



PhD position in Bayesian Causal Graph and uncertainty quantification – Application to the anomaly detection on light line of the Synchrotron

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1 Environment

Within the LIAD laboratory (Laboratory of Artificial Intelligence and Data Science) belonging to the SGLS service (Software Engineering Service for Simulation), you will work in a team specialized in handling uncertainties in numerical simulation. You will contribute to the strengthening of these activities through the DALLIAE project, which aims for Anomaly Detection on Synchrotron Beamlines through Explainable Artificial Intelligence.

This PhD position is part of a collaboration between various CEA teams (LIAD, NRX – Nanostructures and X-Rays Team in Grenoble), the university of Lorraine and the European Synchrotron (ESRF), each bringing distinct skills such as AI, beamline physics, and instrumentation.

2 Subject

The DALLIAE project aims to propose a generic method based on causal (Bayesian) graphs [4, 5] to detect anomalies during beamline experiments and their interpretability. Among causal graphs, we will focus particularly on directed acyclic graphs (DAGs) [1]. The goal is to introduce a hierarchical causal graph and utilize the notion of a surrogate causal model to identify the most pertinent simple (single parameter) and joint (parameter combination) causal links that characterize the causes of an anomaly. This approach is essential due to the multi-scale nature of the instruments and the complete beamline, which requires a nuanced understanding of causal relationships across different scales. We will also focus on quantifying uncertainties associated with identified causal links to ensure their relevance. This search for causality is all the more difficult due to the variety of instruments, parameters [1, 3], their modification during the experiment [2], the combinatorial number of joint effects to study, and the underrepresentation of anomalies in the data.

In practice, this method will limit the impact of operational anomalies of major X-ray or laser instruments for which it is necessary to understand the links between beam characteristics and the physical parameters of the beamline optics. Sudden or slow anomalies/variations can thus be observed over time, such as focusing aberrations that directly affect the quality and speed of measurements. Therefore, understanding and characterizing the causes of these malfunctions and deviations from optimal measurement chain performance is crucial for quick response and maximum reliability in the operation of the beamline or laser. Although there are many anomaly detection methods in AI literature, they are generally based on correlation, which is not effective in conveying cause-and-effect relationships.

Thus, the objective of the project is to propose interpretable AI based on causal graphs to support beamline operators and scientists. The task is to develop a causality-based model to determine the sensor parameters involving anomalies. The method will complement the diagnostic tools for corrective action in suitable time frames. Therefore, the work can be divided into the following tasks:

- Understanding and handling the data produced by the beamlines: measurement instrument parameters and different types of anomalies. This will rely on the expertise of project partners, specialists in physics, optics, and instrumentation related to beamlines.

- Designing the model based on causal graphs that explain the links between different parameters and anomalies. We will focus particularly on :
 - hierarchical causal graphs to represent the multi-scale dimension of application (from the instrument to the beamline),
 - detecting latent variables that can provide error in the causal discovery process,
 - quantifying the uncertainty of the causal link to ensure the reliability of the causal graph,
 - taking into account the heterogeneous data, their dimensionality, and interactions between potential causes,
 - proposing a model to detect the anomaly or estimate the time before failure based on causal graph.

For this, the framework of Bayesian causal graphs will be considered to propose a surrogate model of the simulation model generally used to calibrate the parameters of the instruments.

In this position, you will support and contribute to the work of the LIAD, the Elie Cartan Institute of Lorraine University, the MICS Lab of Centralesupelec at Saclay the NRX, and the ESRF by responding to requests related to uncertainty methodology, AI, or a combination of both. You will promote your research by writing technical notes and publishing papers in specialized conferences and journals, as well as participating in DAL-LIAE project meetings alongside the entire team of experts.

Duration: 36 months

Project start date: By September 2024 at the latest

Job location: CEA Saclay

3 Candidate Profile

Master degree in AI or statistics, machine learning or applied mathematics.

Skills

- Fluency with Python programming for data analysis or machine learning.
- Interest in learning about other disciplines, physics in particular.
- Community-friendly team player.
- Excellent oral and written English communication.

4 Contact

Applicants are requested to submit the following materials:

- A cover letter applying for the position.
- CV.
- Academic transcripts (unofficial versions are fine).

Applications are only accepted through email. All documents must be sent to Aurore Lomet (aurore.lomet@cea.fr), Marianne Clausel (marianne.clausel@univ-lorraine.fr) and Myriam Tami (myriam.tami@centralesupelec.fr)

References

- [1] Clark Glymour, Kun Zhang, and Peter Spirtes. Review of causal discovery methods based on graphical models. *Frontiers in genetics*, 10:524, 2019.
- [2] Biwei Huang, Kun Zhang, Jiji Zhang, Joseph Ramsey, Ruben Sanchez-Romero, Clark Glymour, and Bernhard Schölkopf. Causal discovery from heterogeneous/nonstationary data. *Journal of Machine Learning Research*, 21(89):1–53, 2020.
- [3] Lucie Kunitomo-Jacquín, Aurore Lomet, and Jean-Philippe Poli. Causal discovery for fuzzy rule learning. In *2022 IEEE International Conference on Fuzzy Systems (FUZZ-IEEE)*, pages 1–8. IEEE, 2022.

[4] Judea Pearl. *Causality*. Cambridge university press, 2009.

[5] Jonas Peters, Dominik Janzing, and Bernhard Schölkopf. *Elements of causal inference: foundations and learning algorithms*. The MIT Press, 2017.