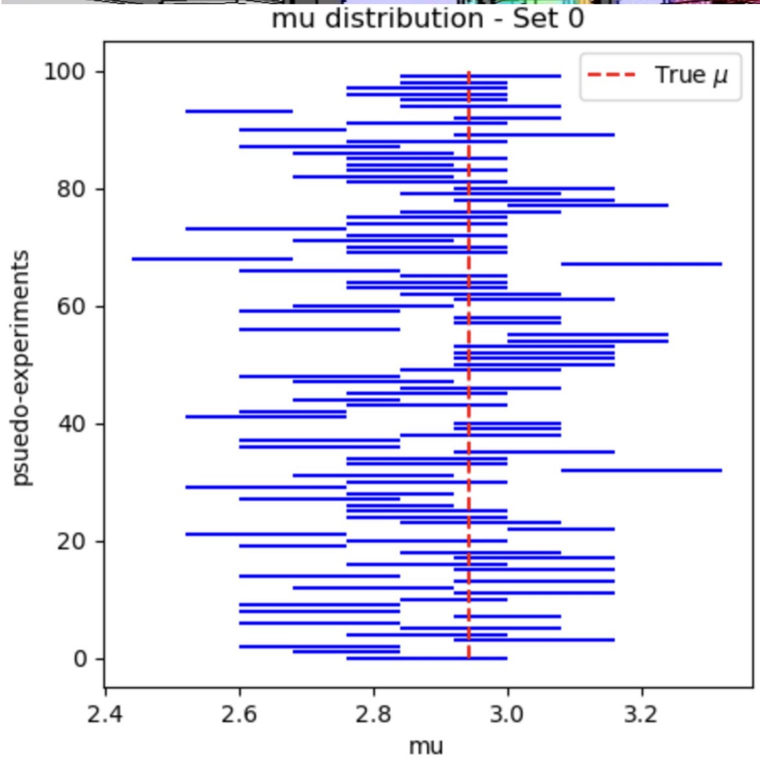
$\mu = \mu_N$

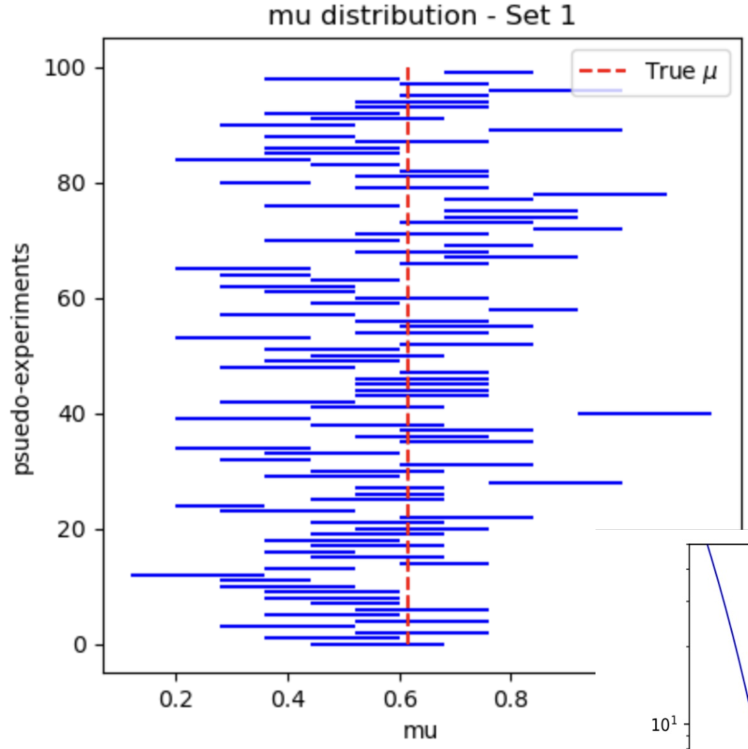




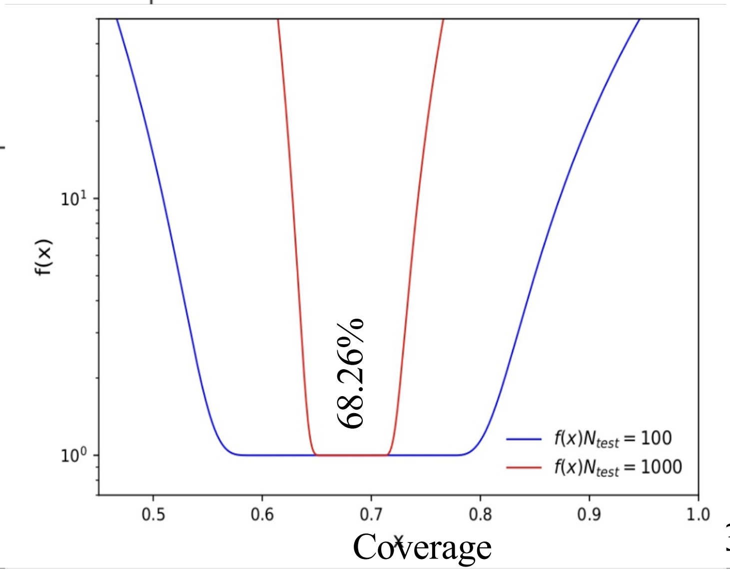


Coverage evaluation





Coverage penalisation function



score : <CI length> x coverage penalisation sd

sd

Task:				Fact Sheet Answers	Higgs Uncertainty Challenge			
#	Participant	Entries	Date of last entry	Method Name	Quantile Score	Interval	Coverage	Detailed Results
1	ragansu	30	2024-01-22	Histogram_10	**1.45**	0.226	0.57	
2	ragansu	30	2024-01-22	One_bin NLL	**1.07**	0.333	0.57	
3	laurensslu	20	2023-12-01	cheat7	**0.68**	0.504	0.63	
4	laurensslu	20	2023-12-01	cheat7	**0.61**	0.544	0.68	
5	laurensslu	20	2023-12-01	cheat4	**0.31**	0.732	0.61	
6	laurensslu	20	2023-12-01	cheat4	**0.16**	0.852	0.71	
7	laurensslu	20	2023-12-01	Cheat2	**-0.44**	1.55	0.62	
8	laurensslu	20	2023-12-01	Cheat2	**-0.74**	1.375	0.55	
9	ragansu	30	2024-01-22	tes_finder	**-0.95**	1.124	0.54	
10	laurensslu	20	2023-12-01	Cheat2	**-1.59**	1.325	0.53	
11	Ihsan Ullah	4	2024-01-18	Sascha sys aware 8	**-2.69**	0.329	0.47	
12	Rafał Masełek	10	2023-12-01	1binNLL	**-2.9**	1.233	0.5	
13	ihsanchalearn	16	2023-12-18	1 bin NLL	**-2.9**	1.233	0.5	
14	Rafał Masełek	10	2023-12-01	1binNLL	**-2.9**	1.233	0.5	
15	ihsanchalearn	16	2023-12-18	Sascha sys aware 8	**-3.01**	0.33	0.46	

Fair Universe Plans

- We're running a second prototype competition as part of ACAT 2024 conference next week
- You're welcome to participate (check Whaid Bhimji's talk on Tuesday)
- We're aiming to run the large scale competition June-Sep 2024, as an official NeurIPS 2024 competition (if accepted)