Mathematics and Statistics for Digitalization

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Abstract

Digitalization is one of the major current societal challenges and its appropriate handling will determine the future economic success of Germany and the EU. The dramatic development over recent years of computational capacities, the introduction of smart sensors and their interconnection via the Internet have enabled new technological advances that will change daily life. Future metrology faces a transition from the assessment of single measurement devices to fully connected sensor systems raising new challenges such as their calibration or uncertainty quantification. Established mathematical and statistical approaches are often no longer sufficient and need to be expanded or even replaced with new methods. This paper intends to identify and discuss the need for the development of novel methods in mathematics and statistics for metrology required to successfully deal with the challenges of digitalization over the next decades.

1 Introduction

Data analysis and mathematical procedures play a key role in today's metrology. Without the application of advanced techniques from signal processing, statistics and numerical analysis, current high-accuracy measurement results would not be possible. M. Sené, I. Gilmore and J. T. Janssen from the National Physical Laboratory (NPL) in the UK, for example, emphasize the role of advanced data analysis and related uncertainty quantification in metrology in a recent viewpoint in Nature [1]:

"Measurement technology is becoming more powerful and complex. … Tracking and quantifying the uncertainty of the final result can get lost amid all this data crunching ... An increasing number of research areas lack a metrological framework, however ... Quantifying uncertainty in complex problems is almost becoming a field in itself. The metrology community needs to step up to this challenge, in particular by engaging more statisticians, data experts."

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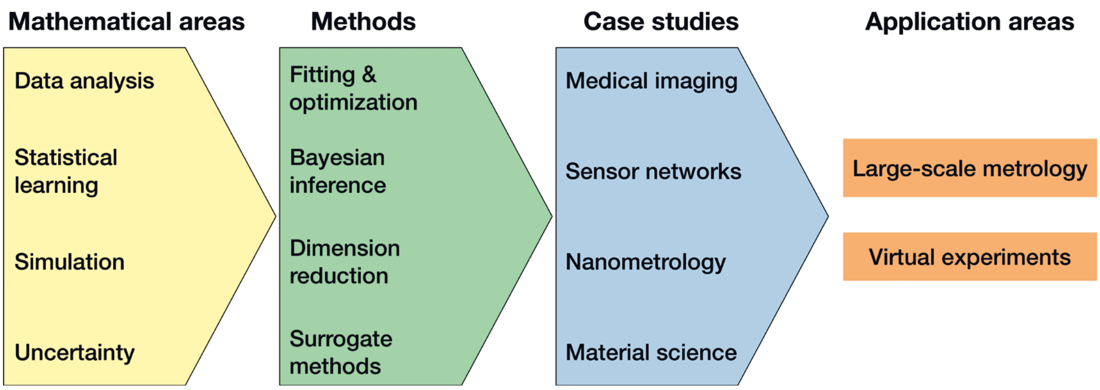

Figure 1: Impact of mathematics and statistics on digitized metrology.

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Digitalization drastically boosts the importance and impact these methods have on metrology. The expertise in mathematical and computational tools will decide about the leading role in future metrology and the speed of the transition of classical metrology to digitized metrology. The impact of statistical data analysis in this transition is underlined in National Science Review [2] by J. Fan, F. Han and H. Liu, statisticians from Princeton University and Johns Hopkins University:

"Big Data bring new opportunities to modern society and challenges to data scientists ... the massive sample size and high dimensionality of Big Data introduce unique computational and statistical challenges…. Valid statistical analysis for Big Data is becoming increasingly important."

Metrology as the science of measurement has always been, and will always be, concerned with quantitative results, including the quantification of their uncertainty. Without a reliable characterization of the measurement uncertainty, measurement results cannot be traced back to the basic units of measurement, a key mission of any National Metrology Institute (NMI). While uncertainty quantification is well understood for conventional metrology, corresponding concepts are lacking for some of the tasks faced in digitized metrology. Examples comprise the uncertainty associated with a sensor network or an empirical model built from a huge amount of data by machine learning techniques. The development of novel methods for uncertainty evaluation therefore is a major challenge for the successful handling of digitalization.

Digitalization will significantly intensify the need for large-scale metrology, i.e. metrology that is concerned with measurands consisting of a large, or even a huge, number of quantities (10^5 or more, say). Sensor networks are just one example, but also for conventional metrology this issue is becoming increasingly relevant, e.g. within dynamic metrology, where the goal is the determination of a whole function such as a time-dependent dynamic force in a crash test, or when characterizing spectral properties in photometry. Metrology is also turning, more and more, towards emerging fields such as health metrology, where imaging methods are often developed into quantitative tools, or nanometrology, where the ever-improving spatial resolution of measurement techniques provides high-dimensional sets of data. Currently, the relevant tasks are solved only approximately, for example by ignoring the presence of correlation in the results. This is because current computational techniques cannot successfully deal with full covariance matrices of such high dimensions.

Modern computer capacities have strongly enhanced the use of **virtual experiments**. Virtual experiments allow the cheap and comprehensive exploration of complex measurement devices. They are particularly suitable when designing such devices. Today, virtual experiments have also become an integral part of measurement devices, used in the analysis of the recorded data. Typically, virtual experiments produce huge amounts of data, and often the modelling of the physical principles is computationally expensive. Issues of large-scale metrology therefore enter the analysis of virtual experiments, as well as surrogate modelling for the approximate, numerically efficient representation of the results of a virtual experiment.

Digitalization leads to a rapid increase of situations where huge amounts of data are produced that shall be used for modelling, prediction and control. Examples comprise such different applications as health monitoring from various modalities or process control via large amounts of interacting sensors in industrial facilities. In order to retrieve the relevant information from such unstructured data, methods from **machine learning** are used for empirical model building and decision-making. Challenges for metrology are that these methods need to be accompanied with an uncertainty quantification. Furthermore, when such methods become an integral part of novel measurement systems, reference procedures and reference data need to be developed to properly assess them.

Statistical process control applies statistical procedures to monitor processes and immediately detect when these processes no longer follow intended specifications. Digitalization poses challenges for these established techniques, and current tools may no longer be applicable. Legal metrology is one field where digitalization can lead to a huge impact of techniques from statistical process control.

In the following, these different challenges in mathematics, statistics and numerical computation are illustrated and discussed.

2 Large-scale metrology

Large-scale metrology is concerned with measurands that consist of large, or even huge, numbers of quantities to be determined simultaneously from measured data. Examples comprise applications in conventional metrology such as dynamic measurements, nanometrology or photometry, where either a whole function is to be determined or large numbers of quantities (10^5 or more). The sheer amount of variables and measured data can already prohibit the estimation and handling of covariance matrices by conventional means. Another challenge is that current computational tools for nonlinear regression problems such as least-squares fitting or state-of-the-art Monte Carlo techniques in statistics do not scale well to dimensions significantly larger

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than 10^4. New statistical methods and computational tools are needed to extend today's metrology to large-scale measurement systems, and their development represents current frontiers in statistical research [3–11].

So far, large-scale metrology has been constrained to a few special areas within metrology such as coordinate measurement techniques. In mainstream metrology, major tasks are still dominated by single device systems and the presence of a small number of quantities, or even of a single quantity, that constitutes the measurand [12]. However, digitalization will drastically change this situation and force metrology to successfully deal with large-scale metrology. Sensor networks (e.g. for environmental monitoring with high spatial and temporal resolution) are just one example that emerges from the new possibilities that digitalization creates. The transition to digitized metrology will move issues of large-scale metrology from the edge to the centre of modern metrology, and all the mathematical and statistical challenges faced for large-scale metrology need to be properly addressed.

3 Virtual experiments

The development of modern computer capacities allows the implementation of virtual experiments that capture the features of complex measurement devices in a realistic way. Virtual experiments enable the comprehensive exploration of possibilities and limitations without the need for carrying out real experiments, thereby providing a cheap way to optimally design new measurement devices. PTB has, for example, developed SimOptDevice, a flexible tool for designing and running virtual experiments for optical form measurements [13, 14] that has proven essential in several industrial projects.

Virtual experiments have meanwhile also become an integral part of novel measurement devices. For example, the tilted-wave interferometer [13] is actually based on a virtual experiment. The tendency of virtual experiments to become a part of measurement devices is growing, and when interconnecting a large number of smart sensors and measurement devices, at least some of them can be expected to depend on a virtual experiment. Metrology is faced with questions such as how to calibrate virtual experiments or the way an uncertainty is assigned to their outputs. At the same time, it can be expected that such questions will often need to be addressed in an online fashion.

Nowadays computational advances also allow the realistic modelling and simulation of measurement processes when the governing physical laws are well understood and easily cast in the form of basic equations such as the Navier-Stokes equations and their variants in flow metrology, or the Maxwell equations in many applications in optics and electromagnetic scattering. Numerical tools such as the finite-element method are applied to explore the behaviour of a measurement device including the object under study. The employed algorithms, however, often produce a large amount of data points in order to adequately reproduce the corresponding continuum functions representing, e.g. flow or electric fields, see e.g. [15, 16].

The mathematical and statistical challenges are then similar to those of large-scale metrology. However, in some cases, virtual experiments are still computationally too expensive, and tools from surrogate modelling are needed. These methods are particularly important for adequate uncertainty characterization in measurements where the relationship between the variables is governed by partial differential equations. Metamodelling techniques use values of a computationally expensive model to determine a computationally cheap surrogate model, which then allows statistical analyses, including uncertainty quantification, to be performed that would have been intractable otherwise.

4 Statistical monitoring and process control

Statistical process control comprises well-established statistical techniques for the control and monitoring of processes [17]. Control charts such as multivariate Shewhart charts are routinely applied nowadays to detect the onset of instabilities. Digitalization poses challenges for these established techniques, for example, when decisions need to be made in view of huge amounts of unstructured data for which current control charts are no longer applicable. Legal metrology is another field in which statistical monitoring can become an important tool. While today conformity assessment is usually done by checking a single device, or a sample of devices (drawn randomly from a large population of devices), digitilization may enable conformity assessments to be made online, and for whole populations of devices at the same time. Proceeding in such a way will result in huge savings. And it will also improve the desired quality assurance significantly as all devices may undergo an ongoing, permanent conformity assessment check. However, in order to meet the specific legal requirements through online statistical quality assurance, corresponding statistical procedures need to be developed which optimally address the specific legal requirements. This in turn calls for individual solutions in different fields due to their different requirements.

5 Machine learning

Machine learning refers to computer algorithms that are able to learn and to make predictions from empirical data. It comprises a large variety of methods that describe how empirical models are extracted from data. These models are typically employed to produce reliable and repeatable decisions and to uncover hidden correlations and structures from data sets. The field has strong relations to computational statistics and statistical learning theory [18] and draws upon the theory and methods from mathematical optimization. While machine learning has been known for decades, recent developments in both computational capacities as well as methodological advances (such as deep convolutional neural networks [19]) have boosted their importance significantly, and meanwhile methods from machine learning represent the state of the art in applications such as the diagnostics of diseases based on medical imaging data or pattern recognition in language processing and computer vision [20]. The aspect of uncertainty associated with the results of methods from machine learning has recently been brought to the fore under the label of probabilistic machine learning, but is still in its infancy [21]. Methods from machine learning are expected to play a major role in future digitized metrology, and the further development of these methods, particularly focusing on issues of uncertainty quantification, represents a statistical research program that will be highly relevant for future metrology.

6 Measurement uncertainty

Comparison of measurement results, reliable decision-making and conformity assessment require the evaluation of uncertainties associated with measurement results. The ability to compare measurements made in different places and at different times underpins international metrology. The Guide to the Expression of Uncertainty in Measurement (GUM [22]) provides the current state of the art for uncertainty evaluation in metrology. JRP EMRP NEW04 (08/12-07/15) [23] extended the methods of the GUM to inverse and regression problems and to computationally expensive systems.

In recent years, metrology has expanded to support new fields to address societal challenges relating to energy and sustainability, climate and environmental monitoring, life sciences and health, using measurement modalities such as imaging, spectroscopy, earth observation and sensor networks. Reliable uncertainty evaluation is particularly important in these applications, e.g. to safeguard diagnostics in medical imaging or to reliably monitor air pollution. However, due to the large numbers of unknown quantities and measured data (10^5 or larger) involved in these applications, e.g. where a sensor network is used to measure and predict environmental quantities with high spatial and temporal resolutions, neither the GUM nor the methods developed within EMRP NEW04 are applicable.

Digitalization will substantially strengthen these developments and the need for novel uncertainty quantification methods. Furthermore, for each of the above-discussed mathematical issues that are becoming relevant in digitized metrology, i.e. large-scale metrology, virtual experiments, statistical process control and machine learning, the adequate evaluation of uncertainties associated with the results is challenging. For example, large-scale metrology is concerned with measurands of large, or even huge, dimensions which already challenges uncertainty characterizations in terms of full covariance matrices, and even more so when characterizing uncertainty through probability distributions. Characterizing the uncertainty associated with results from virtual experiments is often faced with high-dimensional quantities and computationally expensive models, and generally virtual experiments yield a necessarily imperfect image of a real process which needs to be accounted for. Finally, machine learning is usually applied for estimating model relationships or determining a classification only, without providing an uncertainty quantification associated with these results. When applied for digitized metrology, these methods need to be accompanied with an uncertainty quantification. While concepts for the evaluation of uncertainty for machine learning are an issue of current research (e.g. [21]), substantially more research is needed before these techniques can be safely applied for digitized metrology when similar demands on the quality of results shall be posed as in today's metrology.

7 Summary and conclusion

We have identified large-scale metrology, virtual experiments, statistical process control, machine learning and uncertainty quantification as key challenges for metrology in the age of digitalization. Digitalization drastically boosts the already high importance and impact mathematics and statistics have in today's metrology. Furthermore, established mathematical and statistical approaches will need to be expanded, or even be replaced, by new methods in order to successfully face the transition of classical metrology to digitized metrology. Metrology in the decades ahead will strongly depend on mathematics and statistics and their future developments.

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