European Partnership on Metrology
Call 2024 –Digital Transformation, Green Deal, Normative and Research Potential

Selected Research Topic number: **SRT-d09**
Version: 1.0

Title: Machine learning for computationally expensive inverse problems in metrology

Abstract

Currently, many state-of-the-art topics (e.g. nanostructure reconstruction using non-destructive techniques in chip manufacturing, or non-invasive determination of physiological quantities in humans) require the inference of parameters through inverse modelling. This often requires high-dimensional, computationally demanding models of the measurement process and typically includes years of theoretical work in the modelling. In many cases the theoretical model for the measurement itself is also computationally demanding and thus the inverse problem to infer the desired measurement(s) is not well posed. To address this issue novel Machine Learning (ML) approaches need to be developed to bridge the gap between direct and indirect measurements. The ML approaches also need to be applicable to real-world use-cases and to include a comprehensive uncertainty assessment. Once verified for use the ML approaches should be disseminated to end users through good practice guides, benchmark datasets and an open-source software toolbox.

Keywords

machine learning (ML), inverse problems, parameter inference, uncertainty, surrogate modelling,

Background to the Metrological Challenges

ML methods are rapidly becoming integral in advanced measurement applications. This includes the determination of nano structure shape parameters in photolithography, used for process control during semiconductor production, and the determination of physiological parameters such as electrocardiogram (ECG) features or blood pressure through non-invasive measurement of photoplethysmography signals from human subjects in healthcare. Currently, there are two different ways to apply ML to advanced measurement applications, either through (i) data driven approaches using neural networks or (ii) intricate (complex and computationally expensive) approximation techniques integrating knowledge from the physical model. The benefit of the former is that data driven approaches are easy to apply. However, data driven approaches often lack in performance compared to more intricate problem specific modelling techniques. In addition, data driven approaches cannot presently provide accurate estimates for approximation or generalisation errors.

In industrial metrology, inverse problems occur when using scattering measurements to determine critical dimensions or optical constants for nanofilms and -layers. Complex models to address these inverse problems require the use of ML or other surrogates. Therefore, it is essential to determine the uncertainty contributions stemming from the measurement data, the model error and the ML approximation.

In general, the evaluation of measurement uncertainties follows agreed and well-established methods for simple models, however analogous methods for measurement uncertainties in tasks involving ML do not exist. Currently, the propagation of measurement uncertainties for input data in inverse problems is possible using standard metrology tools. But models and approximation errors from ML based surrogates (that replace the original expensive model) need to be developed and their reliability evaluated.

To support the use of ML methods in advanced measurement applications, new state-of-the-art approaches are needed to speed up physical models of computationally expensive measurement simulations including a large number of unknown model parameters. Approaches are also needed to solve the statistical inverse problem and to obtain reliable estimates for the desired quantities alongside their associated reconstruction uncertainties. This must be combined with the influence of different sources of errors, (e.g. measurement noise, model errors or noise model), on the performance of the chosen surrogates and methods to solve the inverse problem.

Objectives

Proposers should address the objectives stated below, which are based on the PRT submissions. Proposers may identify amendments to the objectives or choose to address a subset of them in order to maximise the overall impact, or address budgetary or scientific / technical constraints, but the reasons for this should be clearly stated in the protocol.

The proposal shall focus on metrology research necessary to support digital transformation in ML for computationally expensive inverse problems.

The specific objectives are

1. To investigate at least two computationally complex use-cases requiring ML for computationally expensive inverse problems and produce suitable model training and measurement datasets. The use-cases must be both beneficial and highly relevant to end-users e.g. optical semiconductor manufacturing and digital health.
2. Using the use-cases from Objective 1, to develop at least four different ML surrogates to learn the forward measurement models. Then to benchmark the ML models against (i) quality, (ii) training robustness and (iii) the influence of noise.
3. Using the use-cases from Objective 1, to investigate at least four different ML approaches to solve the inverse problems. Then to compare these different ML approaches in terms of complexity of (i) implementation, (ii) training robustness and (iii) generalisability.
4. To apply the ML methods from Objectives 2 and 3 to the use-cases in Objective 1 in order to verify the results in terms of (i) performance, (ii) applicability and (iii) the validity of the calculated uncertainties. Based on the results, to develop a good practice guide, benchmark datasets and an accompanying software toolbox for the use-cases and ML methods.
5. To develop guidelines with a focus on performance indicators and uncertainty quantification for ML tools in metrological applications based on computationally demanding forward and inverse models. To facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain (NMIs/DIs, calibration & testing laboratories), standards developing organisations (related to the European Chips Act and the EU AI Act) and end users (industry, semiconductor manufacturers, healthcare).

These objectives will require large-scale approaches that are beyond the capabilities of single National Metrology Institutes and Designated Institutes. To enhance the impact of the research, the involvement of the appropriate user community such as industry, standardisation and regulatory bodies, and other European Partnerships is strongly recommended, both prior to and during methodology development.

Proposers should establish the current state of the art and explain how their proposed project goes beyond this. In particular, proposers should outline the achievements of the EMRP NEW04 Uncertainty, EMPIR 18HLT07 MedalCare and 20IND04 ATMOC and Metrology Partnership 22HLT01 QUMPHY projects and how their proposal will build on those.

Proposers should note that the programme funds the activity of researchers to develop the capability, not the required infrastructure and capital equipment, which must be provided from other sources.

EURAMET expects the average EU Contribution for the selected JRPs in this TP to be 1.9 M€ and has defined an upper limit of 2.4 M€ for this proposal.

EURAMET also expects the EU Contribution to the external funded beneficiaries to not exceed 35 % of the total EU Contribution across all selected projects in this TP.

Any industrial beneficiaries that will receive significant benefit from the results of the proposed project are expected to be beneficiaries without receiving funding or associated partners.

Potential Impact

Proposals must demonstrate adequate and appropriate participation/links to the ’end user’ community, describing how the project partners will engage with relevant communities during the project to facilitate knowledge transfer and accelerate the uptake of project outputs. Evidence of support from the “end user” community (e.g. letters of support) is also encouraged.

You should detail how your proposal's results are going to:

- Address the SRT objectives and deliver solutions to the documented needs,
- Feed into the development of urgent documentary standards through appropriate standards bodies,
- Facilitate improved industrial capability, or improved quality of life for European citizens in terms of personal health, protection of the environment and the climate, or energy security,
- Transfer knowledge to the semiconductor, manufacturing and healthcare sectors.

You should detail other impacts of your proposed JRP as specified in the document "Guide 4: Writing Joint Research Projects (JRPs)"

You should also detail how your approach to realising the objectives will further the aim of the Metrology Partnership to develop a coherent approach at the European level in the field of metrology and include the best available contributions from across the metrology community. Specifically, the opportunities for:

- improvement of the efficiency of use of available resources to better meet metrological needs and to assure the traceability of national standards
- the metrology capacity of EURAMET Member States whose metrology programmes are at an early stage of development to be increased
- organisations other than NMIs and DIs to be involved in the work.

Timescale

The project should be of up to 3 years duration.

Additional information

The links provided in this section are only correct at the time of publication up until the end of the Call year.

The references below were provided by PRT submitters; proposers should therefore establish the relevance of any references.

[1] *EMN for Advanced Manufacturing Strategic Research Agenda* https://www.euramet.org/european-metrology-networks/advanced-manufacturing/strategy/strategic-research-agenda

[2] *EMN for Mathematics and Statistics Strategic Research Agenda* https://www.euramet.org/research-innovation/metrology-partnership/strategic-research-and-innovation-agendas