Fundaments of measurement for testing software in computationally-intensive metrology

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Abstract

This talk presents preliminary results from a project between European national laboratories (EUROMET), entitled "Traceability for Computationally-Intensive Metrology" (JRP NEW06 (TraCIM)) to demonstrate metrology software is fit for purpose.

The talk begins by presenting a new mathematical model for measurement, based on "measurement as an inverse problem" that has consequences for reconstruction algorithms in many modern complex measuring instruments such as CT scanners and white light interferometers.

Since metrology software is part of the measuring procedure the "measurement as an inverse problem" model applies and can be used as a foundation to derive properties and build tests for metrology software.

1 Introduction

There is much literature on testing general software, including using datasets (softgauges), with known properties, as input data in which the output results from a given algorithm are also known to a specified tolerance. The question is, is there anything special about measurement computations that can facilitate in the testing the correctness and limitations of measurement computations? Traceability, measurement standards, and quality systems all demand that computational links are demonstrated to be fit for purpose, but:

There is no coherent framework for testing metrology software. Software developers and measuring equipment suppliers have to fill these gaps with their own ad hoc approaches.

- For software performing complex computation, adequate testing is difficult without an effective method of knowing if the software is producing accurate results.

- Computational software depends on finite-precision arithmetic, and it is not sufficient to claim that the software is bug-free.
- For difficult computations, approximate solution methods are used but there is no way of demonstrating that such methods provide sufficiently accurate results.

In order to begin to answer this question, the question of what is measurement also needs to be addressed, since the software for computationally-intensive metrology is part of the measurement procedure. The next section develops measurement theory beyond the current state-of the-art to an enhanced measurement model; the measurement as an inverse problem model (Scott and Forbes [1]) that can begin to answer the questions above.

2 Measurement theory

2.1 State of the art

Measurement is fundamental to obtaining scientific knowledge. For over a hundred years philosophers, physicists, mathematicians, social scientists etc. have pursued the definition or analysis of the concept of measurement. The representational theory of measurement has gained wide support among measurement theorists and is the current dominant paradigm, [2-5].

The representational theory of measurement considers measurement to consist of the following:

1. A set of objects on which a measurand (quantity to be measured, ISO/IEC Guide 99 [6]) is defined together with an empirical relational structure specifying the relationships between measurands.
2. A set of numbers (measured values) together with a numerical relational structure.
3. A set of mappings (homomorphisms), called the measurement procedure, from the set of measurands into a numerical one, under which the empirical relational structure of the measurands are preserved in the numerical relational structure.

The representational theory of measurement can be used to define the topological stability of a measurement procedure. Scott [7] considered that when a measuring procedure is topologically stable a ‘small’ difference in the measured values implies a ‘small’ difference in the measurand.

For finite sets there is a one-to-one correspondence between the topologies on the set and the partial pre-orders[1] defined on the set, see Cameron [8], section 3.9. Scott [7] was able to demonstrate (using the one-to-one correspondence between finite topologies and finite partial pre-orders) that if

[1] A partial pre-order (quasi order) is a relational structure that consists of a collection of objects, (a, b, c, d, …) say, together with a relationship R between these objects that is reflexive (i.e. always aRa, bRb, cRc, ...) and transitive (i.e. if aRb & bRc then always aRc).

for a measurement procedure the relational structures of the measurand and the measured values are both partial pre-orders and the homomorphisms between them are also increasing mappings then the measurement procedure is topologically stable.

In summary, for a stable measurement, in the representational theory of measurement the measurands are defined on a set of objects with a relational system defined on them which is a partial pre-order; this is mapped via an increasing mapping (structure preserving mapping) onto another set of objects (numerical) also with a relational system which is a partial pre-order; further one particular object is identified in the numerical relational system as being the observable result of the measurement. Due to the stochastic nature of physical measurement, repeated measurements result in different particular objects being identified which can be characterised by a probability distribution over the objects in the numerical relational system. This probability distribution contributes to the resulting measurement uncertainty (ISO/IEC Guide 98-3 [9]).

2.2 Measurement as an inverse problem

Modern scientific instruments are becoming more and more complex with the observed measurement being a proxy for the value of the measurand (e.g. sinograms in CT scanners, see Mueller and Siltanen [10], stack of interferograms in white light interferometers see Balasubramanian [11].) with the value of the measurand having to be reconstructed from the proxy observable measurements. This reconstruction can be represented as an inverse mapping from the numerical relational system back to the relational system of the measurand, i.e. as an inverse problem. The inverse problem model of measurement is an extension of the representational theory of measurement model. An example is CT measurement where the observed values are a sinogram constructed from different projections on an object. The inverse problem is then to use the sinogram to reconstruct an inverse solution that is the inference to the 'best' model that directly maps onto the observed data.

A general inverse problem is to compute either the input or the system, given the output and the other quantity (see figure 1).

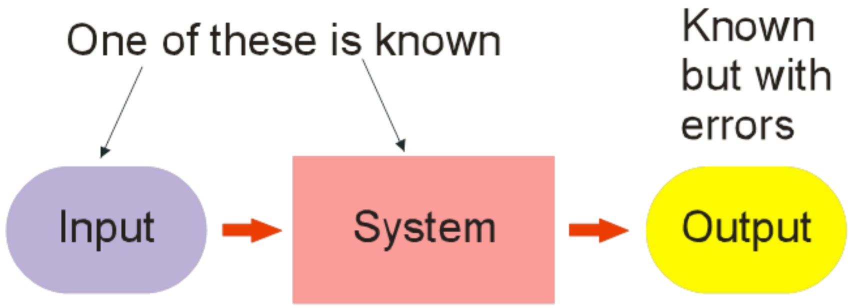

Figure 1 Schematic of the structure of inverse problems

In 1902 Hadamard [12] stated three criteria for an inverse problem to be well posed:

1. Existence: There exists an input that exactly fits the observed data;

2. Uniqueness: There is a unique input that exactly fits the observed data;
3. Stability: There are small changes in the input when there are small changes in the observed data.

An inverse problem is ill-posed if any one of these conditions is not satisfied. It is assumed in this paper that the measurement system is known. The reconstruction of the measurand from the observable data in a stable way that gives a meaningful interpretable measurand is the inverse problem of measurement. Measurement is essential to the scientific approach and stable meaningful interpretation of measurands is crucial to this endeavour. Thus the inverse problem of measurement is a very fundamental scientific problem.

There has been a huge discussion on reconstruction methods within the metrology community. Many approaches are very ad hoc and create artificial features (e.g. “bat wings” on edges for optical surface measuring instruments, Goa et. al [13]). Many cannot give a meaningful scientific interpretation of the reconstructed measurand. This paper addresses this fundamental inverse problem of measurement by exploring the mathematical structure (in terms of category theory) of the problem and giving three properties that are sufficient and necessary for stable and meaningful reconstruction.

Property one: Topological stability

As defined above topological stable measurement implies both the relational structures on the measurand and the observed data are partial pre-orders and the homomorphism from the measurand to the observed data (Forward mapping F) is an increasing function.

Property two: Inverse mapping constraint

The inverse homomorphism from the observed data to the measurand (Inverse mapping I) must map onto measurand objects whose forward mappings are the original observed data; i.e. in terms of mapping compositions $F \circ I \circ F = F$.

Property three: Meaningfulness

Meaningfulness is when the relationships of the observed data can give a meaningful interpretation of the relationships of the measurands. In terms of mappings this implies:

$X \geq Y$ iff $F(X) \geq F(Y)$)

and $I(A) \geq I(B)$ iff $A \geq B$

Where X & Y are measurand events

A & B are observed data

and ‘iff’ means if and only if.

Otherwise it is possible that a relationship in the observed data implies (through the inverse mapping) a relationship in the measurand that does not exist.

It can be shown that Properties P1 to P3 imply that the Forward and Inverse mappings form a Galois Correspondence (Adjoint Functors).

That is to say: $X \geq I(A)$ iff $F(X) \geq A$

Galois Correspondence implies that the corresponding measurement is well posed according to Hadamard's three criteria and that a stable and meaningful reconstruction is possible (called the Ockham inverse solution) and is given by:

$$I(A) = \min\{X \text{ s.t. } F(X) \geq A) \text{ (see Dikranjan and Tholen, [14])}$$

The Galois correspondence model also has additional structure useful for the interpretation of the measurement procedure. The subsets of measurand values that forward map onto particular observable data points partition the measurands into an equivalence relation called the measurand resolution, since the observed data cannot distinguish between measurand values within a subset. Similarly observed data resolution can be defined from the equivalence relation constructed from the subsets of observed data that inverse map onto particular measurands. Both these resolutions can be used in the calculation of the measurement uncertainty due to the metrology software.

Many inverse measurement problems are naturally ill-posed (e.g. CT reconstruction from the sinogram) but the full weight of inverse problem theory techniques can be used (such as regularization) to rectify this situation by turning an ill-posed problem into a well-posed problem that is a close approximation to the original such that useful reconstructions result. Throughout the rest of this paper it is assumed the software under test is part of a well-posed measurement procedure.

3 Testing Metrology Software

Since metrology software is part of the measuring procedure the "measurement as an inverse problem" model applies and can be used as a foundation to derive properties and build tests for metrology software.

A very common approach to test metrology software is through softgauges. These are reference pairs of data comprising reference input data and reference output data for a particular computational aim of the metrology software. The comutational aim metrology software is tested by processing the reference input data using the test software and comparing the results returned (in an appropriate way) with the reference output data.

Softgauges are constructed with data generators which are generally implemented in one of the following two approaches:

- Forward data generation: taking reference input data using Reference Software to produce corresponding reference output data.
- Reverse data generation: taking reference output data and using it to produce corresponding reference input data.

The forward approach to data generation involves developing reference software to take the input reference data to produce the reference output data which in practice can be difficult and costly. The reverse approach to data generation requires a mathematical understanding of the forward process from which the Ockham inverse solution can be constructed to produce the corresponding reference input data. This is often more simple to implement than the forward data generation approach.

Example CT reconstruction

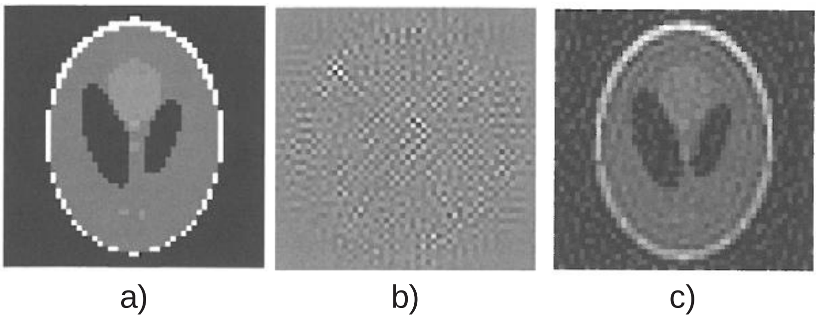

Figure 2 a) original modified Shepp-Logan phantom image; b) reconstruction of a sonogram with 0.1% noise; c) regularization reconstruction using 1500 Eigenfunctions

Reconstruction from the sonogram in a CT scan is ill-posed. As a result adding 0.1% noise to the sinogram makes the reconstruction (figure 2b) unrecognisable from the original image (figure 2a). The reconstruction of the ill-posed problem cannot have an uncertainty statement associated with it as a result of the global instability of the ill-posed problem. Using the first 1500 Eigenvalues, as a regularization technique, converts it into a well-posed approximate model allowing a useful reconstruction with the Ockham solution, with only 48% relative error and also allows uncertainty statements to be made.

4 Conclusions

The "metrology as an inverse problem" has been introduced. Three properties are described that are necessary and sufficient for the forward and inverse mappings to form a Galois correspondence ensuring that the measurement is well posed. The formula for Ockham reconstruction, from the observed data to the measurands, has also been given for well-posed measurement procedures. Further the measurand resolution and the observed data resolution have been given as part of the structure of the Galois correspondence model. There has been a brief discussion on data generators for softgauges to test metrology software, in particular Forward and Reverse data generators and how the Ockham solution can help with reverse data generators for well posed metrology software. Finally an example from CT scanning illustrates how inverse problem techniques are useful for reconstruction in metrology instrumentation.

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