The Structure of a General Type of Inverse Problem in Metrology

By

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Abstract

Inverse problems are ubiquitous in science. The theory and techniques of inverse problems play important roles in metrology owing to the close relation between inverse problems and indirect measurements. However, the essential connection between the concepts of inverse problems and measurement has not been deeply discussed before. This thesis is focused on a general type of inverse problem in metrology that arises naturally in indirect measurements, called the inverse problem of measurement (IPM).

Based on the representational theory of measurement, a deterministic model of indirect measurements is developed, which shows that the IPM can be taken as an inference process of an indirect measurement and defined as the inference of the values of the measurand from the observations of some other quantity(s). The desired properties of solving the IPMs are listed and investigated in detail. The importance of estimating empirical relations is emphasised. Based on the desired properties, some structural properties of the IPMs are derived using category theory and order theory. Thereby, it is demonstrated that the structure of the IPMs can be characterised by a notion in order theory, called 'Galois connection'.

The deterministic model of indirect measurements is generalised to a probabilistic model by considering the effects of measurement uncertainty and intrinsic uncertainty. The propagation of uncertainty from the observed data to the values of measurands is investigated using a method of covariance matrices and a Bayesian method. The methods of estimating empirical relations with probability assigned using the solutions of IPM are discussed in two different approaches: the coverage interval approach and the random variable approach.

For estimating empirical relations and determining the conformity of measurement results in indirect measurements, a strategy of estimating the empirical relations with high resolution is developed which significantly reduced the effect of measurement uncertainty; a method of estimating specification uncertainty is proposed for evaluating the intrinsic uncertainties of measurands; the impact of model resolution on the specifications of the indirectly measured quantities is discussed via a contradiction in the specifications of surface profiles.

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Nomenclature

A	Set of objects with a common measurand
X	Set of the values of a measurand
$\mathcal{M}$	Model space, e.g. $\langle M, \precsim \rangle$
$\mathcal{D}$	Data space, e.g. $\langle D, \precsim \rangle$
F	Forward mapping of an inverse problem, F: $M \rightarrow D$
$F^{\dagger}$	Generalized inverse of F
G	Backward mapping of an inverse problem, G: $D \rightarrow M$
T	Extracting function, T: $M \rightarrow X$
I_A	Identical mapping of set A
$\cong$	Isomorphism
$\leq_M$	Binary relation in the model space
$\leq_D$	Binary relation in the data space
$\precsim$	Preorder
$\sim$	Equivalence relation
$\preceq$	Partial order
$\lhd$	Interval order
$\wr$	Indifference relation
D_S	Function processing dilation filter with a structuring element S
E_S	Function processing erosion filter with a structuring element S

Abbrevations List

IPM	Inverse problem of measurement
ERS	Empirical relational system
NRS	Numerical relational system
Poset	Partcially ordered set
IFK	Fredholm integral equation of the first kind
SVD	Singular value decomposition
MVN	Multivariate normal distribution
PDF	Probability density function
JDF	Joint probability density function
MAP	Maximum a posteriori
ANOVA	Analysis of variance
USL	Upper specification limit
LSL	Lower specification limit

Chapter 1
Introduction

1.1 Background

Inverse problems are problems of inferring the information of the causes from the observations of some effects (Sabatier 2009, Turchin *et al* 1971). Inverse problems are ubiquitous in science, from geophysics (Zhdanov 2002) to imaging (Bertero and Boccacci 2010) and many other disciplines (remote sensing, nondestructive testing, weather prediction, etc.). Many mathematical techniques and theories have been developed for solving inverse problems in different disciplines.

Metrology is the science of measurement and its application, which includes all theoretic and practical aspects of measurement (JCGM 200 2008). It is a common phenomenon that inverse problems arise in different types of measurements. Many techniques of solving inverse problems have been applied in metrology, such as the contact surface measurement (Example 3.1), white light interferometry (Malacara 2007) and tomography (Kak and Slaney 1988). However, it appears that the essential connection between inverse problems and measurement has not been deeply studied before, and the inverse problems which involved in measurement have not been studied and characterised from the perspective of measurement theory. Mroczka & Szczuczyński (2009) pointed out the importance of inverse problems formulated in terms of first-kind Fredholm integral equation in indirect measurements. However, they focused on reviewing the existing methods of solving inverse problems without characterising the special properties of this type of inverse problem. Rossi (Rossi 2006) proposed a framework of measurement that allows (indirect) measurement to be considered as a system of mappings. However, in this framework, the characteristic function of a measurement process (or measuring system) is assumed to be invertible, which in practice is not always true, thus inverse problems or ill-posed problems in the framework of measurement were not considered.

In physics, inverse problems are often regarded as parameter estimation problems (Aster *et al.* 2005), where the parameters are some physical quantities related to a physical system (e.g. the location and origin time of an earthquake). In the perspective of metrology, the solutions

of model parameters are measurements of quantities (measurands), which are measured indirectly via some other quantities (proxy quantities). Thus, these inverse problems are associated with indirect measurements. There is an essential connect between indirect measurements and inverse problems.

In this thesis, a general type of inverse problem involved in indirect measurements is defined and named as the inverse problem of measurement (IPM). The concept of the IPM provides a novel prospect for both inverse problems and indirect measurements in the sense that the inference process of indirect measurement is an inverse problem, and the solution of the IPM is or contains the value of the measurand. It also provides new objective criteria on the way of solving the associated inverse problem.

The structural properties of the IPMs provide a deep understanding of the IPMs and enable the derivation of a typical type of the IPM that possesses the structure properties of Galois connections. Measurement theory (Michell 2007) and category theory (Mac Lane 1971) are used to investigate the structural properties of the IPMs.

Furthermore, understanding the structure of the IPMs allows (i) the development of stable measurement procedures, particularly reconstruction methods in indirect measurement, such as those that occur in computed tomography (CT) scanner and coherence scanning interferometer (CSI) areal texture instruments, (ii) traceability for computational metrology, particularly for computationally intense metrology and the development of the test procedures for reference metrology algorithms and reference software datasets (Soft-gauges).

1.2 Objectives and approaches

The main aim of this thesis is to define a general type of inverse problem in metrology and to determine its basic structural properties. It can be elaborated by the following objectives:

1. To understand the connection between metrology and inverse problem by undertaking a literature review of measurement theory and inverse problems.

2. To determine the common structural properties of different types of inverse problem by undertaking a literature review on the structure of inverse problems. Category theory will be used to investigate and describe the structural properties.

3. To develop a deterministic model of indirect measurements as a system of mappings

based on the representational measurement theory, thereby defining a general type of inverse problem involved in indirect measurements (IPM).

4. To investigate and determine the desired properties of solving the IPMs according to the three essential issues (existence, uniqueness and stability) of ill-posed problems (Hadamard 1902) and the criteria of measured values.

5. To investigate the structural properties of the IPM based on the derived desired properties, and find out the connection between the structure of IPM and the structural properties of the associated Galois connection.

6. To develop a probabilistic model of indirect measurement, which is compatible with uncertainty, based on the deterministic model.

7. To understand the propagation of uncertainty from the measured data to the res, and determine the methods of estimating empirical relations when the measurement uncertainty is contained in the measured data.

8. To find out the possible applications of the structural properties of inverse problems in metrology using case studies.

The author does not intend to cover all the structural properties of the IPMs. Only the basic structural properties that can be used to characterise the IPMs are discussed in this thesis.

1.3 Structure of the thesis

This thesis is divided into two parts: the first part from Chapter 2 to Chapter 4 is the theoretical basis for the model of indirect measurements and the structure of the IPM, and the second part from Chapter 5 to Chapter 7 concerns practical applications of the developed theories to metrology.

In Chapter 2, a literature review on the basic concepts of this study, including inverse problems, mathematical structure, measurement theory and category theory, is conducted. In addition, the methodologies of previous studies on the structure of inverse problems are reviewed. In Chapter 3, a deterministic model of indirect measurements is developed and the inverse problem involved in this model is characterised by its basic structural properties. In Chapter 4, measurement uncertainty is added to the deterministic model, and the metrology of estimating empirical relations in the IPMs is developed. A novel way of estimating

empirical relations is proposed in Chapter 5. A method of estimating the specification uncertainty is proposed in Chapter 6. A contradiction in the specification of surface profile is discussed from the perspective of the IPM in Chapter 7. Chapter 8 includes a conclusion of the important and novel work contained within this thesis, together with recommendations for future work.

The logical structure of this thesis can be described by the following graph, in which the round icons are the objectives of the research, the rectangular icons are the novel contributions, and the icons in the other shape are the applied background knowleges.

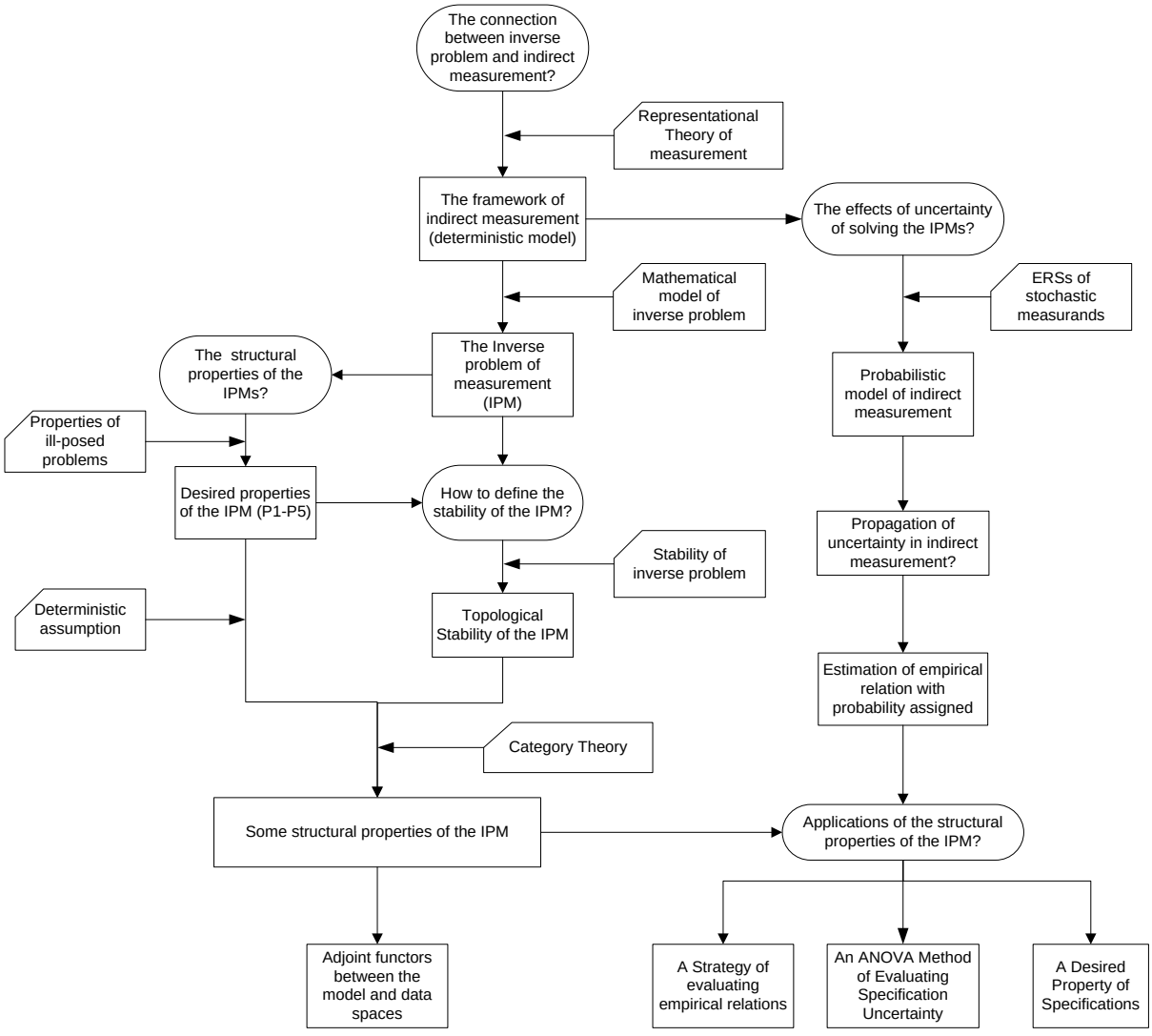


Figure 1.1 The logical structure of this thesis

Chapter 2
Literature Review

2.1 Introduction

To investigate the structure of inverse problems in metrology, the following theories and concepts are essentially important. Representational measurement provides a good theoretical basis for investigating measurement in terms of mathematical structures. The concept of indirect measurement reveals the connection between measurement and inverse problem. The mathematical model and basic concepts of inverse problems are needed to identify and model inverse problems in metrology. Category theory is a useful tool for proving theorems about mathematical structures, which provides an abstract way of investigating and describing mathematical structure in terms of a system of objects and their mappings.

This review starts with the development of measurement theory, which gives a general understanding of measurement theory. Based on the representational theory of measurement, measurement is taken as a structure-preserving mapping between the empirical relational system (ERS) of the measurand and the numerical relational system (NRS) of the measurand values. The measurability of an attribute is discussed from the mathematical and practical points of view. With the assumption of the measurability, a definition of measurement is given with the concepts of quantity and quantity values. The concept of indirect measurement is introduced. The definition and the mathematical model of inverse problems are introduced and some examples of inverse problems in metrology are given. The general concept of mathematical structure is reviewed, and category theory is briefly introduced. The metrologies and results of the previous studies on the structure of inverse problems, including generalised inverse and functional analysis, are reviewed, and the gaps in this research area are discussed in the summary.

2.2 Measurement theory

2.2.1 Development of measurement theory

Measurement theory is a branch of applied mathematics on the theoretical aspects of measurement, which answers the following two fundamental questions.

1) What kinds of attributes can be measured?
2) Are there different types of measurements?

There is more than one theory of measurement, each of which gives a different definition of measurement. Generally speaking, measurement associates numbers to some attribute of a class of phenomena, bodies, or substances (collectively refer to as objects) in such a way to describe the attribute. This kind of activity started much earlier than the development of measurement theory, probably in terms of counting of units, such as days, numbers of animals, which appeared since the invention of number. The earliest figures representing numbers are in the forms of slashes and dots on cave walls, grooves on sticks, which appeared in the early Stone Age. The line of dots in the cave painting (Figure 2.1), which was found in a 17,300-year-old cave at Lascaux, France, is probably used for counting the number of the megaloceros.

Figure 2.1 Megaloceros with a line of dots (Wikipedia contributors 2014)

The measurements of length and weight appeared from the beginning of the Bronze Age. One of the earliest known uniform systems of such measurements was created by the Indus Valley civilisation (ca. 2600 BC), which has an astoundingly high accuracy (Baber 1996). The smallest unit of length was approximately 1.704mm, and of weight was approximately 28 grams.

With the development of natural science, many physical attributes, such as force, velocity and energy, are investigated and defined in terms of quantities, in the sense that their magnitudes can be measured by numbers. After a very long time, Fourier (Fourier 1822) is the first one to

consider the first fundamental question of measurement theory in physics. In his famous work on the theory of heat, he state that in order to measure physical quantities and express them numerically, five different units of measurement are needed, namely, those of length, time, mass, temperature, and heat. This idea is developed into a subject, named dimensional analysis. Maxwell, in his treatise on electromagnetism, also emphasised the fundamental character of the three fundamental units of length, mass, and time. He then went on to derive the units of some other quantities in terms of products of powers of the fundamental units. In theory, if each physical quantity can be defined in terms of a set of fundamental quantities (such as length, mass and time), by assuming the fundamental quantities can be measured and represented by numbers, it's clear that other physical quantities can also be measured in terms of numbers. While the question of why the fundamental quantities can be measured in terms of numbers was not discussed.

It is commonly accepted that Helmholtz's work is the beginning of measurement theory (Diez 1997). Helmholtz (Von Helmholtz 1977) pointed out the question 'we shall have to investigate in which circumstances we can express magnitudes through… numbers'. He calls 'magnitude' the 'attributes of objects which when compared with similar ones allow the distinction greater, alike or smaller'. To answer the question, he defines a 'special relationship … between attributes of two objects' called alikeness, which is now called equivalence relation. He then defines 'a method of connecting the magnitudes', which is a physical concatenation operation similar to addition. With the concatenation operation, he refers to an order relation between magnitudes: 'the whole is greater than the parts of which it is composed'. The magnitudes discussed by Helmholtz are actually the attributes with a concatenation operation, called *extensive* attributes.

Hölder (Hölder 1901) was the first to formally study the conditions of numerically measuring attributes of objects. He treats the objects manifesting a common attribute as a domain of objects with an ordering relation and a concatenation operation, which is now called an *extensive structure*. He then gives seven axioms as the conditions that the extensive structure must the same mathematical structure as the positive real numbers together with the numerical relation < and operation +. This result is known as Hölder's theorem, which is purely mathematical. This importance of Hölder's work is the idea of defining an empirical structure of the measured attribute with axiomatics and searching for conditions for a real

morphism (not necessarily an isomorphism, in general it will be sufficient to be a structure-preserving mapping) from the empirical structure.

N. R. Campbell (Campbell 1921, 1957) characterises measurement as 'the process of assigning numbers to represent qualities', and clearly state the question that concerns us: 'Why can and do we measure some attributes of bodies while we do not measure others?' He distinguishes measurement into two types: fundamental and derived measurement, corresponding to the fundamental and derived quantities respectively. Derived quantities, such as density, are measured in terms of other fundamental measurements. While in fundamental measurement, numbers are assigned to the objects directly according to the qualitative data. There is always one or more fundamental measurement involve in the measurement of an attribute. To prove the attribute is measurable, it's necessary to prove the fundamental quantities involved are measurable. This starts with qualitative statements (in terms of axioms) about the empirical structures (e.g. extensive structure) of the fundamental quantities, and then proves the existence of numerical representations. The detail of empirical structure and its numerical representation will be introduced further in the next section.

Scales	Admissible transformations	Examples
Absolute	$x \to x$	Counting, probability
Ratio	$x \to ax \quad (a \in \mathbb{R}^+)$	Length in meter or inch
Interval	$x \to ax + c \quad (a \in \mathbb{R}^+, c \in \mathbb{R})$	Temperature in Celsius or Fahrenheit
Log-interval	$x \to cx^b \quad (b, c \in \mathbb{R}^+)$	Density (mass/volume)
Ordinal	$x \to f(x)$ (f is any monotonic increasing function)	Moh's scale of hardness
Nominal	$x \to f(x)$ (f is any one-to-one function)	Numbering of football players

Table 2.1 Some common measurement scales

Campbell believed that only extensive quantities (such as length, mass) are measurable. While, for the attributes studied in psychology and social science (such as loudness), no concatenation operation can be defined, thus it seems to him these attributes are not measurable. Stevens (Stevens 1946) replied this opinion by showing that extensive

measurement is not the only type of measurement, there are different kinds of scales and different types of measurements. He points out that the key features of measurement are not only the empirical structure and its numerical representation, but also the degree of uniqueness of the representations which is reflected in the group of admissible transformations between the representations. According to the degree of uniqueness, he classified measurement into four different scales in his paper in 1946 (Stevens 1946), namely ratio scale, interval scale, ordinal scale and nominal scale. Some other types of scales were found later by Steven and others (Narens and Luce 1986), of which the most commonly discussed scales of measurement are listed in Table 2.1.

The absolute scale has the highest uniqueness, of which the only admissible transformation is the identity function. The representation in the ratio scale is unique up to multiplying a positive real number, which means if a set of numbers are the (numerical) representations of the quantity, by multiplying these numbers with a real number, another set of equally meaningful representations can be obtained. The uniqueness of the interval and the log-interval scales is of the same degree, which is weaker than the ratio scale. For the ordinal scale, objects are assigned with numbers such that the order of the numbers reflects the empirical order defined on the attribute. So a representation in the ordinal scale can be transformed to another by any order-preserving function. In the nominal scale, the only rule of assigning number is that a same number should be assigned to two objects if the objects are equivalent in the attribute. So the uniqueness of the nominal scale is the weakest. Since no ordering representation is involved in the nominal scale, it is not generally treated as measurement (Luce and Suppes 2002). It is clear that no concatenation operation is need in an empirical structure for it to be represented in an ordinal or nominal scale. Thus a measurable empirical structure does not need to be extensive.

Steven's result is a big breakthrough in measurement theory, not only because it widen the range of measurable attributes, it also allows us to determine whether a (statistical) statement is meaningful or not. For example, the statement that today's temperature is twice warmer than yesterday because the temperature of today is $30\,^{o}\mathrm{C}$ and of yesterday is $15\,^{o}\mathrm{C}$ is not correct. The ratio between temperature in $^{o}\mathrm{C}$ is meaningless, because temperature in $^{o}\mathrm{C}$ is in interval scale, the $0\,^{o}\mathrm{C}$ does not imply that the object has no temperature. In the interval scale, a magnitude of zero can be arbitrarily set; only the ratio of two intervals or differences

is fixed. So instead, the statement that the range of the temperature of today is twice of the range of yesterday is meaningful.

It's also been demonstrated by Steven that different scales have different collections of appropriate statistics. Only appropriate statistics can be used for each measurement scale. The criterion of an appropriate statistics of a scale is that the statistic should be invariant under the admissible transformations of the scale (Stevens 1946). For instance, it is meaningless to compare the means (averages) of two groups of data obtained from ordinal measurements, because the conclusion can change when the numerical data is transformed by a monotonic increasing function. In contrast, the medians are invariant under monotonic transformations. In general, the weaker the degree of uniqueness is, the smaller the collection of applicable statistics. Thus nearly all statistics are appropriate to the measurement of ratio scale, but only very limited statistics are applicable to nominal scale (such as mode). To be able to make sure the statistical inference of some data reflects something about reality, it's necessary to be clear about the scale of the measurement that generates the data.

The work of Helmholtz, Hölder and Campbell focuses on the conditions that the empirical structure of an attribute must satisfy in order to be represented numerically. The work of Steven focuses on the scale types and transformations between the possible representations within each scale type. These two lines of research need to be integrated in an appropriate way. The fundamental work in Suppes' paper (Suppes 1951) integrates these two lines for the first time, which studies (1) the conditions (weaker than Hölder's) for an empirical domain to have a homomorphism (a structure-preserving mapping which preserves the empirical structure) into the set of real numbers, and (2) the relation between all the possible homomorphisms. The first part of his work, which concerns the existence of a presentation, is referred to as the representation theorem, and the second part, which concerns the degree of uniqueness of the representations, is referred to as the uniqueness theorem. In that paper, only extensive measurements are dealt with, but his theorems can be generalised to other types of empirical domains.

After the integration of the two research lines, measurement theory became a mature theory and started to develop rapidly, especially during the 1950s and 1960s. The method of analysing extensive measurement was extended to other empirical structures. Some of the important extensions are listed as following.

- An axiomatisation of the expected utility theory constructed by Von Neumann and Morgenstern (Von Neumann and Morgenstern 1947) and developed by Savage (Savage 1972) is the first evidence of something different from extensive measurement.
- Conjoint measurement (Luce and Tukey 1964) is the most wildly accepted non-extensive measurement, of which the empirical structure is an order structure, in the form of $\langle A \times P, \precsim \rangle$, with an ordering relation affected by two independent factors.
- Difference measurement (Suppes and Winet 1955) is different from extensive measurement in the sense that the ordering is not of elements, but of 'intervals' between elements.
- Non-transitive indifference relation (Scott and Suppes 1958) is an extension of the equivalence relation (alikeness) in the extensive structure, which can be used to define the relation of measurement results with uncertainties (see Chapter 4).
- Measurement of probability (Kraft *et al* 1959) is close to the extensive measurement, but the concatenation operation is the union of disjoint events, which is a partial operation (not defined between every events).
- Weighted averaging representation is an alternative of the additive representation of extensive structure, which was first studied by Pfanzag (Pfanzag 1959).

By 1960s, most of the foundation for the present-day measurement theory was complete, which is organised systematically in a series of works. The most important is the three volumes book, Foundation of Measurement (Krantz *et al* 1971, Suppes *et al* 1989, Luce *et al* 1990).

2.2.2 Representational theory of measurement

The representational theory of measurement is the current paradigm of measurement which defines measurement as the assignment of numbers to attributes of objects in such a way as to describe them (Finkelstein 1982, p 6). In fact, this particular theory is often referred as the 'modern measurement theory' or simply the 'measurement theory'.

For a set of objects *A* with a common attribute to be measured, if the attribute is comparable, one or more empirical relations would be defined between the objects. For example, by comparing the length between rods, 'rod *a* is not longer than rod *b*' is a binary relation, denoted as $a \precsim b$; 'rod *a* concatenates with (put end to end in a straight line) rod *b* is not

longer or shorter than rod *c*' is a tertiary relation, denoted as $(a \circ b) \square c$. These relations can be precisely described by axioms. For instance, a reflexive and transitive binary relation *R* is a preorder. That means, for all $a, b, c \in A$, *aRa* (reflexive), and *aRb* and *bRc* imply *aRc* (transitive). So by defining the empirical relations with axioms, the set of the objects together with the empirical relations, $R_1, R_2, ..., R_p$, can be taken as a relational structure, $\mathcal{A} = \langle A, R_1, R_2, ..., R_p \rangle$, called an *empirical relational system* (ERS) (Roberts 1979). The elements in set *A* can also be considered as the manifestations of an attribute (Finkelstein and Leaning 1984, p 26), thus an ERS is determined by the corresponding attribute.

Depending on the attribute to be measured, there are many types of ERSs with different mathematical structures. For instance, a common structure of physical quantities is the extensive structure and takes the form of $\langle A, \precsim, \circ \rangle$, where *A* is a set of all the objects under consideration, $\precsim$ is a weak order (also called total preorder) and $\circ$ is a monotonic concatenation operation (Krantz *et al* 1999). Sometimes, the attribute of the objects cannot be combined, e.g. Mohs hardness of minerals, the ERS is simply an ordered set, denoted as $\langle M, \precsim \rangle$. Some attributes need to be determined by two or more quantities, e.g. loudness is depended on intensity and frequency, and the ERS is in the form of $\langle A \times P, \precsim \rangle$, called a 'conjoint structure'. Moreover, not all ERS are totally ordered: For example, let *A*, *B* be two surfaces in a 3-dimension space, an ordered relation $\precsim$ can be defined for the height of the surfaces such that $A \precsim B$ if and only if every point in *B* is not lower than *A*. Then if *A* intersects *B*, we have neither $A \precsim B$ or $B \precsim A$. Without connectedness (either $a \precsim b$ or $b \precsim a$), a weak order becomes a (partial) *preorder*, which is reflexive and transitive.

Some other commonly used ordering relations in measurement theory and their defining axioms are given in Table 2.2 and 2.3 (Roberts 1979). In Table 2.3, simple order, weak order and partial order are respectively the reflective closures[1] of strict simple order, strict weak order and strict partial order. It can be derived from Table 2.2 & 2.3 that the three types of ordering relations, simple order, weak order and partial order, all belong to preorder. Hence preorder is a very general type of ordering relation. A further instruction of order structure is given in Section 2.5.3.

To describe the measured attribute, the numbers should be assigned to the objects corresponding to the empirical relations. For example, the hardness of a mineral can be

[1] A reflective closure of a relation *R* on set *A* is the union of *R* with an equivalence relation on *A*.

measured by comparing it with other known minerals by scratching one with another. In Mohs' scale, the hardness of topaz and diamond are 8 and 10 respectively. If it is observed that the mineral is harder than topaz and softer than diamond, 9 can be assigned to the mineral as its hardness. To measure the objects in an ERS, a set of numbers and their relations are needed, which form a *numerical relational system* (NRS).

Properties of relation R on set A	Axioms
Reflexive	aRa, all $a \in A$
Symmetric	$aRb \Rightarrow bRa$, all $a,b \in A$
Asymmetric	$aRb \Rightarrow$ not bRa, all $a,b \in A$
Antisymmetric	aRb & $bRa \Rightarrow a=b$, all $a,b \in A$
Transitive	aRb & $bRc \Rightarrow aRc$, all $a,b,c \in A$
Negatively transitive	not aRb & not $bRc \Rightarrow$ not aRc, all $a,b,c \in A$
Complete	For all $a \neq b \in A$, aRb or bRa

Table 2.2 Some examples of properties and defining axioms of binary relations

Properties	Preorder	Simple order	Strict simple order	Weak order	Strict weak order	Partial order	Strict partial order
Reflexive	√	√		√		√	
Symmetric							
Asymmetric			√		√		√
Antisymmetric		√				√	
Transitive	√	√	√	√		√	√
Negatively transitive					√		
Complete		√	√	√			

Table 2.3 Some examples of ordering relations and their properties

The answer of whether an attribute can be measured in terms of numbers depends on whether the ERS corresponding to the attribute can be represented or preserved by a NRS, in the sense that there exists one or more homomorphism from the ERS to a NRS. Via a homomorphism, an ERS, $\langle A, R_1, R_2 ... R_p \rangle$ can be represented by a NRS, $\langle X, S_1, S_2 ... S_p \rangle$, where R_i is a relation in

the ERS and S_i is the corresponding relation in the NRS. For example, the extensive structure $\langle A, \precsim, \circ \rangle$ can be represented by a NRS, $\langle \mathbb{R}^+, \leq, + \rangle$, where $\mathbb{R}^+$ is the set of positive real numbers, $\leq$ is a simple order, and + is addition. Mapping ψ is a homomorphism from $\langle A, \precsim, \circ \rangle$ to $\langle \mathbb{R}^+, \leq, + \rangle$ if and only if, for any elements $a, b \in A$,

$$a \precsim b \Rightarrow \psi(a) \leq \psi(b), \text{ and } \psi(a \circ b) = \psi(a) + \psi(b),$$

where $\psi(a), \psi(b) \in \mathbb{R}^+$ (Krantz *et al* 1971). The homomorphism from an ERS to an NRS has certainty degree of uniqueness which is determined by the uniqueness of the numerical representations of the ERS (see Section 2.2.1).

The elements in a NRS are commonly taken as the numerical representations of the objects in ERS. However they are not necessarily numbers, other mathematical objects, such as vectors, functions, and intervals, can also be used to represent the empirical structure (Roberts 1979, p 254). For a homomorphism from an ERS to a NRS, the image of each object is a measurand value. So the elements of a NRS are the possible measurand values of the corresponding measurand.

The basic aim of representational theory is to study the existence and uniqueness of the homomorphism from an ERS to a specified NRS (Narens and Luce 1986). Based on the representational theory, we can use an ERS to model the attribute to be measured, a NRS to model the measured values, and a homomorphism between the ERS and the NRS to describe the measurement process.

2.2.3 Other theories of measurement

Michell (Michell 1986, 2007) distinguished two theories of measurement from the representational theory, namely the operational theory and the classical theory. The operational theory avoids assuming an underlying reality. Attributes and variables are the same, so there is no such thing as the ERS. It requires a precisely specified and consistent measurement procedure. A measurement is defined as any precisely specified operation that yields a number (Dingle 1950). In the classical theory, measurement only refers to attributes which are ordinal and additive, called quantitative attributes. Like the representational theory, an objective reality is also assumed, but unlike the representational theory, numbers are considered as ratios of quantities, which are discovered as relations between empirical

entities in measurement, thus are empirical. In the classical theory, measurement is thought of as the discovery of the numerical relationship between quantities (Michell 1986).

Hand (Hand 1996, p 447) says 'the importance of operational theory hinges on its place in justifying analytic practices that might be regarded as dubious under the representational theory'. It has had practical effect in disciplines such as psychology, and it has achieved a high level of sophistication through statistical models such as latent variable models and linear structural relational models. For the unobserved latent variables, the approach of defining these variables with observable (manifest) variables in an axiomatic system is more naturally described as operational (Hand 1996). However, operationalism has some severe philosophical disadvantages. Because numbers are not assigned to an underlying reality, questions like 'has intelligence increased, or just the test scores' are not able to be answered. Niederée (Niederée 1994) says the operational approach, which removes ambiguity by defining a phenomenon in terms of a specified measurement procedure, is 'suitable for Bureaucrats…who just want to establish plausible formal decision rules'. Robert Klee (Klee 1997, p 53) says 'operationalism did not last long in the physical science…, it survives to this day with considerable influence in the social and behavioural sciences'.

According to Michell, the traces of the classical theory of measurement may be found in the works of Aristotle and Euclid, and the basic concepts can be found in the works of Fechner (Fechner 1966, p 38) and Titchener (Titchener 1905, p xix). Although it is called 'classical', it is relatively new as a theory of measurement. Hand (Hand 1996, p 457) says the Rasch model (a psychometric model for analysing categorical data) might be regarded as fitting naturally into the framework of the classical theory. But he also says that the Rasch model, as a latent variable model, can also be interpreted with the operational theory. Moreover, Sarle (Sarle 1997, p 12) says 'a Rasch model is a form of representational measurement involving probabilistic relationship— a natural extension of Steven's idea of measurement'. Thus the distinctions among the three theories are not always clear. It's difficult to see that some psychological attribute, such as hunger, has a ratio or interval scale as the classical theory assumed. Michell's book (Michell 2014) is devoted to promoting the classical theory, but it seems that so far this theory has not been wildly accepted and applied yet.

Due to the absence of a commonly accepted philosophical assumption, the arguments of measurement theory are not easy to reach a consensus. Klee (Klee 1997) points out that a

similar situation exists with regards to the arguments between realist and anti-realist philosophers of science.

In a pragmatic point of view, it's acceptable that there is more than one measurement theory, just as there is more than one interpretation of probability, such as frequentist probability and Bayesian probability. For defining an attribute, both the theoretical and operational definitions are useful. For example, the theoretical definition of weight is a measurement of gravitational force acting on an object, and an operational definition is a result of measurement of an object on a Newton spring scale. The formal is helpful for understanding the concept, which attempts to construct a theory about the nature of the attribute (Cline n.d.), and the latter is often simpler, which is useful for standardising the measurement unit of the attribute. Although evaluating the measurability of an attribute base on the understanding of its nature is a more acceptable and reliable approach, for some latent (or construct) variables, such as quality-of-life, quantity indices in economics, it is more natural to use the operational approach.

Besides these three theories of measurement (representational theory, operational theory and classical theory), there are some other different schools of thoughts. Kyburg (Kyburg 1983), for example, suggests that 'the value (or interval of values) assigned to an object or event by measurement is a magnitude (or interval of magnitudes), rather than a number'. He also drew attention to the central role of error in measurement. And his study on indirect measurement, which is discussed in Section 2.3, is enlightening for this thesis. Adams (Adams 1966) takes measurement as indictors, of the underlying phenomena, which can be good or bad indicators. To him, laws of measurement connect the phenomenon under investigation with the results of the measurement, but these laws need not be exactly formulated and satisfied for measurement to be useful. IQ, for example, is a useful measurement, but stating the rules of how it related to intelligence is probably impossible.

For the research subject of this thesis, to study the structure properties of inverse problems of measurement, it's necessary to consider measurement as a mapping and understand the empirical structure of the measurement. So the representational theory is suitable for this research subject.

2.2.4 Measurability

In representational measurement theory, the measurement of an attribute is possible only if there exists a homomorphism from the ERS to a specified NRS (Narens and Luce 1986). The measurability of an attribute can be defined mathematically as following.

Definition 2.1: An attribute is *mathematically measurable* only if the ERS can be defined with axioms and the structure of the ERS can be represented by the structure of a NRS.

A basic aim of the representational theory is to study this mathematical measurability. If an attribute is mathematically measureable, it can be taken as a quantity, and thus a *measurand* (the quantity intended to be measured). Usually, this measurability is taken for granted for the quantities of interest in physics, but in other subject areas, such as in the behavioural and social sciences, the attributes of interest maybe not measurable (Krantz *et al* 1999). That's why the research and application of representational theory are mainly focus in the fields of economics and experimental psychology. In this thesis, this mathematical measurability, as a precondition of conducting a measurement, is assumed for the attributes under discussion.

By assuming this measurability, the definition of measurement gives in measurement theory can be simplified to with the concepts of quantity and quantity values. As defined in JCGM 200 (2008), measurement is the process of experimentally obtaining one or more *quantity values* that can reasonably be attributed to a *quantity*. Here a quantity is an *attribute* of an object, where the attribute is (mathematically) measurable. Hence, measurement establishes a correspondence between quantity and quantity values.

In a more practical point of view, measurability of an attribute is not only determined by the existence of a homomorphism from the ERS to a NRS, but also determined by whether the empirical relations can be observed via an empirical operation or not. If not, numbers cannot be assigned accordingly, and thus the measurand values cannot be obtained. For examples, the empirical relations of the length of rods can be observed by placing the rods parallel with each other. While the empirical relations of the electric charge of some objects can only be observed indirectly via the effects of the electrostatic force, such as the angle of torsion of the torsion spring in the Coulomb's torsion balance. Thus to measure electric charge, the relationship between the angle of torsion and the electric charge must be known. The quantities, of which the empirical relations can be observed, are named as *observable quantities*. From this point of view, a quantity is measurable if either it is an observable

quantity, or its quantity values can be inferred via the *measured data* of some related observable quantities. For the latter situation, the quantity is measured indirectly.

2.3 Indirect measurement

A measurement can be classified as a direct measurement or an indirect measurement according to whether the measurand is measured directly via observation or indirectly via other quantities. A definition of indirect measurement is given by Ellis as following.

Definition 2.2: When one or more other quantities are involved in the measurement of a given quantity, the measurement is referred to as an *indirect measurement*. (Ellis 1968)

The values of the indirectly measured quantity are inferred from the measured data of some observable quantities, thus an inference process is involved in every indirect measurement.

The reason of measuring a quantity indirectly is commonly understood as that measurands, such as density, temperature, cannot be measured directly in the sense that the empirical relations cannot be observed. However, it is often ambiguous to claim that a certain quantity can or cannot be measured directly (Kyburg 1983). As claimed by Campbell (Campbell 1921), many quantities can be measured both directly and indirectly, and it is often more reliable or convenient to measure it indirectly. Take the measurement of speed as an example, the speed of moving objects can be compared by direct observation, and thus numbers can be assigned to the objects to rank their speed. This is a direct measurement which assigns numbers to the measured objects in an ordinal scale. But, as we known, speed is usually measured indirectly in terms of the ratio of distance and time. This is because the second way is much more reliable and useful than the first. And more importantly, the second way generates a ratio scale which *conforms to* the ordinal scale of the first way, in the sense that there is a monotonic relation between the indirect scale and the direct scale of the measurand. This monotonic relation is a basic requirement of indirect measurement (Kyburg 1983).

The inference process of indirect measurement can be straight forward or difficult depends on the functional relation between the measurand and the observable quantities involved. A common form of the functional relation can be written as

$$x = g(d_1, d_2, \ldots, d_n), \tag{2.1}$$

where x is the measurand, and d_i are the observable quantities. For instance, density, $\rho = g(m,v) = m/v$, where m is mass, v is volume. This form is wildly used for evaluating measurement uncertainties (JCGM 100 2008), since measurands of precision measurements are normally related with some influence quantity, such as temperature, pressure. More generally, equation (2.1) can be written as

$$x = G(d), \tag{2.2}$$

where x and d can be scalar, vector or function respectively, and G is a mapping, such as a linear operator or a nonlinear system of equations. When the mapping G is known, with the measured values of d_i, the inference of the measurand is straight forward. While, in many cases, the mapping G is unknown. Conversely, the known functional relation is in the form of

$$d = F(x), \tag{2.3}$$

where F is a mapping from the space of the measurand to the space of the observable quantity(s). When F is known, to infer the values of x according to the measured data of d is a typical inverse problem, which can be difficult due to the ill-posedness of inverse problems (Hansen 1998). Equation (2.2) and (2.3) are the mathematical models of the two types of indirect measurements.

Indirect measurement is important in our research because it has close connection with inverse problems. This connection is further discussed in Chapter 3.

2.4 Inverse problems

2.4.1 The mathematical model of inverse problems

The concept of inverse problem is defined opposite to the forward problem. It is commonly considered that two problems inverse to each other if the formulation of each of them requires full or partial solution of the other (Keller 1976). From the mathematical point of view, there is no certain criterion to determine which one of the two problems is the direct or inverse problem (Kirsch 1996). However, for physicists, two problems are not on the same level, the direct problem is considered to be more fundamental than the other, thus it is investigated earlier and, perhaps, in more detail (Bertero and Boccacci 2010).

Moreover, from the perspective of physics, a direct problem is the problem of finding the consequences of the given causes, thus it follows a cause-and-effect orientation (Turchin *et al*

1971). Conversely, an inverse problem is the problem of finding the causes of some given consequences. The causes can be taken as a 'physical state' and modelled by parameters, such as physical quantities (Sabatier 2009). For finding the causes, the consequences are taken as phenomena and described by measured (quantity) values.

Mathematically, it is convenient to treat the parameters of the 'physical state' as an element of a space $\mathcal{M}$ (e.g. a metric space), named as a *model*; and similarly, treat the measured data of the 'phenomenon' as an element of another space $\mathcal{D}$, named as a *data set*, so that the cause-and-effect relation from the model to the data can be represented by a mapping F from $\mathcal{M}$ to $\mathcal{D}$. $\mathcal{M}$ and $\mathcal{D}$ are named as model space and data space respectively. Mapping F is named as the *forward mapping* of the inverse problem.

Thus, when a model m and the mapping F is known, the observations can be predicted by

$$d = F(m). \tag{2.4}$$

Equation (2.4) is called *the mathematical model of the inverse problem* (Aster *et al* 2005).

Depends on the type of forward mapping, there are various methods to solve equation (2.4). For instance, if F is invertible, (2.4) can be solved by its inverse F^{-1}; if F is an arbitrary matrix, the Moore-Penrose generalised inverse $F^{\dagger}$ can be used to find a generalised solution (Moore 1920, Penrose 1955); if F is an Fredholm integral equation of the first kind, the inverse problem can be solved by deconvolution with convolution theorem (Bracewell 2000). Each of these methods can be described by the following equation,

$$\hat{m} = G(d), \tag{2.5}$$

where G is a mapping from the data d to the estimated model $\hat{m}$. As described by equation (2.5), inverse problems can be solved by using a proper mapping G, called a *backward mapping*.

For inverse problems in metrology, the definition of inverse problems given by Sabatier (Sabatier 2009) is adopted in this thesis as the problems of inferring information from observations, which is not only about solving mathematical problems but also using mathematics to solve the problems in natural science. Combining with the cause-and-effect definition, inverse problems can be defined as following.

Definition 2.3 *Inverse problems* are the problems of inferring the information of the causes of some effects from the observations of the effects.

As shown in the last section, the mathematical model of indirect measurements can be similar to the mathematical model of inverse problem (see equation (2.3) and (2.4)). For an indirect measurement in the form of (2.3), the inference process is an inverse problem. Moreover, if the model *m* in (2.4) is or contains the measurand *x*, by solving (2.4), the values of the measurand can be derived.

2.4.2 Examples of inverse problems

Example 2.1 Seismic tomography (Iyer 1993)

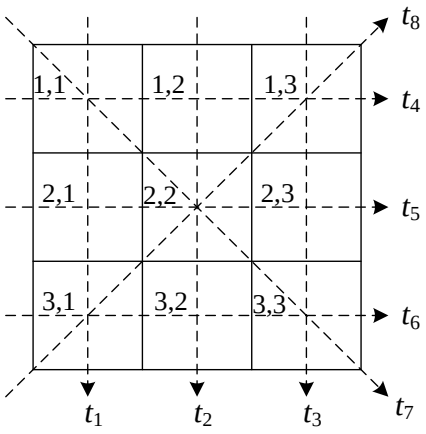


Figure 2.2 The measured area and the wave paths of a simple seismic tomography example

In seismic tomography, the seismic structure of a location in Earth's sub-surface is usually parameterised by the slowness (the reciprocal of velocity) of the seismic waves at that location. The seismic structure of a specified area, such as the square in figure 2.2, can be estimated according to the variation of the slowness in the area. Several sources and receivers of seismic waves are set to measure the travel-time of the seismic waves through the designed wave paths, which are assumed to be straight lines, in the area. The measured area is divided into uniform blocks (see Figure 2.2) to simplify and discretise the mathematical model. The slowness of the nine blocks are indexed in a row-by-row way. By using an 8-by-9 matrix **F**, of which the elements are the lengths of the wave paths within corresponding blocks, the functional relation of slowness $s_{i,j}$ and time t_i can be modelled in the form of $\mathbf{Fs} = \mathbf{t}$,

$$\begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ \sqrt{2} & 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & \sqrt{2} & 0 & \sqrt{2} & 0 & \sqrt{2} & 0 & 0 \end{bmatrix} \begin{bmatrix} s_{1,1} \\ s_{1,2} \\ s_{1,3} \\ s_{2,1} \\ s_{2,2} \\ s_{2,3} \\ s_{3,1} \\ s_{3,2} \\ s_{3,3} \end{bmatrix} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ t_4 \\ t_5 \\ t_6 \\ t_7 \\ t_8 \end{bmatrix}. \tag{2.6}$$

To estimate the vector of slowness from the above equation is a typical linear inverse problem, which can be solved using the Moore-Penrose generalised inverse of the matrix **F** (see Section 2.7.1). Regularisation (e.g zeroth-order Tikhonov regularisation) should be applied if the generalised inverse of **F** is ill-conditioned.

Example 2.2 Geological prospecting (Kirsch 1996, p 1)

The distribution of the mass density of a buried field, $m(x)$ at a fixed depth h can be estimated according to the vertical gravity anomaly, $g(s)$ measured at the surface directly above the field (refer to Figure 2.3). The mathematical model of the inverse problem involved can be expressed by a *Fredholm integral equation of first kind* (*IFK*):

$$g(s) = K\int_{-\infty}^{\infty} \frac{h}{((x-s)^2+h)^{3/2}}\, m(x)dx, \tag{2.7}$$

where K is the gravitational constant, both $m(x)$ and $g(s)$ are continuous functions of x-coordinate (Aster *et al* 2013).

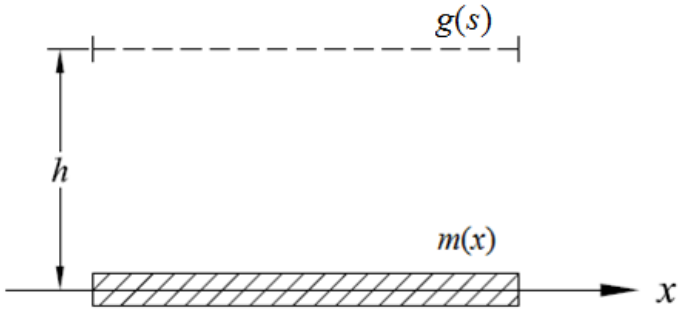


Figure 2.3 The vertical gravity anomaly is measured with a distance h from the buried field

Equation (2.7) can be written in the form of convolution:

$$g(s) = \int_{-\infty}^{\infty} f(x-s)m(x)dx\,. \tag{2.8}$$

This inverse problem can be solved by deconvolution with the convolution theorem (Bracewell 2000) if the function $g(s)$ can be obtained according to the measured data. A discrete method of solving this is to discretise the linear continuous equation (2.8) by the quadrature method (Aster *et al* 2005, p 41) into

$$\mathbf{Fm} = \mathbf{g}. \tag{2.9}$$

The output and input functions are discretised to two sets of discrete points in terms of vectors **m** and **g**, and the forward mapping is transformed from an integral operator to the matrix **F**. Thereby, (2.9) can be solved similarly as Example 2.1.

Example 2.3 Earthquake location problem (Aster *et al* 2013, p 9)

The estimation of the (3-dimensional) location **c** and origin time t_0 of an earthquake according to the data of arrival times **t** collected by the *n* stations of seismographs around the centre of the earthquake is a classic *nonlinear inverse problem*. The mathematical model of this inverse problem can be written as a system of *n* nonlinear equations, in the form of

$$\mathbf{F}(\mathbf{m}) = \mathbf{t}, \tag{2.10}$$

where **m** is the hypocentre of earthquake,

$$\mathbf{m} = \begin{bmatrix} \mathbf{c} \\ t_0 \end{bmatrix}. \tag{2.11}$$

Assume that the seismic waves travel from the hypocentre to the stations in straight lines with a given constant velocity, *v*. The arrival time observed at station *i* can be described as

$$t_i = \frac{\|\mathbf{s}_i - \mathbf{c}\|_2}{v} + t_0 = F(\mathbf{m})_i \tag{2.12}$$

where $\mathbf{s}_i$ is the location vector of station *i*, $i \in \{1, \ldots, n\}$.

By using the iterative methods, such as Newton method and Gauss-Newton method (Thurber 1985), an approximate solution of **m** can be obtained from equation (2.12), which consists of two quantities.

Many other examples of inverse problems in metrology can be found in (Aster *et al* 2005), (Tarantola 2005) and (Kirsch 1996). A review of inverse problems in indirect measurements in terms of IFK equations is given in (Mroczka and Szczuczyński 2009).

2.5 Mathematical structure

Before investigating the structure of inverse problem, it is necessary to understand what mathematical structure is. That is a philosophical problem which has been discussed for a very long time.

2.5.1 What is mathematical structure?

A mathematical structure is essentially a list of mathematical operations and/or relations with their required properties, normally given as axioms, shared by a number of, possibly quite different, mathematical objects (Mac Lane 1996).

Intuitively, the word 'structure' refers to the way of how the components of an entirety, such as a building, a society, link together and form the entirety. In mathematics, the 'entirety' can be considered as a mathematical object, such as an ordered set, natural numbers under addition. The 'components' are the elements of the mathematical object, such as subsets, numbers, or the object itself. Some specified 'aspects' of the object links the 'components' together to form the 'entirety' in a certain way. The 'linking method' is normally given as a list of axioms. And the 'aspects' can be mathematical operations, relations, or other composite features, which are named as the links. Structures are determined by the links and the linking method only.

Nicholas Bourbaki classified mathematical structures into three great types (Bourbaki 2004): algebraic structures (e.g. group, ring, field), order structures (e.g. partial order, linear order, and well order), and topological structures (e.g. metric space, Alexandrov space). To take a more explicit look on mathematical structures, some examples of the three types are demonstrated in the following three sections.

2.5.2 Algebraic structure

Group is a typical structure of algebraic structure. A group $\langle G, * \rangle$ is a set G, closed under a binary operation $*$, such that the following axioms (Fraleigh 2003) are satisfied:

1. Associative: for all $a, b, c \in G$, we have $(a * b) * c = a * (b * c)$;

2. Identity: there is an element *e* in *G* such that for all $x \in G,\ e*x = x*e = x$;

3. Inverse: For each $a \in G$, there is an element *a'* in *G* such that $a*a' = a'*a = e$.

Here the binary operation $*$ is the link, and the linking method is given by the three axioms above.

For example, integers under addition form a group ⟨ℤ, +⟩; four complex numbers {1, *i*, -1, -*i*} under multiplication form a group; and the eight symmetries of a square (the operations of rotation or reflection) also form a group when the group operation is taken to be the composition (e.g. a rotation followed by a reflection).

A binary operation $*$ on a set *G* is a function mapping *G* x *G* into *G*. For each $(a, b) \in G \times G$, $a*b$ denotes the element $*(a,b)$ of *G*. So all the mappings in a group between the elements can be taken as a function $*: G \times G \to G$.

Just like a set can be mapped into another set, a group can also be mapped into other group, such that the group structure is preserved by the mapping. A mapping that preserves the group structure is called a group homomorphism (Fraleigh 2003). A group homomorphism $f: G \to H$ maps each element group *G* to an element $f(x)$ group *H* such that equation (2.13) holds for all $x, y \in G$.

$$f(x*y) = f(x)*f(y) \tag{2.13}$$

Structures	Links[2]	Associative	Identity	Inverses	Commutative	Distributivity
Magma	◦	No	No	No	No	N.A.
Semigroup	◦	Yes	No	No	No	N.A.
Monoid	◦	Yes	Yes	No	No	N.A.
Group	◦	Yes	Yes	Yes	No	N.A.
Abelian group	◦	Yes	Yes	Yes	Yes	N.A.
Ring	+, ·	Yes	+[3]	+	+	Yes
Field	+, ·	Yes	+	Yes	Yes	Yes

Table 2.4 Some examples of algebraic structures

[2] All the links in the table are binary operations.

[3] It means for + only.

By adding or removing the axioms, some other abstract structures can be obtained as listed in Table 2.4. For instances, if the inverse axiom of a group does not hold, the group becomes a monoid. A commutative group is an Abelian group. Thus the group $\langle \mathbb{Z}, + \rangle$ is an Abelian group, since + is commutative. But $\langle \mathbb{N}, + \rangle$ is not a group, it is a monoid, since the inverse axiom does not hold.

In Table 2.4, commutative of $\circ$ means for all $a, b \in G$, we have $a \circ b = b \circ a$. Distributivity is only applicable for more than one operation, e.g. for the operations + and · (addition and multiplication), $a \cdot (b + c) = (a \cdot b) + (a \cdot c)$ and $(a + b) \cdot c = (a \cdot c) + (b \cdot c)$ hold.

A vector space *V* is also an algebraic structure, which consists of a set of vectors, two operators: vector addition and scalar multiplication, and an associated field *F*. Let *u, v* and *w* be arbitrary vectors in *V*, and *a* and *b* be arbitrary scalars in *F*, a vector space *V* can be defined by the following eight axioms:

(1) $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w}$;

(2) $\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$;

(3) For any $\mathbf{v} \in V$, there exists an element $-\mathbf{v} \in V$, such that $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$;

(4) There exists an element $\mathbf{0} \in V$, such that $\mathbf{v} + \mathbf{0} = \mathbf{v}$;

(5) There exists an element $1 \in F$, such that $1\mathbf{v} = \mathbf{v}$;

(6) $a(b\mathbf{v}) = ab\mathbf{v}$;

(7) $(a + b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$;

(8) $a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}$.

Detailed instructions of vector space can be found in most of the books of linear algebra, such as (Meyer 2000).

2.5.3 Order structure

Order structures and ordering relations are essentially important for defining the ERS and NRS in measurement theory. As mentioned in Section 2.1, weak order, partial order and preorder are commonly used to define the empirical relations of measured objects. The properties of these ordering relations are defined by axioms. There are many other relations defined in order theory (Davey and Priestley 2002) and measurement theory (Roberts 1979), some commonly used relations and their properties are listed in Table 2.2 & 2.3. Each ordering relation *R* together with the set *A* it applies form an order structure $\langle A, R \rangle$.

For instances, the real numbers ordered by simple order ≤ is a simply ordered set or a chain. The class of subsets of a given set S (its power set $P(S)$) ordered by inclusion is a partially ordered set (poset), $\langle P(S), \subseteq \rangle$. The set of subspaces of a vector space ordered by inclusion is also a poset.

The models and data of inverse problems can be in the form of finite or infinite dimensional vectors (latter is usually referred to as functions). There are many ways to define the order structure of vectors. For instance, *pointwise order* is a commonly used partial order of vectors, which is defined as, for vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, $\mathbf{x} \preceq \mathbf{y}$ if and only if $x_i \leq y_i$ for $i = 1, \ldots, n$, where x_i, y_i are the entities of $\mathbf{x}$ and $\mathbf{y}$. Lexicographical order is a total order, defined in such a way that in $\mathbb{R}^2$, $(a, b) \leq (c, d)$ if and only if $a < c$ or ($a = c$ and $b \leq d$). By comparing the L^p-norm ($\|\cdot\|_p$, $p = 1, 2, \ldots, \infty$) of vectors, or comparing the sum or product of the entities of each vector, different totally ordered relations can also be defined. More generally, in $\mathbb{R}^n$, the relation of vectors can be defined as

$$\mathbf{a} \preceq \mathbf{b} \qquad \text{if and only if} \quad F(\varphi_1(a_1), \ldots, \varphi_n(a_n)) \leq F(\varphi_1(b_1), \ldots, \varphi_n(b_n)),$$

where $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$, and F and φ_i are real-valued functions. The theory of conjoint measurement (Krantz *et al* 1999) studies the conditions that the joint effects of n factors can be represented in terms of polynomials.

The mapping between two posets can be structure-preserving as well, which is an order preserving mapping (or a monotonic mapping). If a mapping $f : P \to Q$ is order preserving, we have $x \leq y$ in P implies $f(x) \leq f(y)$ in Q.

The structure of poset is closely related to the structure of lattice (Davey and Priestley 2002). Let P be a non-empty poset, and let $a \wedge b$ be the greatest lower bound of $\{a, b\}$ and $a \vee b$ be the least upper bound of $\{a, b\}$, if $a \wedge b$ and $a \vee b$ exist for all $a, b \in P$, then the poset P is a lattice. For a lattice P the following three conditions are equivalent:

1. $a \leq b$,
2. $a \wedge b = a$,
3. $a \vee b = b$.

2.5.4 Topological structure

A topological space $\langle X, \Gamma \rangle$ is a set X together with a topology Γ which specifies that certain subsets of X are regarded as 'open' (Mac Lane 1996). This specification can be considered as the link of the topological structure which must satisfy the following axioms: The set X and its empty subset $\varnothing$ are both open; the intersection of any two subsets of X is open; the union of any collection of open sets is also open.

For any set X, the discrete topology on X is the topology comprising all the subsets of X (Sutherland 1975); the trivial topology on X is the topology $\{\varnothing, X\}$.

The specified open subsets of a topology space are closed under unions and finite intersections. Hence the open subsets of a set X ordered by inclusion form a lattice of sets in which $A \vee B = A \bigcup B$ and $A \wedge B = A \bigcap B$, $A, B \in X$.

Metric space is an important type of topological space for inverse problems. A metric space (M, d) is a set M and a distance function d which defines a distance for any two elements in M (Sutherland 1975). With the distance function, open balls $B(x, r)$ with a point x and a specified distance r can be defined, which are the open sets of the topology of the metric space.

Some vector spaces are endowed with additional topological structures, such as the topologies generated by a norm or inner product, which are called topological vector spaces. Banach spaces and Hilbert spaces are complete topological vector spaces, which are complete in the sense that a Cauchy sequence (a sequence whose elements become arbitrarily close to each other as the sequence progresses) of vectors always converges to a well defined limit that is within the space (Goffman and Pedrick 1983). Banach spaces and Hilbert spaces are important in functional analysis for investigating infinite-dimensional function spaces whose vectors are functions.

2.5.5 Structures and mappings

The definition of mathematical structure mentioned before may look somewhat ambiguous; actually it appears that there are many different definitions. Giving an explicit and useful definition of mathematical structure maybe as difficult as defining what is a game. Bourbaki gave a mathematical definition of structure using the axiomatic method and three basic operations of set: product $E \times F$, power set $P(E)$, and function set E^F of two sets E and F

(Bourbaki 1963). This definition clearly includes most structures, such as group, topological space and combined cases. However it did not really become a useful definition, even not in Bourbaki's own treatise (Corry 2004, p318). It seems that the important thing is not the explicit definition of structure, but the method of characterising and describing the structure of a given kind.

As shown in the above examples, all the different structures have their own structure-preserving mappings respectively, which are called group homomorphism, monotonic mapping, continuous function, etc. Thus these structures can be distinguished by their different structure-preserving mappings. And the axiomatised links, such as binary operation, can also be expressed as mappings, such as f: $G \times G \rightarrow G$. It seems that we should pay more attention to the mappings rather than investigate mathematical object in isolation. In fact, mathematical object are determined by their 'admissible transformations' (Steve 1996).

The axiomatic method (Potter 2004) is widely used for defining structures, because the whole theory of that structure can be developed in a comprehensible way by defining the linking method of the structure with a small numbers of well-chosen axioms. Another more general and effective way of specifying and describing mathematical structure, which also includes the axiomatic notion, was emerged after mathematicians realising the fact that mathematical structure is determined by a system of objects and their mappings. That is category theory: the abstract theory of mathematical objects and their mappings.

2.6 Category theory

2.6.1 Definition of a category

Two mathematicians, Eilenberg and Mac Lane, observed that many properties of mathematical system can be unified and simplified by a presentation with diagrams of arrows (Mac Lane 1971), and then they created a very abstract and powerful theory: Category Theory. The arrows are just the mappings mentioned in the last section. In this thesis, category theory is introduced as the principle of defining and investigating mathematical structure, especially for the structure of inverse problems.

Definition 2.4: A category **C** consists of a collection of objects *A, B, C,...* and mappings *f, g, h,...* such that: (1) every mapping *f* has a unique domain and a unique codomain, written as $f : A \rightarrow B$; (2) given any $f : A \rightarrow B$ and $g : B \rightarrow C$ there is a unique composition,

$g \circ f : A \to C$, and the composition is associative, i.e. $f \circ (g \circ h) = (f \circ g) \circ h$; (3) each object *A* has an identity mapping $I_A : A \to A$ which is a unit for composition, i.e. for any $f : A \to B$, we have $I_B \circ f = f$ and $f \circ I_A = f$. (Pierce 1991)

The categories in which objects can be viewed as 'sets with additional structure' and mappings as 'structure-preserving mapping' are called concrete categories (Adámek *et al* 1990). There are many concrete categories defined for various structures, such as **Vect** for vector spaces, **Grp** for groups and **Top** for topological spaces.

A preordered set $\langle A, R \rangle$ is a category, in which there is at most one mapping between any two objects *a*, *b*, and $a \to b$ if and only if aRb, where the objects are the elements in *A*, and *R* is a binary relation. The transitivity of preorder implies the mapping can be composed, and the reflexivity of preorder implies there is an identity mapping $a \to a$ for each object. Hence the definition of category is satisfied.

A monoid can be taken as a category with one object by considering all the elements in the monoid as the mappings of the category ($f : A \to A$), and taking the monoid operation $*$ as the composition of mappings (Mac Lane 1971). Since there is only one object, all the mappings map from the object to itself. One of these mappings is the identity mapping I_A, which is the identity element of the monoid. By definition of monoid, $*$ is associative. Therefore, the properties of monoid satisfy the definition of category.

2.6.2 How to describe structures in a category?

Having the definition of category in mind, the following example demonstrates how structure can be described by 'diagrams of arrows'.

From the Table 2.4, if a monoid satisfies the inverse axiom, it is a group. Hence a group is a category with one object in which every mapping has an inverse under composition.

In a category of monoid, written as **Mon**, the objects are all monoids, and the mappings preserve the monoid structure, a group *G* can be defined in the category **Mon**, by the diagram below (Steve 2006).

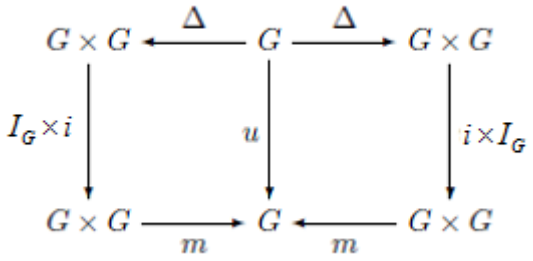


Figure 2.4 Group *G* in category **Mon**

Here Δ is the diagonal function $\Delta : x \mapsto (x, x)$. I_G is an identity function, and *i* is an inverse function, such that $I_G \times i : (x, x) \mapsto (x, x^{-1})$. The function $u : G \to G$ is a constant function, which maps all the elements of monoid *G* to its identity element *e*. And *m* is the function of the monoid operation. When the left and right diagram commute, we have

$$x * x^{-1} = e = x^{-1} * x, \tag{2.14}$$

so this diagram is exactly the same as the inverse axiom.

The other structural properties, such as associativity, commutativity and identity given by axioms, can also be described by some commutative diagrams like this. This diagram makes no explicit mention of monoid elements, so it is applicable to other structures. That's why category notion provides invariant syntax for describing structure.

2.6.3 Mapping properties: isomorphic, monic and epic

Each object in a category may have some elements, but category theory treats each object as a black box (Pierce 1991), and ignores the elements inside, since the details of elements does not affect the structure properties. Thus the non-structural differences of objects cannot be distinguished in a category, and that is what we want for describing structures, just as the topologists do not care to distinguish among homomorphic spaces. When two objects with different elements are not distinguishable by the structural-preserving mappings, the two objects are isomorphic (written as $A \cong B$).

Definition 2.5: In category theory, a mapping $f : A \to B$ is an *isomorphism* if and only if there is an inverse mapping $g : B \to A$ such that $g \circ f = I_A$ and $f \circ g = I_B$. (Mac Lane 1971)

For example, an isomorphism of sets is a bijection; an isomorphism of topological spaces is a continuous function which is bijective and the inverse function is also continuous (Steve 1996).

The other two important mapping properties are monic and epic.

Definition 2.6: An mapping $f : B \to C$ in a category is *monic* if, for all mappings: $g : A \to B$ and $h : A \to B$, the equality $f g = f h$ implies that $g = h$. (Mac Lane 1971)

Definition 2.7: An mapping $f : A \to B$ in a category is *epic* if, for all mappings: $g : B \to C$ and $h : B \to C$, the equality $g f = h f$ implies that $g = h$. (Mac Lane 1971)

In the category **Set** (objects are sets, mappings are functions), monic is same as injective (one-to-one), and epic is same as surjective (onto) (Mac Lane 1971). But a mapping may not be an isomorphism, even if it is monic and epic.

2.6.4 Functors and Natural transformations

Other than the structure-preserving mapping between objects, there are also structure-preserving mappings map between different categories. A mapping between categories that preserves the structure of category is called a *functor*.

Definition 2.8: Let **C** and **D** be categories. A functor $F : \mathbf{C} \to \mathbf{D}$ is a mapping that maps each **C**-objects A to a **D**-object $F(A)$, and each **C**-mapping $f : A \to B$ to a **D**-mapping $F(f) : F(A) \to F(B)$, such that

(1) $F(I_A) = I_{F(A)}$ for every object A in **C**,

(2) $F(f \circ g) = F(f) \circ F(g)$ for all compositions of mappings in **C**.

That means a functor takes a commutative diagram from a category to another category as shown in Figure 2.5 (Steve 2006). For example, a functor between two posets as categories is an monotonic mapping (Arbib and Manes 1975).

A functor can be considered as a kind of projection from **C** to **D**. Imaging, in Figure 2.5, if there are two functors F, U project the diagram of **C** into **D**, there will be two similar images of the diagram in **D**. And if the two images are not coincident, them can be linked by the mappings in **D** that map each $F(A)$ to $U(A)$ for each object A in **C**. This kind of mapping between functors are called *natural transformation*, the explicit definition can be found in

(Steve 2006). If the diagram in **C** looks like a circle, then the images of that diagram in **D** projected by two functors and linked by the natural transformation looks like a cylinder.

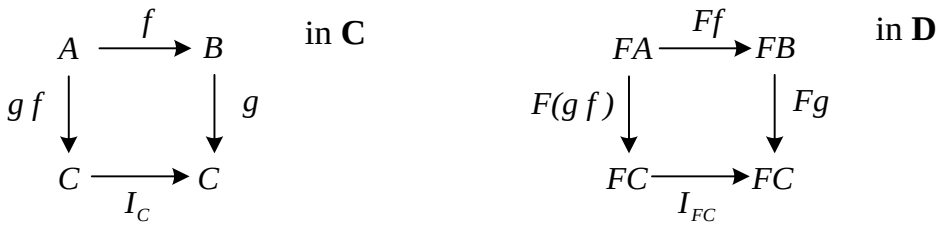


Figure 2.5 Domain and codomain of functor *F*

The concepts of functors and natural transformations are applied in the section of adjoint.

2.6.5 Universal constructions

In mathematics, it can be observed that some similar constructions appear iteratively in different fields. For instance, 'product' appears in vector spaces, groups, topological spaces, etc.; 'free objects' appears in vector spaces, groups, rings, topological spaces, etc. (Adámek *et al* 1990). Category theory, as a language for all the structures, provides the means to understand these special constructions by the notion of *universal mapping property* (UMP). And the UMPs are represented by some special diagrams which are called *universal constructions*. Universal constructions pick out something (objects and the accompanying mappings) unique in the category. Each universal construction has a co-universal construction, which also has a UMP. They are dual to each other, in the sense that they have the same form except that the mappings are reversed.

Product is a simple and common universal construction. A product of two objects *A* and *B* is an object $A \times B$, together with two projection mappings $p_1 : A \times B \to A$ and $p_2 : A \times B \to B$, such that for any object *C* which maps to *A* and *B* by mappings *f* and *g*, there is a unique mapping $\langle f, g \rangle$ making the below diagram commute (Pierce 1991).

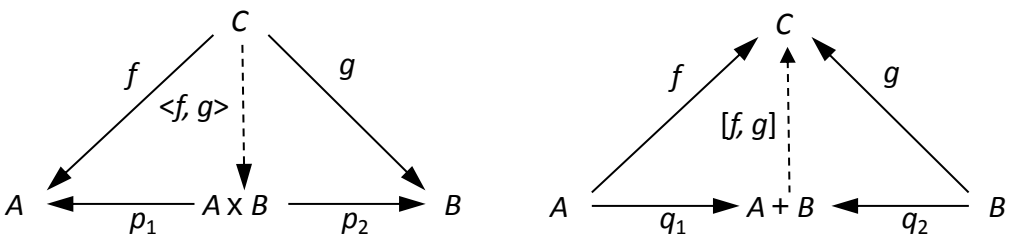


Figure 2.6 Diagram of product (left) and co-product (right)

For example, the product in the category of sets is the Cartesian product; the product in a poset is the greatest lower bound of two elements ($a \wedge b$), if the mappings of **Poset** are inclusions $\subseteq$, the product is the intersection ($A \bigcap B$).

The dual of product is co-product (see Figure 2.6). There are many other pairs of universal contractions, such as pullback and pushout, equaliser and coequaliser, limit and colimit. Product, pullback and equaliser are all basic types of limit in different forms. The definitions of these universal constructions can be found in (Mac Lane 1971).

2.6.6 Adjoint functors

A very important universal construction is adjunction, which is a relationship between two functors. It captures an important mathematical phenomenon that is invisible without the lens of category theory. As Mac Lane (Mac Lane 1971) said, 'Adjoint functors arises everywhere'.

Assume there are two functors F: **C**→**D** and U: **D**→**C** between two categories **C**, **D**, and two natural transformations in each category, $\eta: I_{\mathbf{C}} \to UF$ and $\varepsilon: FU \to I_{\mathbf{D}}$, where $I_{\mathbf{C}}$ and $I_{\mathbf{D}}$ are the identity functor of **C** and **D** respectively, See figure 2.7. (F, U) is an adjoint pair if, for any objects A in **C** and B in **D**, the set of mappings from A to $U(B)$ is isomorphic to the set of mappings from $F(A)$ to B, i.e.

$$\hom(A, U(B)) \cong \hom(F(A), B) . \tag{2.15}$$

This construction is named as an *adjunction*, denoted as $F \dashv U$. Functors F and U are called a pair of adjoint functors. The explicit (and thus more complicated) definition of adjuncation can be found in (Steve 2006).

A Galois connection in order theory, for instance, is an adjunction between two posets (Davey and Priestley 2002).

It is proved in the next chapter that under certain conditions, the forward and backward mappings of some inverse problems involved in measurement are adjoint to each other.

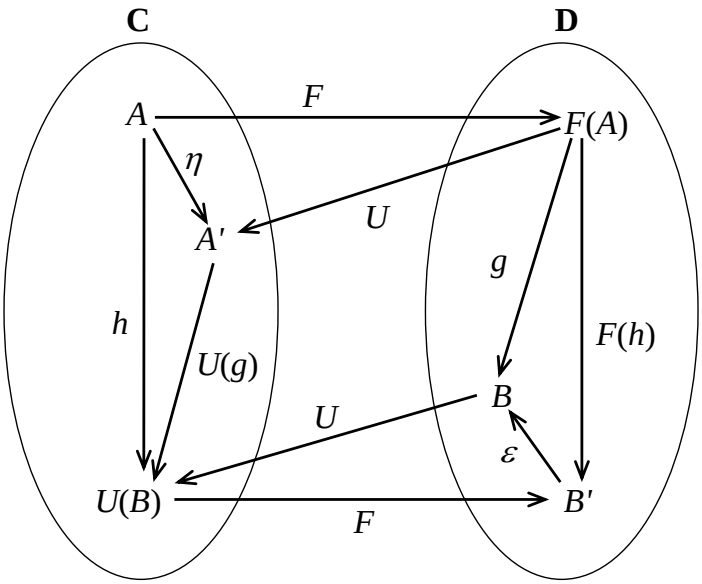


Figure 2.7 Diagram of an adjunction $F \dashv U$

2.7 On the Structure of inverse problems

For inverse problems, the structural properties can also be described in terms of a "diagram of arrows" according to its mathematical model. In Figure 2.8, the objects *M* and *D* are the model space and data space. *F* is the forward mapping, and *G* is a backward mapping as introduced in Section 2.4. R_m is called the *model resolution*, and R_d is called the *data resolution*, $R_m = GF$ and $R_d = FG$, they are self-mappings of *M* and *D* respectively.

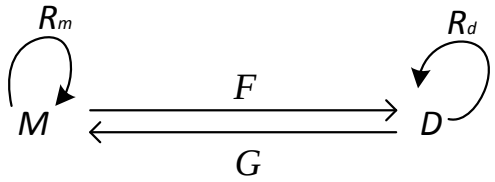


Figure 2.8 The objects and mappings of an inverse problem

In this thesis, "The structure of inverse problems" refers to the following aspects:

1) the system of mathematical objects and their mapping involved in the inverse problem, see figure 2.8,

2) the structures of the model and data spaces, e.g. posets, normed vector spaces and Hilbert space,

3) the mapping properties of *F* and *G*, e.g. isomorphic, monotonic, compact, continuous and linear,

4) the relationship of *F* and *G*, e.g. $FGF = F$, *F* is left adjoint to *G*,

5) the results that can be derived from these structural properties.

The structural study of measurement basically belongs to measurement theory, especially the representational theory introduced in Section 2.2.2. The structural properties of inverse problems are studied mainly in two fields, generalised inverse and functional analysis.

2.7.1 Generalised inverse of a linear operator

It is well known that a matrix **F** has an inverse $\mathbf{F}^{-1}$only if it is a square and non-singular matrix. In many of cases, the forward mapping of an inverse problem is a singular matrix **F**. To be able to solve the inverse problems in the form of

$$\mathbf{Fm} = \mathbf{d}, \tag{2.16}$$

where $\mathbf{F}: M \to D$, a more general type of 'inverse' of **F** is needed, which should (1) exist for a larger class of matrices than the class of non-singular matrices, (2) have some of the properties of the usual inverse, and (3) reduce to the usual inverse when **F** is non-singular. Ben-Israel and Greville (Ben-Israel and Greville 2001) name this type of 'inverse' as a *generalised inverse* of a given matrix **F**, some authors also use the term 'pseudo-inverse'.

It can be easily verified that the three conditions of a generalized inverse can be satisfied by a matrix $\mathbf{G}: D \to M$ with equation (2.17) satisfied.

$$\mathbf{FGF} = \mathbf{F} \tag{2.17}$$

If **F** is non-singular, equation (2.17) can be reduced to $\mathbf{G} = \mathbf{F}^{-1}$ by multiplying $\mathbf{F}^{-1}$ two times. It can be proved that for every finite matrix **F,** there exists a matrix **G** satisfies (2.17), which is not uniquely defined by (2.17) unless **F** is nonsingular (Ben-Israel and Greville 2001, p.29).

A unique generalised inverse for every finite matrix **F** was defined by Moore (Moore 1920) and proved by Penrose (Penrose 1955) to be the unique matrix **G** satisfying equation (2.17) and the following three equations:

$$\mathbf{GFG} = \mathbf{G}, \tag{2.18}$$

$$(\mathbf{FG})^* = \mathbf{FG}\,, \tag{2.19}$$

$$(\mathbf{GF})^* = \mathbf{GF}\,, \tag{2.20}$$

where $\mathbf{F}^*$ denotes the conjugate transpose of **F**. The unique generalised inverse **G** is commonly known as the *Moore-Penrose inverse* of **F**, and normally denoted as $\mathbf{F}^\dagger$. The Moore-Penrose inverse can be used not only for solving the consistent equations to obtain a minimum norm solution, but also for obtaining the least-square solutions of the inconsistent equations in the form of (2.16) (Aster *et al* 2013).

Although the concept of generalised inverse became thriving only after the paper of Penrose (Penrose 1955), it was first mentioned by Fredholm (Fredholm 1903) (called by him 'pseudo-inverse') referring to integral operators, earlier than Moore (Moore 1920) referring to matrices. The class of all pseudo-inverses of integral operator was characterised by Hurwitz (Hurwitz 1912). Comparisons of these pseudo-inverses with the Moore-Penrose generalised inverse are given in (Rail 1976). Generalised inverses of differential operators have been discussed by Hilbert (Hilbert 1912) in terms of generalised Green's functions. A review of generalised inverses of integral and differential operators can be found in (Reid 1968).

For the discrete linear inverse problems, of which the forward mapping F is a matrix **F**, the Moore-Penrose inverse $\mathbf{F}^\dagger$ can be used as a backward mapping G to obtain the minimum norm least-square solution, called generalised solution. Hence, by letting $F = \mathbf{F}$ and $G = \mathbf{F}^\dagger$, the relationships between F and G can be described by the equation (2.17) ~ (2.20). The model resolution and data resolution are thus, $R_m = \mathbf{F}^\dagger\mathbf{F}$ and $R_d = \mathbf{F}\mathbf{F}^\dagger$, respectively. The *singular value decomposition* (SVD) method (Golub and Van Loan 2012) is commonly used to compute and analyse the Moore-Penrose inverse, the data resolution and the model resolution. In real situations, due to the noise effect, the Moore-Penrose inverse can be very unstable, and regularisations are often needed to reduce the noise effect.

Surprisingly many continuous inverse problems are in the form of Fredholm integral equations of the first kind (IFK), such as Example 2.2; they can normally be discretised into discrete linear inverse problems with good approximation. Techniques of discretising integral operators into matrices, such as quadrature methods and Backus & Gilbert method, are discussed in (Engl *et al* 1996, Aster *et al* 2013). After discretisation, the inverse problems can then be analysed or solved with the Moore-Penrose inverses of the discretised forward mappings.

Generalised inverse is not only an important analytical method of solving the inverse problem, but also a useful tool for investigating the structure of inverse problems. The model resolution of generalised solution shows the inevitable bias of the inverse solution, which is an intrinsic property of the forward mapping. The data resolution can be used as a filter to detect and partially remove the noise in the measured data owe to its idempotent property.

2.7.2 Application of functional analysis

In functional analysis, by investigating the structural properties of inverse problems, many useful theorems are derived. These theorems are powerful tools for analysing the solutions of inverse problems and the principle of solving inverse problems, especially when the models are infinite dimensional (i.e. functions). For instance, in the book of Lebedev *et al.* (Lebedev *et al* 2000) on functional analysis, the following theorems and results on inverse problems are derived.

1. By assuming the model space $\mathcal{M}$ and data space $\mathcal{D}$ in the mathematical model of inverse problem (2.4) are normed vector spaces, and F is a compact linear operator, it can be derived that if $\mathcal{M}$ is infinite dimensional, F cannot have a bounded inverse, i.e. F^{-1} , if it exists, is not stable.
2. Let $\mathcal{M}$ and $\mathcal{D}$ be normed vector spaces, when F is a continuous one-to-one operator from $\mathcal{M}$ to $\mathcal{D}$, a continuous inverse of F can be obtained by restricting the domain of F to be a compact subspace of $\mathcal{M}$ (Tikhonov and Arsenin 1977).
3. By assuming $\mathcal{M}$ and $\mathcal{D}$ are Banach spaces, and $\mathcal{M}$ is infinite dimensional, it can be proved that the solution of an arbitrary observation in D cannot be both unique and exist.
4. By assuming $\mathcal{M}$ and $\mathcal{D}$ are Hilbert spaces, and F is a continuous linear operator, the existence of a unique generalised solution (the least square solution of minimum norm) can be proved.
5. Under the same assumption, it can be proved that the generalised inverse $F^{\dagger}$, which associates the data to the generalised solution, is a closed operator, and $F^{\dagger}$ is continuous if and only if the range $R(F)$ is closed.

Moreover, for inverse problems in the infinite dimensional context, the theory behind Tikhonov regularisation is established base on functional analysis (Groetsch 1984). A general regularisation theory is given in (Kirsch 1996).

2.8 Conclusions

In this chapter, the basic theories and concepts for investigating the structure of inverse problems in metrology, including measurement theory, inverse problems, mathematical structures and category theory, are briefly reviewed. The structure of measurement is introduced via the representational theory of measurement, and some structural properties of inverse problems are reviewed base on the theories of generalised inverse and functional analysis. A connection between the mathematical models of indirect measurements and inverse problems can be observed, which is demonstrated with some examples of inverse problems in metrology. This connection enables us to define and investigate a general type of inverse problem in metrology called IPM, which is, to the best of the author's knowledge, not yet studied before in any literature from the perspective of mathematical structure. This is perhaps because:

1. It is commonly believed that the objective of measurement is to obtain the values of the measurand (JCGM 100 2008); the fact that measurand values should represent the empirical relations is often ignored.

2. Inverse problems are often treated as pure mathematical problems of estimating the model parameters; the fact that the model normally is or contains a quantity to be measured is often ignored.

It is demonstrated in the next chapter that the connection between indirect measurements and inverse problems implies the necessity of embedding a relational structure into the model and data spaces of the inverse problems of measurement. This makes the structure of IPMs different from other inverse problems, and thereby a series of new results, such as the desired properties of solving the IPMs, can be derived.

Chapter 3
Deterministic Model of Indirect Measurements and the Inverse Problem of Measurement

3.1 Representational model of indirect measurements

It is introduced in last chapter that measurement is the process of experimentally obtaining quantity values that can be reasonably attributed to a quantity. This process assigns numbers to the objects manifesting the measurand, in such a way to represent the empirical relations of the objects. In this chapter, to study the basic structure properties of the inverse problems of measurement, it is being assumed that the measurement process of a quantity can be modelled by a deterministic homomorphism φ of the ERS, such that for any objects $a, b \in A$,

$$a \square b \Leftrightarrow \varphi(a) = \varphi(b)\,, \tag{3.1}$$

where $\varphi(a)$ and $\varphi(b)$ are the measured values. This is called the *deterministic assumption* of measurement, which implies that the measured values contain no random errors.

The deterministic assumption enables us to establish a simple and universal model of indirect measurements based on the representational theory of measurement. From that model, a general type of inverse problem involved in indirect measurements can be identified, which is the inverse problem of measurement to be studied in this thesis.

3.1.1 Direct measurements

By the representational theory, a measurement process can be modelled as a homomorphism from the ERS of the quantity to a specified NRS, which maps each object in the ERS to a measurand value in the NRS. In direct measurements, the empirical relations can be directly observed via an empirical operation, and the measurand values can be assigned accordingly. For example, the empirical relations of the length of rods can be observed by placing the rods parallel with each other. No other quantities and the related measurement processes are involved in a direct measurement. Hence a direct measurement maps the measured objects directly to their measured values, which can be modelled as a homomorphism from the ERS to a NRS.

The schema of direct measurement can thus be described by the diagram in Figure 3.1. But practically, some random measurement error is always involved in the measured values. Thus, it is not always suitable to model a measurement process as a deterministic and structure-preserving mapping depending on the noise effect. The deterministic assumption of measurement is used to simplify the model and reveal the basic structure of measurement.

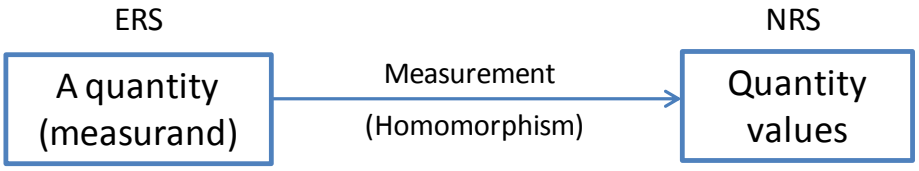


Figure 3.1 The schema of direct measurement

3.1.2 The framework of indirect measurement

For an indirect measurement of a measurand, one or more other quantities are involved to infer the measurand values. These quantities, named as *proxy quantities*[4], can be measured directly or in an easier and/or more reliable way comparing to the measurand. They are related with the measurand in the sense that the measurand can be considered as the cause (or part of the cause) of the observable effects manifest in terms of the proxy quantities. According to the relationship of the measurand and the associated proxy quantities, the proxy quantities can be used to infer the information of the measurand. For example, the thermal expansion of the mercury in a thermometer is an observable effect of temperature, which can be measured in length. According to the length of the mercury, the temperature can be inferred. So there is a *cause-and-effect relationship* between the measurand and the proxy quantities. From this point of view, inferring the values of the measurand from the measured values of the proxy quantity(s) (called the *measured data*) is an *inverse problem*.

For a direct measurement, the homomorphism from the ERS of the measurand to the NRS of the measurand values can be implemented by a measurement process. While for an indirect measurement, this mapping is not implemented directly, instead it takes the following steps:

a. Relate the measurand to some proxy quantity(s), which manifesting its observable effect(s), with a functional relation, such as equation (2.2) or (2.3).
b. Measure the proxy quantity(s) to obtain some measured data.

[4] An proxy quantity is also an influence quantity which is defined in GUM (JCGM 100 2008), since it affects the result of the measurement, but they are not the same concept.

c. Infer the measurand values using the measured data and the functional relation.

These steps can be described by the three mappings (a, b, c) in Figure 3.2. The combination of these three mappings maps the objects manifesting the measurand into the measurand values, which is desired to be a homomorphism according to the representational theory of measurement. The schema in figure 3.2 reveals *the framework of indirect measurement*. Comparing this schema with the schema of direct measurement, the measurement process of indirect measurement is implemented via the combination of the three mappings.

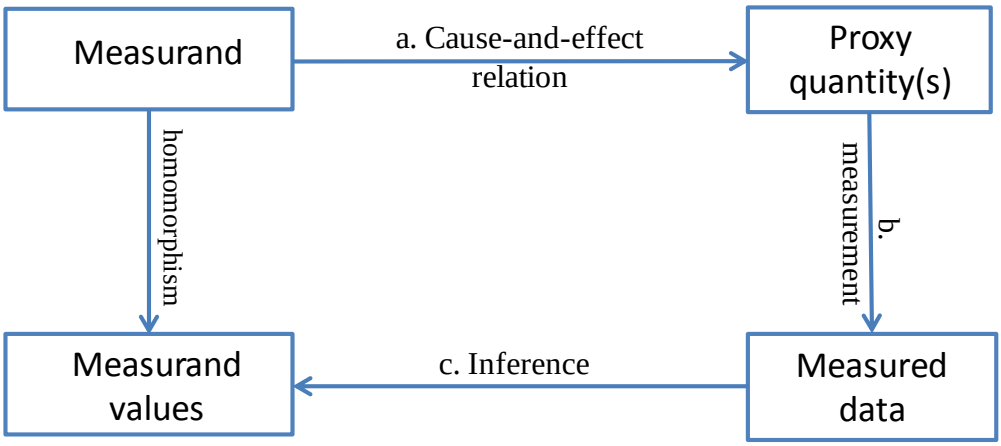


Figure 3.2 The schema of indirect measurement

3.1.3 The inverse problem in the framework of indirect measurement

Since the inference process of indirect measurement can be considered as an inverse problem, there is an essential connection between inverse problem and indirect measurement. An inverse problem is involved in an indirect measurement if the value of the measurand can be obtained by solving the inverse problem. This type of inverse problem is called as the inverse problem of measurement.

Definition 3.1: The *inverse problem of measurement* (IPM) is the problem of inferring the values of a measurand from the observations of some other quantity(s).

Comparing to the definition of inverse problem, the IPM is a general type of inverse problem involved in measurement. For direct measurements, since the measurand values can be directly obtained from the measurement process, no inverse problem is involved. The IPMs arise from indirect measurements.

As an inverse problem, the mathematical model of an IPM should conform to equation (2.4), and the framework of an IPM can be described by the diagram in Figure 2.8. The next

question is how to describe the IPM in the framework of indirect measurement. To see this, some examples of inverse problems in indirect measurements are needed.

Example 3.1 Contact measurement of surface profile

In surface metrology, a tactile spherical stylus is used to measure the surface profile of a free-form surface. As shown in Figure 3.3, during the measurement the stylus *S* moves along the surface profile, the locus of the centre point of *S*, which is called a traced profile in ISO 3274 (1998), is recorded as the measured data in an *x*-*y* coordinate system.

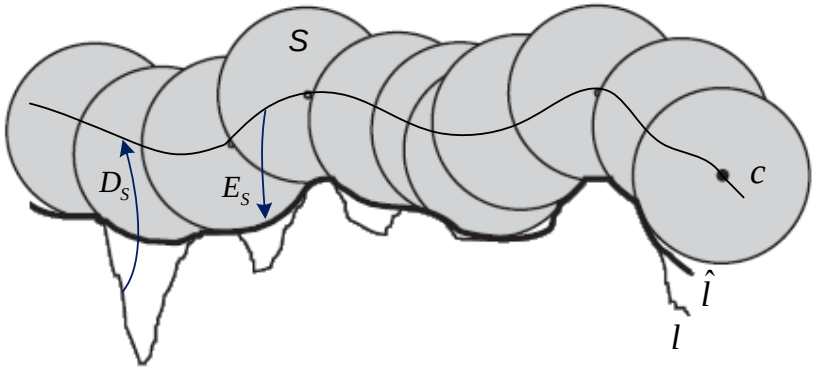


Figure 3.3 Contact measurement of surface profile *l*

c is the locus of centre point, *l'* is the estimation of the surface profile

$D_S : l \mapsto c$ is a dilation operator, and $E_S : c \mapsto \hat{l}$ is an erosion operator

Let $l(x)$ be the function of the height of a surface profile, and $c(x)$ be function of the recorded locus of *S*, $l(x)$ and $c(x)$ are defined within a specified evaluation interval *I*. It is clear that the observed locus is different from the actual surface profile, and the distortion is determined by the actual shape and size of the stylus *S* (see Figure 3.3).

Take the stylus *S* as a structuring element of morphological operators, the transformation from $l(x)$ to $c(x)$ can be formulated as a *function processing dilation operator* (Maragos and Schafer 1987), denoted as D_S. Thus the recorded locus can be described as

$$c = D_S(l). \tag{3.2}$$

To estimate the surface profile *l* from the locus *c* is an inverse problem. The best estimation of the surface profile can be obtained by applying a *function processing*

erosion operator, denoted as E_S, to the locus c (Gröger *et al.* 2005). The estimated profile is

$$\hat{l} = E_S(c) = E_S D_S(l), \tag{3.3}$$

which is named as a real mechanical profile in ISO 14406 (2010). By solving the inverse problem in the form of (3.2), the real surface profile can be indirectly measured via the locus of the stylus.

Example 3.2 White light interferometry

White light interferometry is a technique to measure the topography of surface. For each point on the surface, it is observed by one pixel, and the height is measured indirectly according to the variation of the light intensity at that point during an axial scan of the measurement process. The light intensity varies in terms of the interference fringes of the white light, which can be described as (Malacara 2007)

$$I(z) = I'[1+\gamma(z)\cos(k_0 z)] \tag{3.4}$$

where I' (the background intensity) and k_0 (the number of fringes under the envelope) are both constants, $\gamma(z)$ is the envelope function of the fringes, and z is the axial position (see Figure 3.4).

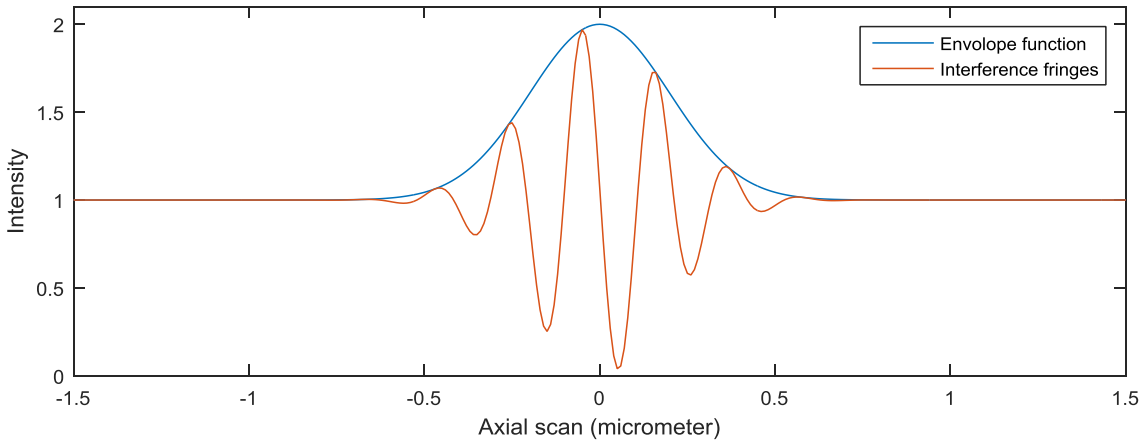


Figure 3.4 The interference fringes and the envelope function of white light

From equation (3.4), $\gamma(z)$ can be estimated according to the observation of $I(z)$. A simple Fourier method proposed by Kino and Chim (1990) can be used to solve this inverse problem. First the Fourier transform of the signal $I(z)$ is computed, which is transformed to a function of three lobes in the frequency domain. The right side-lobe is

isolated and shifted to the centre (origin) to lower the frequency of the signal. And then the envelope function $\gamma(z)$ is calculated using an inverse Fourier transform.

The measurand is the height h of each measured point, which can be determined from the centre of mass of $\gamma(z)$. Thus if function $\gamma(z)$ is symmetric, such as a Gaussian function, then $h = z_0$ such that $\gamma(z_0) = \max(\gamma(z))$.

It is worth to take note that, by definition, an IPM always refers to a specified measurand, rather than several measurands of a general type. This is because the empirical relations and the ERS of a measurement can be defined only when the measurand is specified. For example, in the measurement of surface texture, the heights of all the points on the surface are collected, but only when the measurand is specified to be roughness Ra, a number can then be assigned to the measured surface, and different surfaces can be compared according to their values of roughness. If the specified measurand can be obtained from the model of an inverse problem, then this inverse problem can be considered as an IPM.

In some cases, the model of an IPM m and the measurand x can be a same quantity. But, for estimating the value of the measurand, the model does not necessarily be the same quantity as the measurand. The model can be any mathematical object contains the information of the measurand, as long as the values of the measurand can be extracted from the model via a given function. In the example of white light interferometry, the function from the envelop function $\gamma(z)$ to its centre of mass z_0 is used to extract the measurand h. This function is called an *extraction function*, denoted as T. In the example of contact surface measurement, the extract function is an identity function, since the model $l(x)$ itself is the measurand. If the model and the measurand are the same, the extraction function, T is simply an identical function I.

Many inverse problems can be taken as an IPM in an indirect measurement. In Example 2.1, the inverse problem of estimating the slowness distribution can be taken as the inference process of the indirect measurement of the average slowness $\overline{s}$ of the measured area. The measurand value $\overline{s}$ is simply the average of the entities of vector $\mathbf{s}$ (the inverse solution), which can be obtained using a function $T:\mathbf{s}\rightarrow\overline{s}$. Similarly, in Example 2.2, the inverse problem of estimating the distribution of the mass density can be taken as an IPM in the indirect measurement of the average density of the buried field, the measurand values can be

extracted from the inverse solution[5] **m**. In Example 2.3, the technique of solving the inverse problem of estimating the earthquake hypocentre can be applied in the indirect measurement of the location or the origin time of the earthquake.

In an indirect measurement, when the mapping from the measured data to the measurand values is not known, an IPM arises. Assume that the inverse problem can be solved with a backward mapping G from the data space $\mathcal{D}$ to the model space $\mathcal{M}$, such as the inverse or a generalised inverse of the forward mapping F. By using the mappings G followed by an extraction function T, the measurand values can be estimated from the measured data. Therefore, based on the schema in Figure 3.2, the schema of indirect measurements with the IPM can be described by Figure 3.5.

To estimate the measurand values, it's important to know the mathematical model of the inverse problem involved in the indirect measurement. A proper backward mapping should be chosen according to the forward mapping to derive the model which contains the information of the measurand.

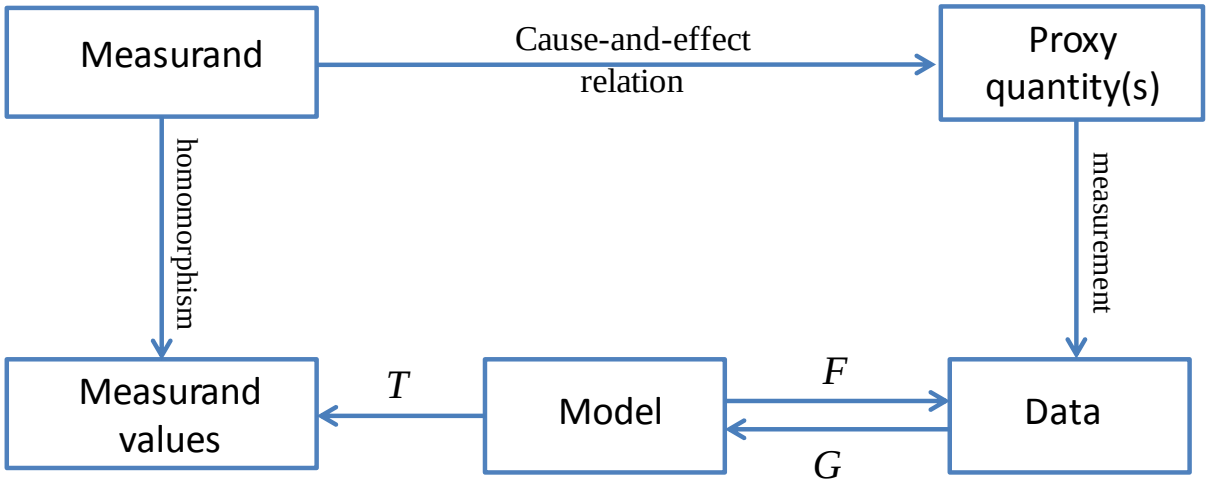


Figure 3.5 The schema of indirect measurements and the IPM

F is a forward mapping, G is a backward mapping, T is an extraction function.

3.2 Desired properties of solving the inverse problems of measurement

A well-posed problem has following three defining properties (Hadamard 1902):

1) a solution exists (existence);
2) the solution is unique (uniqueness);

[5] Inverse solution refers to the 'solution' of the inverse problem which may not exactly fit the measured data.

3) the solution continuously depends on the measured data (stability).

If at least one of the defining properties is not satisfied, the problem is called an ill-posed problem. Some of the inverse problems are ill-posed, which are interesting due to the difficulty of solving the ill-posed problems. Not being able to satisfy the existence, the uniqueness, and the stability are the three essential issues of inverse problems (Aster *et al.* 2013). Due to the essential issues, solving an inverse problem is no just about finding a solution exactly fitting the observation. More than one property of the solution is desired, which are normally difficult to be satisfied all together, a trade-off between these properties should be considered. Moreover, for the IPMs, due to the special properties of measurement, some more desired properties should be considered. These desired properties characterise the IPM, and can be used to derive the structural properties of the IPM.

Based on the essential issues and special characters of the IPMs, the following five properties are desired for solving the IPMs.

P1. The forward mapping *F* should be known.

P2. The inverse solutions should adequately fit the measured data.

P3. The backward mapping *G* should be topologically and numerically stable.

P4. The estimated measurand values should reflect the empirical relation.

P5. The inverse solution should satisfy the principle of Occam's razor.

These properties, indexed with P1~P5, are elaborated in this section following a logic order. Some properties of the mappings *F* and *G* of the IPMs can be derived from these desired properties, which are important for understand the structural properties of the IPMs.

3.2.1 Forward mapping (P1)

First, as a precondition of solving the inverse problem, when the model parameters are unknown, *the forward mapping F should be known* (P1), so that the mathematical model of the inverse problem can be described in the form of

$$F(m) = d. \tag{3.5}$$

The forward mapping *F* refers to a mapping that *correctly* models the functional relation between the model and the data. This should be verified by calibration.

Under the deterministic assumption, data d does not contain any random error, any data $d \in D$ can be written as $d = F(m)$ with some $m \in M$ when F correctly models the relationship between the model and the data, thus F is surjective.

3.2.2 Fitting criterion (P2)

For an inverse solution $\hat{m} = G(d)$ derived by the backward mapping, since the actual model m is unknown, the best way to verify the solution is to check whether it fits the data, in the sense that

$$F(\hat{m}) = d\,,$$

$$\text{or} \qquad FG(d) = d\,. \tag{3.6}$$

In the simplest case, equation (3.5) can be solved using the inverse of F, and the backward mapping G is desired to be F^{-1}, so that (3.6) can be satisfied. But when F is not injective, the solution is not unique, thus the inverse of F does not exist.

For any data d in the range (image) of F, d is equal to $F(m)$ for some $m \in M$. Thus (3.6) can be written as

$$FGF(m) = F(m)$$

$$\text{or} \qquad FGF = F\,. \tag{3.7}$$

Under the deterministic assumption, all the measured data is in the range of F. Hence the inverse solution can fits with the data if G satisfies (3.7). Mapping G in (3.7) is a generalised inverse of F, which derives an inverse solution belonging to the preimage of d. If F is not injective, the element in the preimage (solution) is not unique, and thus G is also not unique. A criterion of choosing the solution is needed.

In practice, due to the noise in the data, some data is not in the range of F. Thus no solution can be found to fit the data exactly. Moreover, due to the stability issue, fitting the data too precisely may cause significant noise effect in the solution. Hence, when the noise is under consideration, the inverse solution is desired to be *adequately fit the observations* (P2). Uncertain degree of misfit between the solution and the data should be accepted, which is usually specified as $\left\|F(\hat{m}) - d\right\|_2 \le \varepsilon$, where ε is a small number. In linear inverse problem, least-square method and Moore-Penrose generalised inverse can be used to find the inverse solution with minimum misfit.

3.2.3 Stability criterion (P3)

In different context, stability is defined in many different ways. For instance, in general system theory, the general concept of stability is described as follows. Let *c* and *e* represent the cause and effect of a phenomenon, respectively, and $e = F(c)$. The cause-effect pair (c, e) is stable if small deviations from *e* are caused by small deviations from *c* (Mesarovic & Takahara, 1975, p.160). Similarly, in signal processing, a linear time invariant (LTI) system is said to be BIBO (bounded-input, bounded-output) stable if every bounded input produces a bounded output (Rabiner & Gold, 1975, p.14). For partial differential equations, the solution is stable if it depends on the auxiliary conditions in a continuous manner in such a way that a small change in the auxiliary conditions only produces a small change in the solution (Jeffrey 2003).

In this section, the stability of an IPM is investigated in two different forms: *topological stability* and *numerical stability*, which are determined by the properties of the backward mapping. The former gives the necessary condition of stability, and the latter determines the degree of stability. The stability discussed here should be distinguished from the concept of measurement stability which is closely related with measurement repeatability and uncertainty.

a. Topological stability of the IPMs

An inverse problem is considered as stable if a 'small' change in the data implies a 'small' change in the inverse solution (Aster *et al* 2013, p.19). This is analogous with the definition of the *continuity* of a function (or a mapping): 'small' changes in the input result in 'small' changes in the output. For the IPMs, *G* is the mapping from the measured data to the inverse solution, thus the stability can be determined by *the continuity of the backward mapping G*. This type of stability is named as *topological stability*.

Depends on the types of topology of the input and output spaces, the continuity of a mapping can be defined in different ways, and have different meanings.

Example 3.3 The continuity of a mapping $f : X \to Y$ between two metric spaces $\langle X, d_1\rangle, \langle Y, d_2\rangle$ can be defined with the distances in the metric spaces: *f* is uniformly continuous, if for any $x, y \in X$, distance, $d_1(x, y)$ is arbitrarily small implies distance, $d_2(f(x), f(y))$ is also arbitrarily small (Hadamard 2003, p.34).

Example 3.4 Alexandrov space is a topological space, which can be uniquely determined by a preordered set. In Alexandrov spaces, magnitude of difference is not definable, thus the continuity of the mapping between Alexandrov spaces is defined in a more general way with *neighbourhoods*: a mapping $f:\langle X,\Gamma_X\rangle\to\langle Y,\Gamma_Y\rangle$ is continuous if for any neighbourhood Q of $f(x)$, there always exist a neighbourhood P of x such that $f(P)\subseteq Q$, where x is an arbitrary point in set X (Sutherland 1975).

If the model and data spaces of inverse problems are metric spaces or normed vector spaces, the magnitudes of differences in model space and data space can be defined by the distances or the norms of the space, and then the stability of those inverse problems can be defined.

While for the IPMs, not all measurands can be represented numerically with an additive operation (see Section 2.2.2). The empirical structures of some measurands (e.g. loudness) are conjoint structure; the representations of some measurands (e.g. hardness, preference) are in the ordinal scale. For these types of measurands, the magnitude of difference is not definable. Thus, instead of using differences in metric spaces, a more general way to define the stability of the IPMs is needed. Topological stability is the solution to this problem.

There are many types of empirical structure, such as extensive structure, conjoint structure and order structure. An ERS always has an ordering relation (such as a weak order or a preorder) called empirical relation[6], so it can be taken as a set with an ordering relation, namely an ordered set. To preserve and represent the empirical relational structure, the model space $\mathcal{M}$ and the data space $\mathcal{D}$ of an IPM are determined by the ERS. Hence $\mathcal{M}$ and $\mathcal{D}$ are also ordered sets.

To investigate the topological stability of the IPM, the topologies of the model and data spaces should be defined. It has been shown by Naturman (1991) that every preordered set, $\mathcal{A}=\langle A,\precsim\rangle$ can be converted to a unique topological space, $T(\mathcal{A})=\langle A,\Gamma\rangle$, named *Alexandrov space*, by the following construction of open sets: call a subset U of A open if, whenever $x\subseteq U$, we have $R(x)\subseteq U$, where $R(x)=\{y: x\precsim y\}$. In Alexandrov space, each element x has a minimal neighbourhood (Arenas 1999) which is the intersection of all open sets containing x, and $R(x)$ is the minimal neighbourhood of x in $T(\mathcal{A})$.

[6] Unless otherwise specified, an empirical relation means a binary empirical relation.

Therefore, if the ordered sets $\mathcal{D}$ and $\mathcal{M}$ can be converted into Alexandrov spaces, denoted as $T(\mathcal{D})$ and $T(\mathcal{M})$. The continuity of G can be defined with the neighbourhoods in $T(\mathcal{D})$ and $T(\mathcal{M})$, and the topological stability of the IPMs can be defined between Alexandrov spaces.

Definition 3.2: An IPM is *topologically stable* if and only if the backward mapping is a continuous mapping between the Alexandrov spaces associated with the ordering relations in the data and model spaces.

If difference is defined in the ERS, such as concatenation structure $\langle A, \precsim, \circ \rangle$, then $\mathcal{D}$ and $\mathcal{M}$ are both preordered metric spaces. In this case, the stability means G is not only continuous between Alexandrov spaces (topological stability) but also between metric spaces.

Proposition 3.1: Let G: $\mathcal{D} \longrightarrow \mathcal{M}$ be a mapping between two preordered sets, $T(\mathcal{D})$ and $T(\mathcal{M})$ are the Alexandrov spaces convert from $\mathcal{D}$ and $\mathcal{M}$. The *continuity* of G: $T(\mathcal{D}) \longrightarrow T(\mathcal{M})$ is equivalent to the *monotonicity* of G: $\mathcal{D} \longrightarrow \mathcal{M}$.

A proof of this proposition is given by P. J. Scott (2004) using open sets. It can also be proved using neighbourhoods as following.

Proof: For any element $d \in D$, let U be a minimal neighbourhood of d in $T(\mathcal{D})$,

and let V be a minimal neighbourhood of $G(d)$ in $T(\mathcal{M})$.

If G is monotonic, we have

$$d \precsim d' \Rightarrow G(d) \precsim G(d'), \qquad \text{for any } d' \in D. \tag{3.8}$$

Since $U = R(d) = \{c \in D: d \precsim c\}$, and $V = R(G(d)) = \{x \in M: G(d) \precsim x\}$,

(3.8) is equivalent to

$$d' \in U \Rightarrow G(d') \in V,$$

which is equivalent to the following statement.

$$G(U) \subseteq V \tag{3.9}$$

Hence G is monotonic if and only if (3.9) is true.

By the neighbourhood definition of continuous mapping, G: $T(\mathcal{D}) \longrightarrow T(\mathcal{M})$ is continuous if and only if the following statement (S1) is true.

S1: for any neighbourhood Q of $G(d)$, there always exist a neighbourhood P of d such that $G(P) \subseteq Q$.

Firstly, we prove S1⇒(3.9). For any neighbourhood P of d, we have $U \subseteq P$, which implies $G(U) \subseteq G(P)$. Let $Q=V$, if (3.9) is not true, i.e. $G(U) \not\subset V$, then $G(P) \not\subset V = Q$, i.e. S1 is also not true. Hence we have S1⇒(3.9).

Secondly, we prove (3.9)⇒S1. For any neighbourhood Q of $G(d)$, we have $V \subseteq Q$. Let $P = U$, we have $G(U) \subseteq V \Rightarrow G(P) = G(U) \subseteq V \subseteq Q$, i.e.

$$G(U) \subseteq V \Rightarrow G(P) \subseteq Q.$$

So we get S1⇔ (3.9),[7] which proves the proposition. □

For an IPM, this proposition means G is continuous between the Alexandrov spaces if and only if it is monotonic (i.e. order-preserving). Hence we have the following equivalence relations: topological stability of an IPM ⇔ continuity of G ⇔ monotonicity of G.

Assume that the topological stability of an IPM is satisfied. Then the relational structures of model and data spaces must be preordered so that they can be converted into Alexandrov spaces. Thus, the empirical structure, which determines the structures of $\mathcal{M}$ and $\mathcal{D}$, must also be preordered. In other words, the topological stability of the IPM leads to the empirical structure being preordered.

b. Numerical stability

Although every linear transformation between finite dimensional spaces is a continuous mapping (Schechter 1997), the inverse solution may still be very sensitive to the error in the data such that the noise effect dominates the solution. Thus besides the topological stability, the degree of sensitivity of the backward mapping to the changes or errors in the input data, namely the *numerical stability* of the inverse problem, should also be considered.

The numerical stability can be measured by the *condition number* (Aster *et al* 2013, p.67) of the backward mapping. For a matrix **G**, the condition number is the ratio of the maximum and the minimum non-zero singular values. When the condition number is large, the output of **G** can be very sensitive to the changes in the input. If a backward mapping G satisfying equation (3.7) has a large condition number, G should be adjusted to improve the stability, which can be done by different regularisation methods, such as truncated singular value decomposition (TSVD) and Tikhonov regularisations (Aster *et al* 2013). The regularisation

[7] This proof also shows that the continuity of a mapping between two Alexandrov spaces can be defined with minimal neighbourhoods.

introduces a restriction on the inverse solution; meanwhile, it causes some bias in the inverse solution. For example, the objective function of 0^{th} order Tikhonov regularisation is

$$\min(\|\mathrm{Fm}-\mathrm{d}\|_2+\alpha^2\|\mathrm{m}\|_2), \tag{3.10}$$

where α is a scalar parameter to be optimised. As demonstrated in (Aster *et al* 2013, p 99), an inverse solution can be obtained from (3.10) as

$$\mathbf{m}_\alpha=(\mathbf{F}^T\mathbf{F}+\alpha^2\mathbf{I})^{-1}\mathbf{F}^T\mathbf{d}\,. \tag{3.11}$$

Hence, after the regularisation, the backward mapping becomes $\mathbf{G}=(\mathbf{F}^T\mathbf{F}+\alpha^2\mathbf{I})^{-1}\mathbf{F}^T$, which does not satisfy the fitting criterion (3.7). As a result, the inverse solution $\mathbf{m}_\alpha$ will not fit the data exactly. The objective function of regularisation provides a trade-off between fitting the data and the numerical stability.

In summary, *the backward mapping G should be both topologically and numerically stable*. This is the desired property P3.

3.2.4 Posets of the model and data spaces

Before the discussion of the next two desired properties, a general method of defining the ordering relations in the model and data spaces is needed.

To be able to define the topological stability of the IPMs, the model and data spaces should be modelled as preordered sets. Sometimes, there is more than one way to define an ordering relation in a space. For instance, in a vector space, the order between vectors can be defined by comparing the norms or defined in the pointwise order. In metrology, numerical relations are used to represent empirical relations. Hence a meaningful way of defining the ordering relations in $\mathcal{M}$ and $\mathcal{D}$ should be chosen according to the empirical relation.

a. Partial order between measurand values

The elements in a preordered ERS can be divided into equivalence classes according to their measurand values. For example, rods with a same length are equivalent (but not exactly the same), and they can be allocated to an equivalence class. For a preordered set A, two elements a and b are equivalent, if $a \precsim b$ and $b \precsim a$, denote as $a \sim b$. A preorder $\precsim$ with anti-symmetric property (if $a \precsim b$ and $b \precsim a$, then $a=b$, for all $a,b \in A$) is a partial order $\preceq$. So, as shown in Figure 3.6, a preordered set can always be converted to a partially ordered set (poset) by merging the equivalent elements into equivalence classes.

It's not necessary to distinguish the equivalent objects with numbers, thus the equivalent objects in the preordered ERS can be represented by a single number in the NRS. Hence a preordered ERS, such as $\langle A, \precsim \rangle$, can be represented by a partially ordered NRS, such as $\langle X, \leq_X \rangle$. Each measurand value in the NRS corresponds to an equivalence class in the ERS. The homomorphism, which models the measurement process, converts a preordered ERS to a partially ordered NRS. Hence, in the deterministic model of the IPM, the ordering relations between measurand values always belong to the type of partial order.

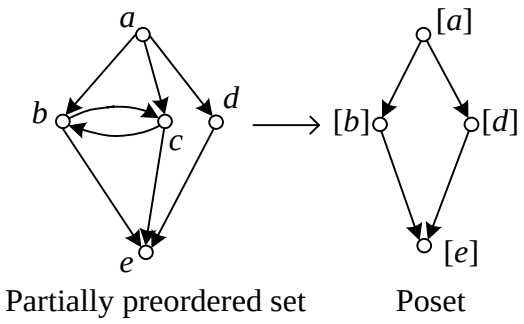


Figure 3.6 From a partially preordered set to a poset

$a \rightarrow b$ stands for $a \precsim b$.

b. Ordering relation in model space

In some case, such as Example 3.1, the model of an IPM and the measurand are the same, so the ordering relation in the model space is the same as the ordering relation between the measurand values. While, in many cases, such as Example 2.1, 2.2 and 2.3, the model and the measurand are different, an ordering relation $\leq_M$ should be defined in order to set the model space to be an ordered set, and this relation must be *empirically meaningful* in the sense that it is related with the empirical relation of the measured objects.

In Example 3.1, surface profile $l(x)$ is the measurand and also the model of the IPM. Since the empirical relation of surface profile (above or below) is determined by every point of the profile, the order between models should be the pointwise order of vectors. If $l_1(x) \leq l_2(x)$ for all $x \in I$, then $l_1 \preceq l_2$; if there is any intersection between the curves of l_1 and l_2, they are incomparable (neither $l_1 \preceq l_2$ nor $l_2 \preceq l_1$). In the example of seismic tomography (Example 2.1), let the measurand be the average slowness of the measured area, then the order between the models (vectors of slowness) should be determined by the average of the entities of slowness vector, i.e. $\mathbf{s}_1 \leq \mathbf{s}_2$ if and only if $T(\mathbf{s}_1) \leq T(\mathbf{s}_2)$, where $\mathbf{s}_1, \mathbf{s}_2$ are the slowness vectors

of two measured areas and T is the function of averaging of the entities of a vector. Therefore, the ordering relation $\leq_M$ of the model space $\mathcal{M}$ can be defined according to the magnitude of the measurand.

Definition 3.3: For any two objects a, b in the ERS, their models $m_a \leq_M m_b$ if and only if $T(m_a) \leq_X T(m_b)$, where $\leq_X$ is the (partial) order of measurand values and T is a extraction function.

As demonstrated before, the relation $\leq_X$ of measurand values is a partial order. Thus Definition 3.3 implies the model space is a poset.

c. Ordering relation in data space

In the data space, a measured data is a collection of the measured values of one or more proxy quantities related to the measurand, which can be 'decoded' into a estimated value of the measurand via the inference process. Hence, for each measured object, the measured data can be considered as a label to be decoded.

Similar to the model space, the ordering relation $\leq_D$ in the data space $\mathcal{D}$ should also be defined in an empirically meaningful way. In many cases, the proxy quantity(s) and the measurand are different quantities (see Example 2.1, 2.2, 2.3 and 3.2). In this situation, the only possible way to relate $\leq_D$ with the empirical relation is to use the estimated values of the measurand from the data. The estimated values can only be obtained using a proper backward mapping G. Hence relation $\leq_D$ can be defined in the following way.

Definition 3.4: For any two objects a, b in the ERS, their data $d_a \leq_D d_b$ if and only if $TG(d_a) \leq_X TG(d_b)$.

Since $\leq_X$ is a partial order, the data space is also a poset.

In some cases, there is only one type of quantity involved in the IPM. For instance, in Example 3.1, the measured data is the locus of centre point, and the model is the surface profile, i.e. the measurand. They both belong to a more generic type of quantity (functions of height), which can both be ordered in the point-wise order. The indirect measurement of the height of a building according to the length of its shadow is also a typical example. Here the height and the length are both belong to a generic quantity, length. In this situation, the orders in the model and data spaces can be naturally defined in the same way as the partial order of the measurand values, instead of using definition 3.4.

3.2.5 Estimation of empirical relations (P4)

For the IPMs, there is one more desired property on the inverse solutions which is related with the special character of IPM. By definition, the information to be derived in an IPM is the values of a measurand, and according to the representational theory, measurand values should be able to represent the (relational) structure of the ERS. Hence, *the relation of the estimated measurand values should reflect the empirical relation in the ERS* (P4). That means, the following relation between the measurand values, x_1, x_2 and their estimations, $\hat{x}_1, \hat{x}_2$ is expected to be satisfied:

$$x_1 \leq_X x_2 \Rightarrow \hat{x}_1 \leq_X \hat{x}_2 . \tag{3.12}$$

It is clear that (3.12) may not be satisfied due to the noise in the measured data, but the noise effect is not the only factor of the correctness of estimated empirical relation. With the deterministic assumption, a necessary condition of satisfying P4 can be deduced.

Proposition 3.2: The monotonicity of the model resolution *GF* is a necessary condition of satisfying the desired property P4.

Proof: The estimated measurand values are extracted from the inverse solutions, thus

$$\hat{x}_i = T(\hat{m}_i) \text{ and } \hat{m}_i = G(d_i), \tag{3.13}$$

where $\hat{m}_i$ and d_i are respectively the estimated model and the measured data of the *i*th object. Thus (3.12) can be written as

$$x_1 \leq_X x_2 \Rightarrow TG(d_1) \leq_X TG(d_2) . \tag{3.14}$$

By the deterministic assumption, the measured data contain no noise, any data $d \in D$ can be written as $d = F(m)$, with some $m \in M$. For the measured data d_i, the estimated measurand value is

$$\hat{x}_i = TG(d_i) = TGF(m_i) . \tag{3.15}$$

Thus the desired property (3.14) can be written as

$$x_1 \leq_X x_2 \Rightarrow TGF(m_1) \leq_X TGF(m_2) . \tag{3.16}$$

By Definition 3.3,

$$m_1 \leq_M m_2 \Leftrightarrow T(m_1) \leq_X T(m_2) \Leftrightarrow x_1 \leq_X x_2 .$$

Hence (3.16) can be written as

$$m_1 \leq_M m_2 \Rightarrow GF(m_1) \leq_M GF(m_2). \quad (3.17)$$

Therefore, to satisfy the desired property P4, the combination *GF*, which is the model resolution, must be *monotonic*. □

If (3.17) is not satisfied, the empirical relation cannot be correctly estimated even without the noise effect. Different from the other four desired properties mentioned this important property (P4) has not been systematically studied yet. Some other derived properties of P4 are given in Section 3.4.

3.2.6 Selection of inverse solution (P5)

a. Occam's solutions of the IPMs

When two competing explanations make exactly the same predications, the simpler one is better (Thorburn 1915). This is the basic idea of a philosophy principle, called *Occam's razor*, and it can be used as the principle of choosing the inverse solution to solve the uniqueness issue.

The inverse solutions can be taken as the explanations of the observations (measured data), since they can be used to predict the observations. When there is a set of inverse solutions which are able to explain the observation equally well in the sense of fitting with the observation, the set is called an *equivalent class of solutions*. For an arbitrary model m_1, its equivalent class $[m_1]$ is the set $\{m \in M: F(m) = F(m_1)\}$, since all the models in $[m_1]$ fit with the data $d_1 = F(m_1)$. The inverse solution of the measured data d_1 derived by a backward mapping *G* is $G(d_1) = GF(m_1)$. If *G* satisfies equation (3.7), then $GF(m_1) \in [m_1]$, since $FGF(m_1) = F(m_1)$. By the principle of Occam's razor, the 'simplest' solution should be chosen from the equivalent class, so the inverse solution $GF(m_1)$ is desired to be 'simpler' than any $m \in [m_1]$ including m_1. The 'simplest' solution in the equivalent class is called as the *Occam's solution*. An Occam's solution can be obtained by minimising the 'complexity' of the solution.

There are some different criteria for determine the 'complexity' of an inverse solution. The preference of the solution, such as smoothness, sparsity, or smaller norm, varies according to the prior information of the actual model. Depends on the preferred type of the model, the

meaning of the 'simplest' solution can be different. Generally speaking, the Occam's solution of the inverse problem is a limit element (minimum or maximum), in terms of some property related to the preferred type of the model, in the equivalent class.

Example 3.5 The estimated model in Example 2.1 (a vector of slowness) is preferred to be a vector with smaller L^2-norm, since the L^2-norm of the model is a measure of the feature complexity. By using the 0^{th} order Tikhonov regularisation in the form of (3.10), the inverse solution, which has a minimum L^2-norm and adequately fits the observation, can be obtained.

Example 3.6 If the true model of mass density distribution in Example 2.2 is expected to be a smooth function, the inverse solution is preferred to be a smooth vector (i.e. the discretisation of a smooth function). The most smoothness inverse solution can be found by minimising the L^2-norm of the first or second derivative of model **m** (denoted $\|\mathbf{Lm}\|_2$). The 1^{st} or 2^{nd} order Tikhonov regularisation is commonly used for this propose (Tikhonov and Arsenin 1977).

Example 3.7 In compressive sensing, it is well-known that many natural signals are spare in the sense that they have concise representations when expressed in a proper basis (Candes and Wakin 2008). Let **m** be a unknown signal (model) which has a sparse basis **W** (e.g. the basis of a vector space), and $\mathbf{m}=\mathbf{Wx}$, where **W** is a matrix, and **x** is the vector of coefficients. The sparsity of **m** is useful for solving the underdetermined inverse problem in the form of $\mathbf{m}=\mathbf{Fd}$, when the dimension of **d** is much lower than the dimension of **m**. By minimising the L^1-norm of **x** (denoted $\|\mathbf{x}\|_1$) subject to $\|\mathbf{FWx}-\mathbf{d}\|_2 \le \varepsilon$, a sparse inverse solution can be obtained.

Formally, an element $m \in Q$ is the maximum of a subset Q of poset $\langle P, \preceq \rangle$ if $q \preceq m$ for any $q \in Q$. A minimum is defined dually. Maximum and minimum are also called as greatest element and least element for posets in some books. There are a unique maximum and minimum in a subset when they exist, which should be distinguished from the least upper bound (join) and the greatest lower bound (meet) (Davey and Priestley 2002). Join and meet of Q do not necessarily belong to Q. A maximum or minimum element of Q is named as a *limit element* of Q in this thesis.

For the IPMs, the models are used to estimate the measurand values, and the measurand values should reflect the empirical relation. Thus the solution (the estimated model) which is most useful for estimating the empirical relation of the measurand is preferred. The model space of an IPM is a poset $\langle M, \leq_M \rangle$ with a (partial) order $\leq_M$ related to the empirical relation (see definition 3.3). If a solution of *m* is a minimum or maximum of the equivalent class $[m]$, it provides a least upper bound or greatest lower boundary of all the solutions (including the actual model) in the equivalent class, and thus it is useful for estimating the range of the measurand value and evaluating the empirical relation. For example, if a solution of *m* (denoted as $\hat{m}$) is a minimum element in $\langle [m], \leq_M \rangle$, then for any $b \in M$, if $b \leq_M \hat{m}$, it can be derived that $b \leq_M m$. Therefore, the solution of an IPM is desired to be a limit element in the equivalent class, when it exists. If the minimum and maximum elements both exist, the Occam's solution should be chosen from the two elements according to the prior information of the actual model.

b. Existence of Occam's solutions

To find a maximum or minimum in a subset *Q* of an ordered set *P*, the existence of such an element should be considered first. The existence of a limit element in *Q* can be assured when *Q* is a finite subset of a totally ordered set *P*. In other situations, the existence should be carefully examined.

For the linear IPMs, usually the mathematical models are in the form of

$$\mathbf{Fm} = \mathbf{d}, \tag{3.18}$$

or in the form of IFK:

$$\int_b^a f(x,s)m(x)ds = d(x). \tag{3.19}$$

where *x* and *s* are variables of a same quantity. As mentioned in Example 2.2, IFK can be discretised into (3.18) using the quadrature method (also called simple collocation). Hence, equation (3.18) can be taken as a general mathematical model of the linear IPMs. If the forward mapping **F** is an *m*-by-*n* matrix, where $m < n$, and the measurand values are scalar, then the existence of limit elements can be examined using the basis vector(s) of the null space of **F**.

Example 3.8 Let x be a measurand value which is a scalar value,

$$x = T(\mathbf{m}) = \mathbf{c}^T\mathbf{m}. \tag{3.20}$$

where $\boldsymbol{c}^T\boldsymbol{m}$ is a linear combination of the parameter of $\boldsymbol{m}$. And let the dimension of the null space of $\mathbf{F}$, $dim\left(N\left(\mathbf{F}\right)\right) = 1$.The mathematical model of the inverse problem is $\mathbf{Fm} = \mathbf{d}$. For a measured data $\mathbf{d}$ (without noise), the collection of the vectors fit with $\mathbf{d}$ forms an equivalent class, denoted as [$\mathbf{m}$]. The vectors in [$\mathbf{m}$] can be expressed as

$$\mathbf{m}_\alpha = \mathbf{F}^\dagger\mathbf{d} + \alpha\mathbf{p}, \tag{3.21}$$

where $\mathbf{p}$ is a (n-by-1) unit vector in the null space of $\mathbf{F}$, $\mathbf{F}^\dagger$ is the Moore-Penrose inverse of $\mathbf{F}$, and $\alpha \in \mathbb{R}$. For model $\mathbf{m}_\alpha$. The measurand value corresponding to $\mathbf{m}_\alpha$ is

$$x_\alpha = \mathbf{c}^T\mathbf{m}_\alpha = \mathbf{c}^T\mathbf{F}^\dagger\mathbf{d} + \alpha\mathbf{c}^T\mathbf{p}. \tag{3.22}$$

Since $\mathbf{c}^T\mathbf{p}$ is normally a non-zero number, $\alpha\mathbf{c}^T\mathbf{p}$ can be any real number. By changing α, x_α can be any real number. Hence, there is no maximum or minimum in the equivalent class [$\mathbf{m}$]. In other words, the solution of the following objective function does not exist.

$$\begin{aligned} &\min \mathbf{c}^T\mathbf{m} \\ &\mathbf{Fm} = \mathbf{d} \end{aligned} \tag{3.23}$$

Hence, for this type of IPM, without other constraints, there are normally no limit elements in the equivalent classes.

However, for real situations, the model parameters are physical quantities. A lower bound and/or an upper bound of the physical quantities often exist naturally, or can be estimated reasonably. For example, if the model parameters are mass density, zero is the lower bound; if the parameters are concentration of contamination in water, according to the range of solubility limit of the contamination in water, a lower bound $\mathbf{l} = \mathbf{0}$ and an upper limit $\mathbf{u}$ are known. A lower bound or upper bound of model parameters assures the existence of a minimum or maximum of the equivalent class of solutions. The bounds can be used as constraints in the objective function (3.23). Assuming a lower bound $\mathbf{l}$ and an upper limit $\mathbf{u}$ are known, the problem of finding the minimum solution can be formulated as

$$\begin{aligned} &\min \mathbf{c}^T\mathbf{m} \\ &\mathbf{Fm} = \mathbf{d} \ , \\ &\mathbf{l} \preceq \mathbf{m} \preceq \mathbf{u} \end{aligned} \tag{3.24}$$

where $\preceq$ is a pointwise order. The problem of finding maximum solution can be formulated by simply changing the objective function in (3.24) to $\max \mathbf{c}^T\mathbf{m}$ or $\min(-\mathbf{c}^T\mathbf{m})$.

Let *p* the rank of **F**, by the theorem of null space and rank of matrices (Aster *et al* 2013, p 297), the dimension of the null space of **F** is

$$dim\left(N\left(\mathbf{F}\right)\right) = n - p \, . \tag{3.25}$$

Let $k = n - p$, then any solution in the equivalent class [**m**] can be written as

$$\mathbf{m} = \mathbf{m}_\dagger + z_1\mathbf{p}_1 + z_2\mathbf{p}_2 + ... + z_k\mathbf{p}_k \, , \tag{3.26}$$

where $\mathbf{m}_\dagger = \mathbf{F}^\dagger\mathbf{d}$, $\mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_k$ are the basis vectors of the null space *N*(**F**), and $z_1, z_2, ..., z_k \in \mathbb{R}$.

Let $\mathbf{z} = [z_1, z_2, ..., z_k]^T$ be the vector of variables, and $\mathbf{P} = [\mathbf{p}_1 \ \mathbf{p}_2 \ ... \ \mathbf{p}_k]$ be the matrix consists of $\mathbf{p}_i$ as the *i*th column, then (3.26) can be written in a more concise form as

$$\mathbf{m} = \mathbf{m}_\dagger + \mathbf{Pz} \, . \tag{3.27}$$

By substituting (3.27), (3.24) can be simplified as

$$\begin{aligned} &\min \ \ \mathbf{c}^T(\mathbf{m}_\dagger + \mathbf{Pz}) \\ &\mathbf{l} \preceq (\mathbf{m}_\dagger + \mathbf{Pz}) \preceq \mathbf{u} \end{aligned} \ . \tag{3.28}$$

For an IPM, **F** and **c** are known, and **d** is the measured data, thus $\mathbf{m}_\dagger$ and **P** can be calculated directly. Parameters in vector **z** are the only variables (called *design variables*) to be determined. Since $\mathbf{c}^T\mathbf{m}_\dagger$ is fixed, (3.28) can be written as

$$\begin{aligned} &\min \ \ f(\mathbf{z}) \\ &\mathbf{l} - \mathbf{m}_\dagger \preceq \mathbf{g}(\mathbf{z}) \preceq \mathbf{u} - \mathbf{m}_\dagger \end{aligned} \tag{3.29}$$

where $f(\mathbf{z}) = \mathbf{c}^T\mathbf{Pz}$, and $\mathbf{g}(\mathbf{z}) = \mathbf{Pz}$ is a vector-valued function. (3.29) is a typical optimisation problem which can be solved by the method of linear programming.

Linear programming is a technique for the optimisation of a linear objective function, subject to linear inequality constraints. The optimal solution exists when the inequality constraints

form a bounded and nonempty region, called feasible region, which is a convex polyhedron (Luenberger 1973).

If an optimal solution **z** for (3.29) exists, a minimum solution **m** of the IPM can be found via (3.27), and the minimum measurand value $x = \mathbf{c}^T\mathbf{m}$ can be obtained. The maximum solution can be obtained similarly by changing $f(\mathbf{z})$ into $f(\mathbf{z}) = -\mathbf{c}^T\mathbf{P}\mathbf{z}$.

Example 3.9 Let a (3-by-5) matrix **F** be the forward mapping of an IPM,

$$\mathbf{F} = \begin{bmatrix} 75 & 70 & 55 & 26 & 81 \\ 26 & 89 & 14 & 84 & 24 \\ 51 & 96 & 15 & 25 & 93 \end{bmatrix} \tag{3.30}$$

Suppose the measurand value is equal to the average of the elements in the model, and the upper and lower bounds of the model parameters are respectively equal to 5 and 1. Find the minimum model which fits with a noise-free data

$$\mathbf{d} = [631.52,\ 516.66,\ 579.72]^T . \tag{3.31}$$

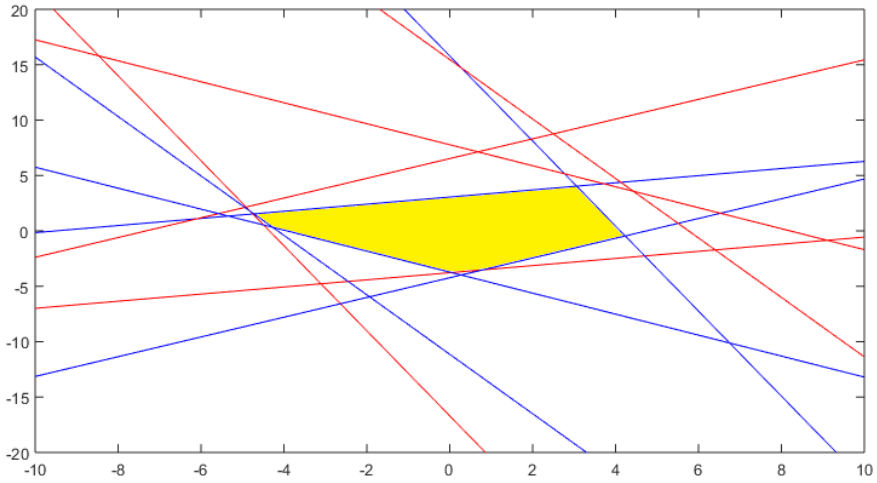


Figure 3.7 The feasible region (The yellow polygon) of the optimisation problem
The red lines and blue lines are corresponding to the upper bound and lower bounds respectively.

This is an optimisation problem can be formulate into a objective function in the forms of (3.28) and (3.29), of which $\mathbf{c} = [0.2, 0.2, 0.2, 0.2, 0.2]^T$, **l** is a vector with all elements equal to 1, and **u** is a vector with all elements equal to 5. An estimation of **m** can be obtained as $\mathbf{m}_\dagger = \mathbf{F}^\dagger\mathbf{d}$, and the matrix **P** in (3.29) can be obtained by a command '*null*' in Matlab. By substituting these vectors and matrix into (3.29), ten linear inequality

constraints (five pairs) can be obtained. Each element in $\mathbf{g}(\mathbf{z})$ provides two constraints corresponding to upper and lower bounds respectively, which are two parallel lines. The region between the parallel lines satisfied the two constraints. By sketching all the inequality constraints, a feasible area satisfies all the constraints can be obtained. As shown in Figure 3.7, the highlighted region is the feasible region of this example. By the theorem of linear programming, the optimal solution is one of the six vertexes of the highlighted polygon, which is the vertex corresponding to the smallest value of $f(\mathbf{z})$.

For the nonlinear IPMs, the problem of finding the minimum solution can be formulated in a general form as

$$\begin{array}{l} \min \ T(\mathbf{m}) \\ \mathbf{F}(\mathbf{m}) = \mathbf{d} \\ \mathbf{l} \preceq \mathbf{m} \preceq \mathbf{u} \end{array} , \tag{3.32}$$

where T is a scalar (linear or nonlinear) function, and $\mathbf{F}$ is a nonlinear vector function (i.e. a system of nonlinear functions). Since there is no universal way of defining the preimage of $\mathbf{d}$, solving (3.32) is far more complicated than solving (3.24). This problem is a nonlinear optimisation problem with equality and inequality constraints which belongs to the field of nonlinear programming. The necessary conditions of the existence of an optimal solution of (3.32) are given by Kuhn and Tucker (1951), known as the Karush–Kuhn–Tucker (KKT) conditions. There is no universal method for solving this type of problem. Different methods should be used depends on the properties (convex, concave or nonconvex) of the objective function and the constraints. A type of algorithm in the field of artificial intelligence, named as the genetic algorithm is commonly used for searching the optimal solution of this type of problem (Guan and Aral 1999) (Michalewicz and Nazhiyath 1995). Due to the complexity of the problem, we shall not discuss it in detail in this thesis.

Example 3.1 is also a typical nonlinear IPM, of which the maximum solution can be directly obtained by the backward mapping (erosion) due to the special properties of the closing operator which is a combination of a dilation followed by an erosion. As shown in Figure 3.8, the output of a closing operator is always above the input. Thus the inverse solution obtained in Example 3.1 naturally satisfies the principle of Occam's razor.

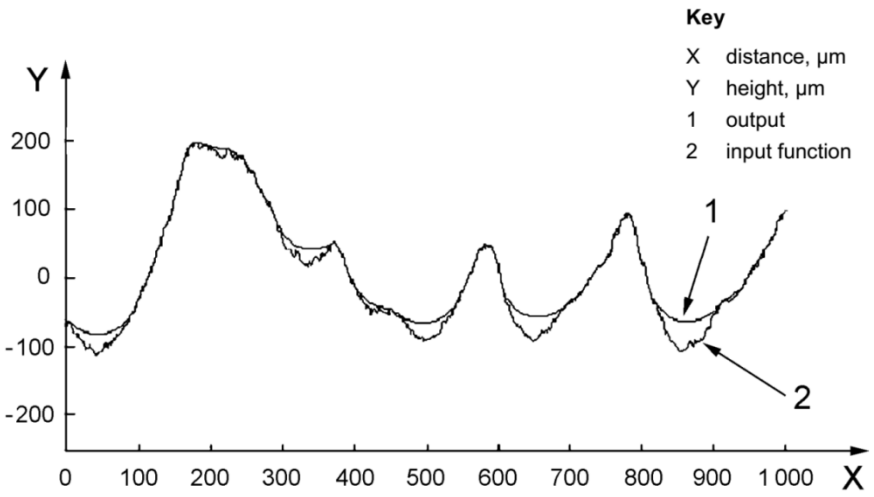


Figure 3.8 Input and output of a closing filter (ISO 16610-41 2006)
The structuring element is a circular disk of 50 µm radius.

c. An algorithm for finding the Occam's solution

When the model is a high dimensional-vector, the number of constraints can be very large, and an efficient algorithm is needed for finding the vertex of the feasible region corresponding to the optimal solution. There are two popular algorithms of finding the optimal solutions in linear programming, one is Dantzig's simplex algorithm, and the other is Karmarkar's interior point algorithm (Illés and Terlaky 2002). These two types of algorithms can be implemented by a '*linprog*' command in the optimisation toolbox of Matlab. Using this command, a universal algorithm is designed for finding the minimum and maximum solutions of the IPMs when the model parameters are bounded, which is named as the algorithm of *bounded parameters Occam's solution* (*bpos*). Here the Occam's solution refers to the solution of (3.24), which is derived with the optimal solution of (3.29). The Matlab code of the *bpos* algorithm is given in Appendix A.

The *bpos* algorithm is implemented in the following steps:

1. Input the forward mapping **F**, the coefficient vector **c** of the extraction function, and the upper and lower bounds *u* and *l* of the model parameters.
2. Calculate the generalised inverse solution $\mathbf{m}_{\dagger} = \mathbf{F}^{\dagger}\mathbf{d}$ using the measured data.
3. Find the basis vectors of the null space of **F** with the *null* command, and combine these vectors into a matrix **P**.

4. Set vectors $\mathbf{f} = \mathbf{c}^T\mathbf{P}$, $\mathbf{b} = \begin{bmatrix} \mathbf{u} - \mathbf{m}_\dagger \\ \mathbf{m}_\dagger - \mathbf{l} \end{bmatrix}$ and matrix $\mathbf{A} = [\mathbf{P}, \mathbf{P}]^T$ so that problem (3.29) can be solved by the *linprog* function of Matlab.
5. Solve the linear programming problem (3.29), and get the optimal solution $\mathbf{z}_0$.
6. Get the minimum solution using $\mathbf{m}_{\min} = \mathbf{m}_\dagger + \mathbf{P}\mathbf{z}_0$.
7. Set vector $\mathbf{f} = -\mathbf{c}^T\mathbf{P}$ to find the optimal solution $\mathbf{z}_1$, and get the maximum solution $\mathbf{m}_{\max} = \mathbf{m}_\dagger + \mathbf{P}\mathbf{z}_1$.
8. Evaluate the measurand values of the minimum solution and the maximum solution respectively using $x = \mathbf{c}^T\mathbf{m}$.

The following example demonstrates that the *bpos* algorithm can be used to solve the objective function in the form of (3.24).

Example 3.10 Let the forward mapping of an IPM be a 40-by-50 matrix **F**. Suppose that the true model $\mathbf{m}_{\text{true}}$ is a vector with 50 elements depicted in Figure 3.9, and the measurand value is equal to the average of the model parameters. According to the prior information of the model, the upper and lower bounds of the model parameters are respectively equal to 10 and 2. Test the *bpos* algorithm using the noise-free data $\mathbf{d} = \mathbf{F}\mathbf{m}_{\text{true}}$.

An arbitrary 40-by-50 matrix **F** is used for the testing. The generalised inverse solution $\mathbf{m}_\dagger = \mathbf{F}^\dagger\mathbf{d}$ is calculated using the *pinv* command, which is shown in Figure 3.9 together with the true model. It can be observed that, although no noise is involved in the data, $\mathbf{m}_\dagger$ does not fit with the true model very well, and $\mathbf{m}_\dagger$ is out of the lower bound. The measurand value of the true model is $x_{\text{true}} = \mathbf{c}^T\mathbf{m}_{\text{true}}$, where every element of **c** equals to 1/50. Giving matrix **F**, vectors **c**, **l**, and **u** as the inputs, the algorithm *vpos* calculates the results $\mathbf{m}_{\min}$ and $\mathbf{m}_{\max}$ as depicted in Figure 3.10 and 3.11 respectively. The minimum solution fits with the true model quiet well. More importantly, this algorithm provides a range of measurand values corresponding to the minimum and maximum solutions using $x = \mathbf{c}^T\mathbf{m}$. The measurand values of the true model, the minimum solution, and the maximum solution are respectively $x_{\text{true}} = 3.8672$, $x_{\min} = 3.8668$, and $x_{\max} = 3.8772$

. The interval [3.8668, 3.8772] is a range of the measurand values of the models within the bounds.

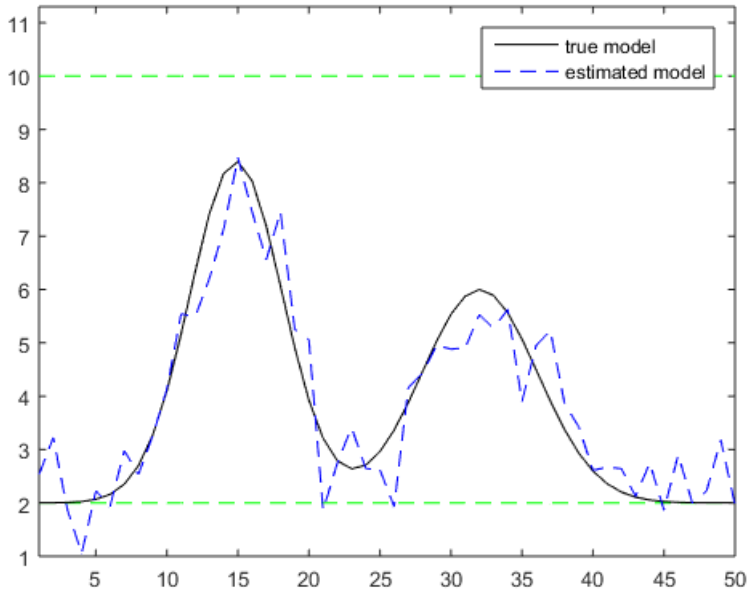


Figure 3.9 The true model and the generalised inverse solution of the IPM

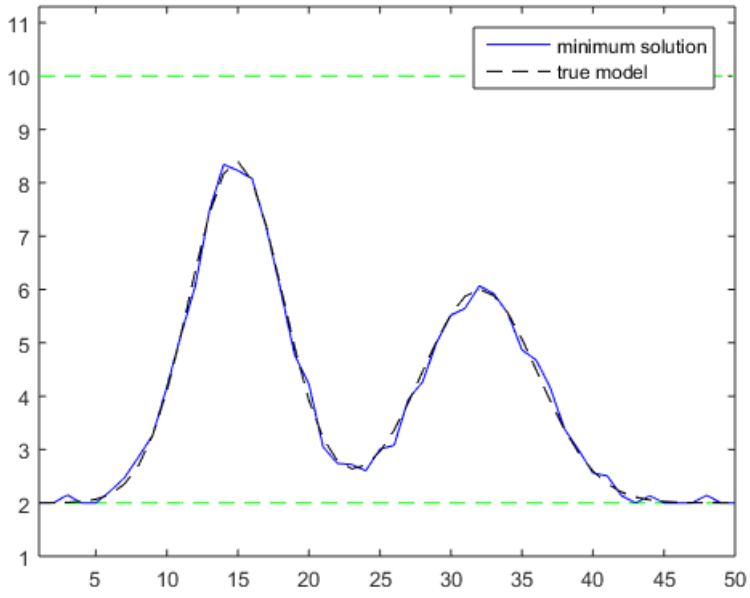


Figure 3.10 The minimum solution of the IPM

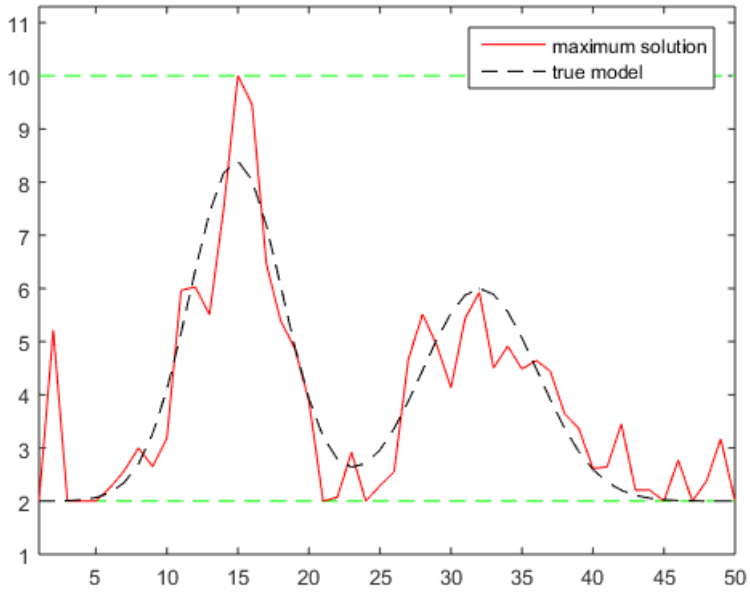


Figure 3.11 The maximum solution of the IPM

3.3 Generalised inverse of *F*

3.3.1 Generalised inverse of a mapping

As mentioned in Section 3.2.2, the backward mapping *G* is desired to be a generalised inverse of *F*. As reviewed in Section 2.7.1, the generalised inverses of linear operators have been extensively studied since 1955. However, the forward mapping of an inverse problem can be an arbitrary (linear or non-linear) mapping, so the properties of the generalised inverse of an arbitrary mapping are also important.

The concept of Moore-Penrose inverse has been extended to the mappings (morphisms) in categories by Davis & Robinson (1972) and others. Base on the proof of the existence of Moore-Penrose inverse, the existence of the generalised inverses of an arbitrary mapping *F* is proved by Puystjens & Robinson (1981) with a condition that *F* has a (epic, monic) factorisation.

The first two defining equations of Moore-Penrose inverse can be used to generalise some of the properties of Moore-Penrose inverse from linear operators to arbitrary mappings.

Definition 3.5: Let $F: M \to D$ be an arbitrary mapping. A mapping $F^{\dagger}: D \to M$ satisfies equation (3.33) is called an *inner inverse* of *F*; and if $F^{\dagger}$ satisfies with the both (3.33) and (3.34), it is called a *quasi-inverse* of *F*.

$$FF^{\dagger}F = F \tag{3.33}$$

$$F^{\dagger}FF^{\dagger} = F^{\dagger} \tag{3.34}$$

Proposition 3.3: If a forward mapping *F* has an inner inverse $F^{\dagger}$, the model resolution $F^{\dagger}F$ and data resolution $FF^{\dagger}$ are both idempotent.

Proof: By (3.33), we have $(FF^{\dagger})(FF^{\dagger}) = (FF^{\dagger}F)F^{\dagger} = FF^{\dagger}$.

Hence $FF^{\dagger}$ is idempotent.

And $FF^{\dagger}F = F$ implies $F^{\dagger}FF^{\dagger}F = F^{\dagger}F$, thus $F^{\dagger}F$ is also idempotent. □

Monic, epic or isomorphic are the general mapping properties of any mappings (see Section 2.6.3), so the properties derived from these mapping properties are universal for any mappings. The following propositions are proved using category theory.

Proposition 3.4: If a forward mapping $F : M \to D$ is monic, and it has an inner inverse $F^{\dagger}$, then the model resolution $F^{\dagger}F$ is an identical mapping I_M.

Proof:

By definition, *F* is monic means for any pair of mappings $g : A \to M$ and $h : A \to M$, $Fg = Fh$ implies $g = h$.

By (3.33), we have $FF^{\dagger}F = F \Rightarrow F(F^{\dagger}F) = F\, I_M$.

Replace *g* and *h* by $F^{\dagger}F$ and I_M respectively, we get $F^{\dagger}F = I_M$. □

Proposition 3.5: If a forward mapping *F* has a quasi-inverse $F^{\dagger} : D \to M$, and $F^{\dagger}$ is monic, then the data resolution $FF^{\dagger}$ is an identical mapping I_D.

Proof: Similar to the proof of Proposition 3.4, by (3.34)

$$F^{\dagger}(FF^{\dagger}) = F^{\dagger} I_D \ . \tag{3.35}$$

And since $F^{\dagger}$ is monic, we get $FF^{\dagger} = I_D$. □

Proposition 3.6: If the forward mapping $F : M \to D$ is epic, and it has an inner inverse $F^{\dagger}$, then the data resolution $FF^{\dagger}$ is an identical mapping I_D.

Proof: By (3.33), $FF^{\dagger}F = F$, which implies $(FF^{\dagger})F = I_D F$.

Since *F* is epic, by definition (Section 2.6.3), for any pair of mappings $g: D \to C$ and $h: D \to C$, $gF = hF$ implies $g = h$.

Replace *g* and *h* by $FF^{\dagger}$ and I_D, we get $FF^{\dagger} = I_D$. □

3.3.2 Range isomorphism theorem

Theorem 3.1: For an arbitrary mapping $F: M \to D$, if it has a quasi-inverse $F^{\dagger}: D \to M$, then the ranges (images) of *F* and $F^{\dagger}$ are isomorphic, i.e.

$$F[M] \cong F^{\dagger}[D]. \tag{3.36}$$

Proof: Since $F^{\dagger}$ is a quasi-inverse of *F*, by (3.33), for any $m \in M$,

$$FF^{\dagger}F(m) = F(m). \tag{3.37}$$

Here *F*(*m*) is an arbitrary element in the range of *F*, $F[M]$. Therefore,

$$FF^{\dagger}(p) = p, \quad \text{for any } p \in F[M]. \tag{3.38}$$

Similarly, for any $d \in D$, by (3.34),

$$F^{\dagger}FF^{\dagger}(d) = F^{\dagger}(d). \tag{3.39}$$

Here $F^{\dagger}(d)$ is an arbitrary element of $F^{\dagger}[D]$. Therefore,

$$F^{\dagger}F(q) = q, \quad \text{for any } q \in F^{\dagger}[D]. \tag{3.40}$$

Two objects *A*, *B* are said to be isomorphic if there exists maps $f: A \to B$ and $g: B \to A$, such that $g\ f = 1_A$ and $f\ g = 1_B$.

Hence, according to equations (3.38) and (3.40), we have proved that $F[M]$ is isomorphic to $F^{\dagger}[D]$. □

The isomorphism between the ranges of *F* and $F^{\dagger}$ can be described by Figure 3.12. The symbol ~ stands for isomorphism.

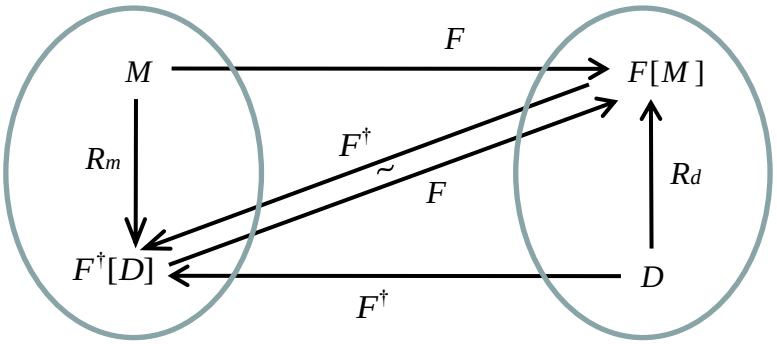


Figure 3.12 Isomorphism between the ranges of *F* and $F^{\dagger}$

Corollary 3.1: If $F^{\dagger}$ is the quasi-inverse of *F*, then the range of *F* is isomorphic to the range of $FF^{\dagger}$, and the range of $F^{\dagger}$ is isomorphic to the range of $F^{\dagger}F$. That is

$$F[M] \cong FF^{\dagger}[D], \tag{3.41}$$

$$F^{\dagger}[D] \cong F^{\dagger}F[M]. \tag{3.42}$$

Proof: Since $F^{\dagger}$ is the quasi-inverse of *F*, by (3.33) we have

$$FF^{\dagger}(F[M]) = F[M], \tag{3.43}$$

$$F^{\dagger}F(F^{\dagger}F[M]) = F^{\dagger}F[M]\ . \tag{3.44}$$

Therefore, by definition of isomorphic,

$$F^{\dagger}F[M] \cong F[M]. \tag{3.45}$$

Similarly, by (3.34), we can get

$$FF^{\dagger}[D] \cong F^{\dagger}[D]. \tag{3.46}$$

By Theorem 3.1,

$$F^{\dagger}[D] \cong F[M]. \tag{3.47}$$

Since isomorphism is transitive, from (3.45), (3.46) and (3.47), we can get

$$F^{\dagger}F[M] \cong F^{\dagger}[D] \quad \text{and} \quad FF^{\dagger}[D] \cong F[M]. \qquad \square$$

Corollary 3.2: If both *G* and *H* are quasi-inverse of $F: M \to D$, then the ranges of *G* and *H* are isomorphic, i.e.

$$G[D] \cong H[D]\ . \tag{3.48}$$

Proof: Let $P = GF$, $Q = HF$.

By the definition of quasi-inverse, it can be observed that

$$GFHFGF = GFHF = GF \text{, i.e. } PQP = P; \tag{3.49}$$

$$HFGFHF = HFGF = HF \text{, i.e. } QPQ = Q. \tag{3.50}$$

According to Theorem 3.1, from (3.49) and (3.50) we can get

$$GF[M] \cong HF[M]. \tag{3.51}$$

By Corollary 3.1, we have $GF[M] \cong G[D]$ and $HF[M] \cong H[D]$.

Therefore, (3.51) becomes $G[D] \cong H[D]$. □

Corollary 3.2 implies that the quasi-inverse of a mapping is unique up to isomorphism.

3.4 Monotonicity of *F* and *G*

Proposition 3.2 states that the monotonicity of *GF* is a necessary condition of P4. To study the monotonicity of *GF*, it's necessary to investigate the monotonicity of *F* and *G* respectively. The monotonicity of a mapping *h* between two posets $\langle A, \leq_A \rangle$ and $\langle B, \leq_B \rangle$ depends on the how the relations $\leq_A$ and $\leq_B$ are defined.

3.4.1 General monotonicity of *G* and *F*

By using the partial orders of the model and data spaces defined in Section 3.2.4, the monotonicity of *G* and the desired monotonicity of *F* can be easily proved. This monotonicity of *F* and *G* is always satisfied as long as $\leq_M$ and $\leq_D$ are defined with Definition 3.3 and 3.4 respectively.

Proposition 3.7 The backward mapping *G* between the posets of data space and model space is *monotonic*.

Proof: Let $m_a = G(d_a)$ and $m_b = G(d_b)$. By Definition 3.4, we get

$$d_a \leq_D d_b \Leftrightarrow TG(d_a) \leq_X TG(d_b) \Leftrightarrow T(m_a) \leq_X T(m_b).$$

And, by Definition 3.3, we get

$T(m_a) \leq_X T(m_b) \Leftrightarrow m_a \leq_M m_b \Leftrightarrow G(d_a) \leq_M G(d_b)$. Hence,

$$d_a \leq_D d_b \Leftrightarrow G(d_a) \leq_M G(d_b). \quad \square \tag{3.52}$$

Proposition 3.8 When the desired property P4 is satisfied, *F* is monotonic between the posets of data space and model space, i.e. *F* is *desired to be monotonic*.

Proof: As shown in Section 3.2.5, P4 implies

$$m_1 \leq_M m_2 \Rightarrow GF(m_1) \leq_M GF(m_2). \tag{3.53}$$

And by (3.52), $GF(m_1) \leq_M GF(m_2) \Leftrightarrow F(m_1) \leq_D F(m_2)$.

Therefore, P4 implies

$$m_1 \leq_M m_2 \Rightarrow F(m_1) \leq_D F(m_2). \quad \square \tag{3.54}$$

This desired monotonicity of *F* is equivalent to the monotonicity of *GF*.

3.4.2 Special monotonicity of *G*

In Proposition 3.7, the backward mapping *G* is proved to be monotonic when the orders in the model and data spaces are defined by Definition 3.3 and 3.4. However, as mentioned in Section 3.2.4, in some cases, it's not necessary to define $\leq_D$ with Definition 3.4. When Definition 3.4 is not applied, the general monotonicity of *G* and *F* is also not applicable.

In many cases, *F* is monotonic. For instance, any non-negative matrix is monotonic between the vector spaces with pointwise orders, and the forward mappings of many linear inverse problems (e.g. Example 2.1 and 2.2) can be modelled as non-negative matrices. Moreover, the deterministic assumption implies that *F* is surjective (see Section 3.2.1). The following proposition shows that, under some condition, the monotonicity of *G* can be proved with the monotonicity of *F*.

Proposition 3.9: Let $h: \langle A, \leq_A \rangle \to \langle B, \leq_B \rangle$ be a monotonic and surjective mapping, where $\langle A, \leq_A \rangle$ is a totally ordered set, and $\langle B, \leq_B \rangle$ is a poset, then the quasi-inverse $h^\dagger$ is strictly monotonic.

Proof: By the definition of quasi-inverse, $hh^\dagger h = h$ and $h^\dagger h h^\dagger = h^\dagger$.

By Theorem 3.1, the ranges of *h* and $h^\dagger$ are isomorphic,

i.e. $h[A] \cong h^\dagger[B]$, where $h^\dagger[B] \subseteq A$, and $h[A] = B$, since *h* is surjective.

Let $A^* = h^\dagger[B]$, and let $h^*: A^* \to B$ be the restriction of *h* to A^*.

Then between A^* and *B*, $h^\dagger$ is the inverse of h^*.

Same as h, h^* is monotonic, thus for any $a_1, a_2 \in A^*$,

$$a_1 <_A a_2 \Rightarrow h^*(a_1) \leq_B h^*(a_2). \tag{3.55}$$

By the isomorphic property, h^* is injective, thus

$$a_1 \neq a_2 \Rightarrow h^*(a_1) \neq h^*(a_2). \tag{3.56}$$

By (3.55) and (3.56), we have

$$a_1 <_A a_2 \Rightarrow h^*(a_1) <_B h^*(a_2). \tag{3.57}$$

For any $b_i \in B$, let $a_i = h^\dagger(b_i)$, then $b_i = (h^\dagger)^{-1}(a_i) = h^*(a_i)$.

Assume $b_1 < b_2$, then $h^*(a_1) < h^*(a_2)$.

By (3.57) h^* is strictly monotonic, thus

if $a_2 \leq_A a_1$, then $h^*(a_2) \leq_B h^*(a_1)$, which contradicts with the assumption;

if $a_1 <_A a_2$, then $h^*(a_1) <_B h^*(a_2)$, which matches with the assumption.

Since $\langle A, \leq_A \rangle$ is totally ordered, $a_2 \leq_A a_1$ and $a_1 <_A a_2$ are the only two options.

So $b_1 <_B b_2$ implies $a_1 <_A a_2$, i.e. $h^\dagger(b_1) <_A h^\dagger(b_2)$.

Thus $h^\dagger$ is strictly monotonic. □

This proposition is useful for the IPMs of which the empirical relation is a total order (e.g. weak order).

3.5 Adjoint functors between the model and data spaces

3.5.1 Adjoint functors between posets

As mentioned in Section 2.6.1, a preordered set, $\langle X, \precsim \rangle$ itself is a category **X** whose objects are the elements of X, and mappings are the ordering relations. A monotonic mapping F: $\mathcal{M} \rightarrow \mathcal{D}$ between two preordered sets can be taken as a *functor* between two categories (Steve 2006, p.191). Let G: $\mathcal{D} \rightarrow \mathcal{M}$ be another functor, if for all $m \in M$, $d \in D$, (3.58) is satisfied, the pair (F, G) is called a *Galois connection* (Davey and Priestley 2002), and G is *right adjoint* to F, and F is *left adjoint* to G. Galois connection is a particular case of adjoint pair of functors (see Section 2.6.6).

$$F(m) \preceq d \Leftrightarrow m \preceq G(d) \tag{3.58}$$

For a functor *F* between two categories of preordered sets, if *G* is right adjoint to *F*, by the properties of Galois connection, we have

G1. both *F* and *G* are monotonic,

G2. $FGF = F$ and $GFG = G$,

G3. $FG(d) \preceq d$ and $m \preceq GF(m)$, for all $m \in M$, $d \in D$.

It can be proved that when G1, G2 and G3 are satisfied, (3.58) is also satisfied, a proof can be found in (Davey and Priestley 2002, p.159).

By G2, *G* and *F* are the quasi-inverse of each other. The adjoint functor of the forward mapping *F* can be used as a quasi-inverse of *F* for deriving the solution. In contrast, a quasi-inverse of *F* is not necessarily an adjoint functor of *F*, since it does not always satisfy (3.58).

For example, let $\lceil\ \rceil : \mathbb{R} \to \mathbb{R}$ denotes the ceiling function, which maps real numbers to integers such that $\lceil x \rceil = \min\{n \in \mathbb{Z} \mid n \geq x\}$, and let $I : \mathbb{Z} \to \mathbb{R}$ be an identity function that embeds the integers into the real numbers, e.g. $\lceil 3.2 \rceil = 4$, $I(4) = 4$. It can be easily verified that for any $a \in \mathbb{R}$, $b \in \mathbb{Z}$, $\lceil a \rceil \leq b \Leftrightarrow a \leq I(b)$ is true. Hence the condition (3.58) is satisfied; the ceiling function is left adjoint to the identity function.

3.5.2 From the desired properties to the Galois connection

For an IPM, if the topological stability (P3) is satisfied, the ERS must be preordered, and thus the model and data spaces, $\mathcal{M}$ and $\mathcal{D}$, are posets, which are also preordered. Under the deterministic assumption, if the estimated measurand values reflect the empirical relation (P4), *F* and *G* are proved to be monotonic (Section 3.4.1). Hence, when P3 and P4 are satisfied, G1 is satisfied.

By P2, *G* is desired to be an inner inverse of *F*, i.e. $FGF = F$ (see Section 3.2.2). And by Proposition 3.6, if *F* is epic and *G* is an inner inverse of *F*, we have

$$FG = I_D. \tag{3.59}$$

By multiplying each side of (3.59) with *G*, we get

$$GFG = G. \tag{3.60}$$

In Section 3.2.1, it has been demonstrated that under the deterministic assumption, F is surjective, and thus epic. Therefore, if P2 is satisfied, G is the quasi-inverse of F, and G2 is satisfied.

By (3.59), for any $d \in D$, $FG(d) = d$, so the 1st inequality in G3 are satisfied.

It is demonstrated in Section 3.2.6 that P5 implies that the solution of an IPM should be a limit element of its equivalent class when it exists. If a maximum element is chosen as the inverse solution, then the 2nd inequality of G3 can be satisfied, thus G3 is satisfied.

If a minimum element is chosen as the inverse solution, we have

G3*. $GF(m) \leq_M m$ and $d = FG(d)$, for all $m \in M$, $d \in D$.

It can be easily proved that G1, G2 and G3* implies that G is left adjoint to F (Davey and Priestley 2002, p 159), i.e. $G(m) \preceq d \Leftrightarrow m \preceq F(d)$. The following proposition concludes this section.

Proposition 3.10: For the IPMs, if the desired properties P1 to P5 are all satisfied, under the deterministic assumption, F and G setup a Galois connection between the model and data spaces.

Therefore, the IPM is a general type of inverse problem in metrology which is expected to process the structure of Galois connection. The logical relation between the desired properties and Galois connection is summarised in the diagram of Figure 3.13.

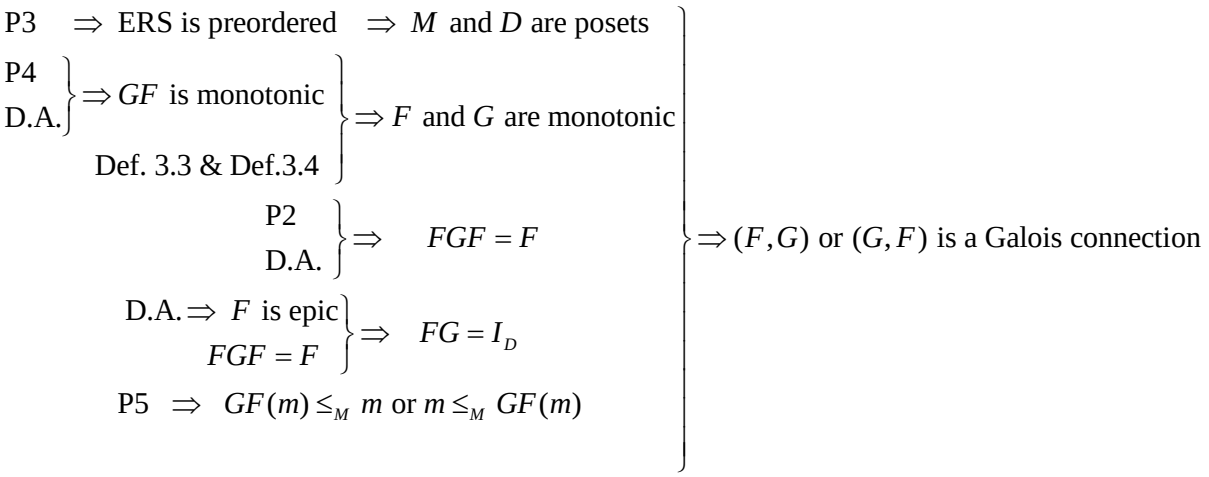


Figure 3.13 The logical relation between the desired properties and Galois connection

D.A. stands for the deterministic assumption

3.6 Conclusions

This chapter is the main part of the theoretical basis of this thesis. A deterministic model of indirect measurements is proposed based on the representational theory of measurement. In this model, the inverse problem of measurement (IPM) is defined, which shows the connection between indirect measurements and inverse problems. Five desired properties of solving the IPMs with a backward mapping G are proposed and elaborated, which correspond to the forward mapping (P1), the fitting criterion (P2), the stability (P3), estimation of empirical relation (P4) and selection of inverse solution (P5). Topological stability, as one of the desired properties, is defined to generalise the concept of the stability of inverse problems for the situation of measurement, which implies that the model and data spaces are desired to be preordered. According to the topological stability, the model and data spaces of IPM are modelled as partially ordered sets. Moreover, the monotonicity of the model resolution (GF) is deduced from the desired property P4. The principle of Occam's razor is applied for choosing inverse solutions. The existence of the maximum and minimum solutions of the IPMs is discussed, and an algorithm is designed for finding the solutions. The generalised inverse of the forward mapping F is investigated using category theory, and some structural properties of inverse problems are derived. Under the deterministic assumption, it is proved that the IPMs possess the structural properties of Galois connections when the five desired properties are satisfied. This characterises the structure of the IPMs.

Chapter 4
Probabilistic Model of Indirect Measurements and the Inverse Problems of Measurement

4.1 Introduction

4.1.1 Uncertainty of the measurement process

As pointed out by Gauss (1821) in his famous work on the theory of least squares: 'however much care is taken with observations of the magnitude of physical quantities, they are necessarily subject to more or less considerable errors.' Some errors vary randomly with each observation, and are independent of the measurement result; some errors are identical for all observations of the same nature, or depend on the measurement results. The former type of error is called random error, and the latter is called systematic error (JCGM 200 2008). These two types of errors normally arise simultaneously in a measurement. The variation of the error can be characterised by a parameter named the measurement uncertainty.

In the deterministic model of indirect measurement, for investigating the structural properties of the IPM, the measurement process is modelled to be a deterministic mapping. However, in practice, due to measurement error, the measured value of an object is not always fixed, thus the deterministic assumption is not satisfied. To be able to involve the effect of measurement error, the deterministic model should be generalised to a probabilistic model.

In the processes of indirect measurements, measurement uncertainty first appears in the measured data, which then affects the reliability of the estimated measurand value, and results an uncertainty in the measurand value. To be able to compare measurement results among themselves or with reference values, it is necessary to assess the reliability of the measurement results using uncertainty (JCGM 100 2008). Solving the associated IPM is not only about estimating the measurand value; the evaluation of the uncertainty of the measurand value is also important. To do that, it is necessary to understand the propagation of uncertainty via the backward mapping.

For inverse problems, the noise in the measured data is an important issue, which includes the measurement error and the rounding error. It cannot be ignored in the process of solving the

inverse problem, since it is directly related to the existence issue and the stability issue of inverse problems. Due to the noise, the data can be out of the range of the forward mapping F, thus it is possible that no solution exactly fits the data. Furthermore, due to the noise, if the backward mapping is sensitive to small changes, the noise effect can dominate the inverse solutions. To include the noise under consideration, the mathematical model of the inverse problem is often written as

$$d = F(m) + \eta\,, \tag{4.1}$$

where η is a random variable representing the noise in the data and F is assumed to be the exact functional relation between the model and the noise-free data.

The noise also affects the desired properties of solving the IPM. It is known that there is certain amount of noise in the measured data and the magnitude of the noise can be estimated in terms of an interval; thus, it becomes not necessary to find a solution that fits the data exactly. Instead, a small misfit should be acceptable. Hence the fitting criterion (P2) can be weakened from $FGF = F$ to $\|F(m) - d\|_2 \leq \varepsilon$, where $\boldsymbol{\varepsilon}$ is a small number. This allows a trade-off between fitting the data and minimising the complexity of the inverse solution, and thereby, improves the stability of the solution.

Under the deterministic assumption, the desired property of selecting the solution of the IPM (P5) is formulated in terms of the objective function (3.24). By weakening the fitting criterion, the objective function (3.24) can be written as

$$\begin{gathered} \min \mathbf{c}^T\mathbf{m} \\ \|\mathbf{Fm} - \mathbf{d}\|_2 \leq \varepsilon\,, \\ \mathbf{l} \preceq \mathbf{m} \preceq \mathbf{u} \end{gathered} \tag{4.2}$$

where $\boldsymbol{c}^T\boldsymbol{m}$ is a linear combination of the parameter of the model $\boldsymbol{m}$. The algorithm for solving this objective function is given by Aster *et al.* (2013, p 170) based on the bounded value least square algorithm given by Stark and Parker (1995). By using this algorithm, an inverse solution with the minimum (or maximum) value of the measurand can be obtained.

Lastly, in the probabilistic model, the estimation of empirical relations is a big concern. The empirical relations, estimated with the measurand values, become uncertain when the uncertainties of the estimated measurand values are significant. Therefore, the empirical relations should be estimated and described in a probabilistic approach.

4.1.2 Measurands with intrinsic uncertainties

The uncertainty of measurement results can be generated not only from the measurement process but also from the measurand itself. In the deterministic model of measurement, the measurand values are considered as fixed numbers or vectors. This is because, in classical physics, it is commonly believed that a physical quantity of an object can always be measured as a value. However, in quantum mechanics, it is impossible to measure a property of some microscopic particle without creating a significant disturbance to the state of the particle. This inevitable disturbance is called the observer effect, which makes the measurement of the exact values of some quantity at the quantum level impossible. For example, the exact positions of electrons at any moment are unobservable. Many physicists, followed by Heisenberg (1925), believe that a quantity is physically meaningful only if it can be observed via experiments. Thus, it is meaningless to use an exact value to describe the position of an electron; instead, an uncertainty should be given for the position.

In Heisenberg's celebrated paper (1927), he demonstrated a universal principle called the uncertainty principle, which states that some pairs of quantities at quantum level, such as position and momentum or position and velocity, cannot be measured accurately at the same time. The more precisely one is known, the less precisely the other can be known. This principle can be expressed by an inequality of the standard deviations. In the case of position and momentum, the inequality is

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}, \tag{4.3}$$

where $\hbar$ is the reduced Planck constant, and σ_x and σ_p are the standard deviations of position and momentum, respectively. Thus, if the product of the position and momentum of a small particle is taken as a measurand *q*, there is an intrinsic minimum uncertainty of *q* that cannot be eliminated by any measurement method.

This kind of intrinsic uncertainty exists not only in the cases of microscopic particles, but also in general situations. As pointed out in the GUM (guide to the expression of uncertainty in measurement) standard (JCGM 100 2008, p.49), a measurand cannot be completely specified without an infinity amount of information. A limited description of a measurand, such as the velocity of sound in air, is incomplete since it leaves room for interpretation. This inevitable incompleteness introduces a component of uncertainty into the uncertainty of the

measurement result, which is called *definitional uncertainty* in JCGM 200 (2008). Thus, at some level, every measurand has such an intrinsic uncertainty.

If the intrinsic uncertainty is significant, there is no such thing as the 'true' value of the measurand. Instead, the measurand should be represented by a probability distribution. A measurand with an intrinsic uncertainty is called as a *stochastic measurand*. For a stochastic measurand, the measurand value of an object should be described by a random variable with a specified distribution. This completely affects the way of estimating empirical relations.

In this chapter, a methodology of estimating empirical relations according to the measured data is developed, which includes a method of evaluating the uncertainty of measurement results and a method of estimating empirical relations with probabilities assigned.

4.2 Propagation of uncertainty in indirect measurement

4.2.1 A law of propagation of uncertainty

A law of propagation of uncertainty from measured data to measurement results is introduced in GUM (JCGM 100 2008), which provides a method to treat the uncertainty components identically so that they can be combined to estimate the uncertainty of the measurand. In this method, it is assumed that the measurand x can be written in the form of $x = g(d_1, d_2, \ldots, d_n)$, and function g is known, where d_i are the random variables representing the values of the proxy quantities. By means of a first-order Taylor series, an approximation of a small deviation of x about its expectation, μ_x, can be obtained in terms of small deviations of d_i about their expectations, μ_i (JCGM 100 2008):

$$x - \mu_x = \sum_{i=1}^{n} \frac{\partial g}{\partial d_i}(d_i - \mu_i). \tag{4.4}$$

Thus, the square of $x - \mu_x$ can be written as

$$(x - \mu_x)^2 = \sum_{i=1}^{n} (\frac{\partial g}{\partial d_i})^2 (d_i - \mu_i)^2 + 2\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\partial g}{\partial d_i} \frac{\partial g}{\partial d_j} (d_i - \mu_i)(d_j - \mu_j). \tag{4.5}$$

The variance of x is equal to the expectation, $E[(x - \mu_x)^2]$, and the covariance of d_i, d_j is equal to the expectation, $E[(d_i - \mu_i)(d_j - \mu_j)]$. Thus equation (4.5) implies that

$$u(x)^2 = \sum_{i=1}^{n}\left(\frac{\partial g}{\partial d_i}\right)^2 u(d_i)^2 + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\frac{\partial g}{\partial d_i}\frac{\partial g}{\partial d_j}\mathrm{cov}(d_i, d_j), \tag{4.6}$$

where $u(x)$ is the estimated standard deviation of x and $\mathrm{cov}(d_i, d_j)$ is the covariance of d_i, d_j. If the observable quantities are independent of each other, equation (4.6) can be simplified as

$$u(x)^2 = \sum_{i=1}^{n}\left(\frac{\partial g}{\partial d_i}\right)^2 u(d_i)^2 . \tag{4.7}$$

The method of estimating the uncertainty of the measurand with equations (4.6) and (4.7) can be found in detail in GUM (JCGM 100 2008).

4.2.2 Transformation of covariance matrices

Equation (4.6) is applicable only when function g in equation (2.1) is known. For an IPM, g is a backward mapping, which is normally unknown, and the measurand can be a vector. For the situation that the forward mapping is a matrix, **F**, as mentioned in Chapter 3, the backward mapping is desired to be the Moore–Penrose inverse (i.e. a quasi-inverse) of **F**, namely $\mathbf{F}^{\dagger}$. If the stability of $\mathbf{F}^{\dagger}$ is acceptable (depends on the condition number), $\mathbf{F}^{\dagger}$ can be used as a backward mapping, and the distribution of the model **m** can be estimated by transferring the uncertainty in data **d** to **m** via $\mathbf{F}^{\dagger}$.

To characterise the distribution of a random vector, the distribution of each component of the vector and the covariance between the components should be specified. A random vector is said to have a *multivariate normal distribution* (MVN) if each linear combination of the components of the vector is normally distributed (Genz and Bretz 2009). If a random vector $\mathbf{d} = [d_1, d_2, ..., d_m]$ has a MVN distribution, **d** can be completely characterised by a vector $E(\mathbf{d}) = [E(d_1), E(d_2), ..., E(d_m)]$ of the expected values and a covariance matrix **C** of **d**. The elements in **C** are

$$C_{i,j} = \mathrm{cov}(d_i, d_j). \tag{4.8}$$

The multivariate normality can be tested via Mardia's test (Mardia 1970), the BHEP test (Henze and Wagner 1997) and some other methods. A detailed survey of these testing methods is available in the paper by Henze (2002).

For an IPM, let **d** denotes the random vector of measured data, if **d** has the MVN distribution, the distribution can be specified as $\mathbf{d} \sim N(E(\mathbf{d}), \mathbf{C})$, where $E(\mathbf{d})$ and **C** can be obtained according to the measured data.

The vector of model **m** can be estimated as

$$\mathbf{m} = \mathbf{F}^{\dagger}\mathbf{d} . \tag{4.9}$$

It can be proved that, for a multivariate normal random vector, $\mathbf{x} \sim N(E(\mathbf{x}), \mathbf{C_x})$, after multiplying a matrix **A**, the output vector **y** is still multivariate normal, and the mean and the covariance of **y** are $E(\mathbf{y}) = \mathbf{A}(E(\mathbf{x}))$ and $\mathrm{cov}(\mathbf{y}) = \mathbf{A}\mathbf{C}_{\mathbf{x}}\mathbf{A}^{T}$, respectively (Searle 1982). Thus, **m** has an MVN distribution, and the mean and the covariance of **m** can be obtained as

$$E(\mathbf{m}) = \mathbf{F}^{\dagger}(E(\mathbf{d})) , \tag{4.10}$$

$$\mathrm{cov}(\mathbf{m}) = \mathbf{F}^{\dagger}\mathbf{C}(\mathbf{F}^{\dagger})^{T} . \tag{4.11}$$

By the properties of the Moore–Penrose inverse, the estimated distribution of **m** obtained from equations (4.10) and (4.11) is the distribution of the least square solutions of the model. According to the definition of the multivariate normal random variable, the PDF (probability density function) of **m** is

$$f(\mathbf{m}) = \frac{1}{\sqrt{(2\pi)^{n} \det\left(\mathrm{cov}(\mathbf{m})\right)}} \exp\left(-\frac{1}{2}(\mathbf{m} - E[\mathbf{m}])^{T} \mathrm{cov}(\mathbf{m})^{-1}(\mathbf{m} - E[\mathbf{m}]) \right), \tag{4.12}$$

where *n* is the dimension of vector **m** (Chatfield and Collins 1981).

Geometrically, the contours of equal probability density of a MVN vector **m** are (hyper-) ellipsoids centred at $E[\mathbf{m}]$ (Hansen 2005). Thus, the range of the MVN vector at a confidence level (such as 99%) is an ellipsoid. The directions of the principal axes of the ellipsoids are given by the eigenvectors of the covariance matrix, cov(**m**). The lengths of the principal axes are scaled by the square roots of the corresponding eigenvalues.

An example of the distribution of a two-dimensional MVN vector **m** is depicted in Figure 4.1. The green ellipse is the 99% confidence region of the random vector.

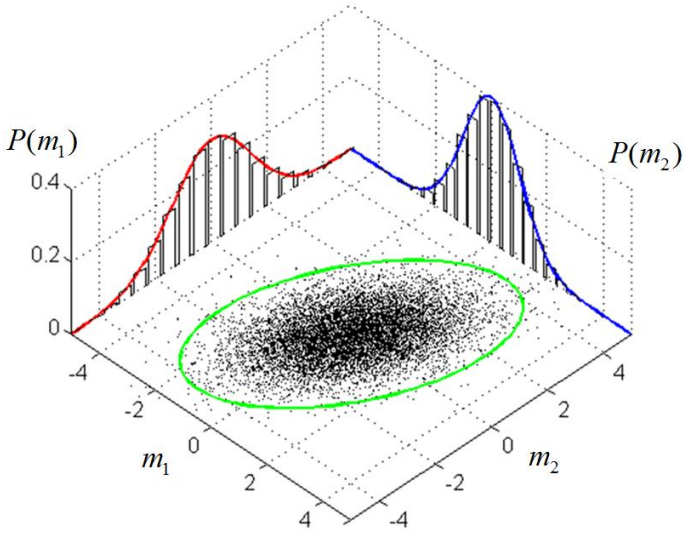


Figure 4.1 An example of a two-dimensional multivariate normal distribution with the contour of 99% confidence level (Wikipedia contributors 2015)

It is clear that the ellipsoid confidence region of **m** obtained by equations (4.10) and (4.11) is correlated with the ellipsoid confidence region of **d** at the same confidence level. Let E_m be the set of points in the former region and E_d be the set of points in the latter region, which are open sets in vector spaces. It can be directly derived from the range isomorphism theorem in Chapter 3 that E_m is isomorphic to the subset of E_d in the range of **F**, i.e.

$$E_m \cong \left(E_d \bigcap R(\mathbf{F})\right). \tag{4.13}$$

(4.13) implies that if **F** is surjective, E_m is isomorphic to E_d.

Due to the isomorphism, there is a one-to-one correspondence between the points in $E_d \bigcap R(\mathbf{F})$ and the points in E_m; hence E_m can be considered as an open set transformed from $E_d \bigcap R(\mathbf{F})$. Since the linear mapping $\mathbf{F}^\dagger$ is continuous, the transformation is a deformation.

With the singular value decomposition (SVD) method, **F** can be decomposed as

$$\mathbf{F} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \tag{4.14}$$

where **U** and **V** are orthogonal matrices, and **S** is a diagonal matrix with diagonal elements called singular values (Golub and Van Loan 2012). From equation (4.14), it can be easily deduced that

$$\mathbf{F}^\dagger = \mathbf{V}\mathbf{S}^\dagger\mathbf{U}^T. \tag{4.15}$$

Geometrically, $\mathbf{V}$ and $\mathbf{U}^T$ can be taken as rotation matrices, and $\mathbf{S}^\dagger$ can be taken as a scaling matrix. Hence, the transformation from $E_d \bigcap R(\mathbf{F})$ to E_m is a rotation, a stretching and another rotation. The deformation is determined by the singular values in $\mathbf{S}$. The larger the ratio of the maximum and minimum the singular values (conditional number), the larger the deformation will be. This explains how a small change in the measured data can be extremely enlarged in the inverse solution. An example of the transformation from a circular region of data points to an ellipse region of points via a 2-by-2 matrix $\mathbf{G}$ is demonstrated in Figure 4.2, where $\mathbf{G} = \begin{bmatrix} 7 & 9 \\ -5 & -3 \end{bmatrix}$.

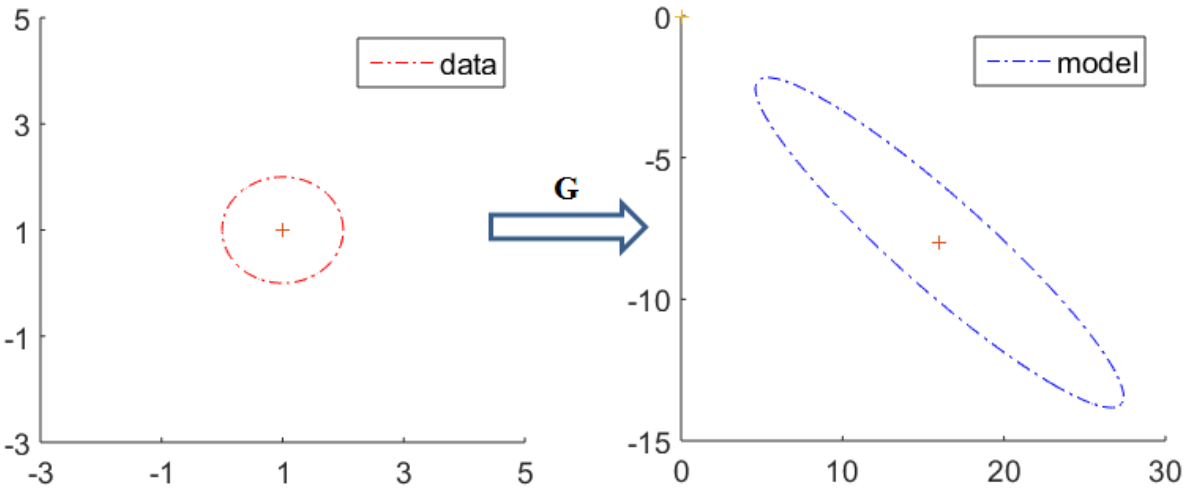


Figure 4.2 A demonstration of the transformation from a circular region of data points to an ellipse region of points via a 2-by-2 matrix $\mathbf{G}$

4.2.3 The Bayesian approach

The method of evaluating the uncertainty of a model by transforming the covariance matrix of the measured data to a covariance matrix of the model with equation (4.11) has some limitations. Firstly, it is applicable only when the data has the MVN distribution; secondly, the Moore–Penrose inverse of $\mathbf{F}$ can be ill-conditioned, which is not suitable for estimating the expected values of a model due to the stability issue. To solve the stability issue, a regularisation is often applied to obtain a regularised backward mapping $\mathbf{G}$ which is more stable then $\mathbf{F}^\dagger$. But, as mentioned before, a bias of the inverse solution will be introduced when the stability is improved by the regularisation. Due to the bias, after regularisation, the estimated result of the model is not statistically meaningful.

The Bayesian approach allows the estimation of the distribution of the model according to the distribution of the data and the prior information of the model in an inverse problem. It has been widely applied for solving ill-conditioned inverse problems since it avoids the bias of regularisation.

In this approach, the model to be estimated is taken as a random variable or random vector. It is assumed that based on some prior information of the model, such as constraints of physical laws and experience-based intuition, a *prior distribution* of the model is known, which is expressed as a PDF, $p(\mathbf{m})$. Let $f(\mathbf{d}|\mathbf{m})$ denote the PDF of the measured data **d** of the model **m**. It can be assumed that the measurement errors corresponding to the components d_i of the data **d** are independent, so $f(\mathbf{d}|\mathbf{m})$ can be expressed as a JDF (joint probability density function) of the PDF of d_i as follows:

$$f(\mathbf{d}|\mathbf{m}) = f(d_1|\mathbf{m}) f(d_2|\mathbf{m}) ... f(d_n|\mathbf{m}). \tag{4.16}$$

If d_i is normally distributed with a standard deviation, σ_i, the PDF of d_i is

$$f(d_i|\mathbf{m}) = \frac{1}{\sigma_i\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{d_i - (\mathbf{Fm})_i}{\sigma_i} \right)^2 \right). \tag{4.17}$$

It is well known that Bayes theorem can be expressed in the following equation:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}, \tag{4.18}$$

where *A*, *B* are events. This theorem can be used to update the prior probability for a hypothesis $P(A)$, according to some acquired evidence $P(B|A)$ and $P(B)$. The updated result, $P(A|B)$, is called a posterior probability.

Bayes theorem is also applicable to updating the PDF of a random variable, from the prior distribution to a *posterior distribution*. Based on this theorem, the probability distribution of the model parameters can be estimated as a posterior distribution:

$$q(\mathbf{m}|\mathbf{d}) = \frac{f(\mathbf{d}|\mathbf{m})p(\mathbf{m})}{g(\mathbf{d})}, \tag{4.19}$$

where $g(\mathbf{d})$ is the PDF of the data independent of the model. By the law of total probability (Zwillinger and Kokoska 1999), we have

$$g(\mathbf{d}) = \int_{\text{all models}} f(\mathbf{d}\,|\,\mathbf{m})\,p(\mathbf{m})\,d\mathbf{m}. \tag{4.20}$$

In equation (4.19), $g(\mathbf{d})$ is simply a constant c that normalises the distribution $q(\mathbf{m}\,|\,\mathbf{d})$ so that its integral in model space is equal to 1 (Aster *et al.* 2013, p 256). In many cases, it is not necessary to know the constant c, so equation (4.19) is often expressed by a proportional relationship:

$$q(\mathbf{m}\,|\,\mathbf{d}) \propto f(\mathbf{d}|\mathbf{m})p(\mathbf{m}). \tag{4.21}$$

It is often reasonable to assume that the data $\mathbf{d}$ has a MVN distribution, and the prior distribution is also MVN. For a linear inverse problem, let $\mathbf{d}_0$ be the mean of the measured data, $\mathbf{C}_D$ be the covariance matrix of corresponding data, $\mathbf{m}_0$ be the mean of the prior distribution and $\mathbf{C}_M$ be the covariance matrix of the prior distribution. According to the PDF of multivariate normal random vector, the PDF of the $\mathbf{d}$, given $\mathbf{m}$, is

$$f(\mathbf{d}\,|\,\mathbf{m}) = \frac{1}{\sqrt{(2\pi)^n \det(\mathbf{C}_D)}} \exp\left(-\frac{1}{2}(\mathbf{Fm}-\mathbf{d}_0)^T \mathbf{C}_D{}^{-1}(\mathbf{Fm}-\mathbf{d}_0)\right). \tag{4.22}$$

Thus

$$f(\mathbf{d}\,|\,\mathbf{m}) \propto \exp\left(-\frac{1}{2}(\mathbf{Fm}-\mathbf{d}_0)^T \mathbf{C}_D{}^{-1}(\mathbf{Fm}-\mathbf{d}_0)\right) \tag{4.23}$$

Similarly, for the prior distribution, we have

$$p(\mathbf{m}) \propto \exp\left(-\frac{1}{2}(\mathbf{m}-\mathbf{m}_0)^T \mathbf{C}_M{}^{-1}(\mathbf{m}-\mathbf{m}_0)\right) \tag{4.24}$$

Thus, from equation (4.21), we get

$$q(\mathbf{m}\,|\,\mathbf{d}) \propto \exp\left(-\frac{1}{2}\left((\mathbf{Fm}-\mathbf{d}_0)^T \mathbf{C}_D{}^{-1}(\mathbf{Fm}-\mathbf{d}_0) + (\mathbf{m}-\mathbf{m}_0)^T \mathbf{C}_M{}^{-1}(\mathbf{m}-\mathbf{m}_0)\right)\right). \tag{4.25}$$

It has been demonstrated by Tarantola (2005) that equation (4.25) can be simplified to

$$q(\mathbf{m}\,|\,\mathbf{d}) \propto \exp\left(-\frac{1}{2}\left((\mathbf{m}-\mathbf{m}_{MAP})^T \mathbf{C}_{M'}{}^{-1}(\mathbf{m}-\mathbf{m}_{MAP})\right)\right), \tag{4.26}$$

where $\mathbf{m}_{MAP}$ is the *maximum a posteriori* (MAP) model, which is the model maximising the value of $q(\mathbf{m}\,|\,\mathbf{d})$, and

$$\mathbf{C}_{M'} = \left(\mathbf{F}^T \mathbf{C}_D{}^{-1} \mathbf{F} + \mathbf{C}_M^{-1}\right)^{-1}. \tag{4.27}$$

The MAP model can be obtained by maximising the exponent in equation (4.25), or minimising its negative, which is equivalent to the following linear least squares problem (Aster *et al.* 2013):

$$\min \left\| \begin{bmatrix} \mathbf{C}_D^{-1/2} \mathbf{F} \\ \mathbf{C}_M^{-1/2} \end{bmatrix} \mathbf{m} - \begin{bmatrix} \mathbf{C}_D^{-1/2} \mathbf{d}_0 \\ \mathbf{C}_M^{-1/2} \mathbf{m}_0 \end{bmatrix} \right\|_2^2. \tag{4.28}$$

The proportional relation in equation (4.26) implies that the posterior distribution is also a MVN distribution, of which the mean is $\mathbf{m}_{MAP}$, i.e. the solution of equation (4.28), and the covariance is $\mathbf{C}_{M'}$.

In theory, the Bayesian approach can also be applied when measurement errors are not normally distributed, but, in practice, the associated analytical computations can be difficult. For situations of not normally distributed measurement errors and nonlinear inverse problems, the Markov chain Monte Carlo method can be used to obtain samples from a posterior distribution, which is a computational method and not in the scope of this thesis. The details of this method can be found in the work by Hastings (1970) and Aster *et al.* (2013).

4.3 The ERSs of stochastic measurands

The measured value of a measurand is meaningful only if it can be used for estimating the empirical relation. Before discussing how to estimate empirical relations according to the measurement results with uncertainty, it is helpful to understand the ERSs of stochastic measurands and the way of representing these ERSs.

4.3.1 Semiorder and interval order

It is obvious that the ERS of a stochastic measurand is different from the ERSs discussed before. If the measurand values of a stochastic measurand are considered as intervals of the possible values, when two intervals of objects *a*, *b* intersect, both $a \prec b$ or $b \prec a$ are possible. Thus, the empirical relation is neither an equivalence relation nor a weak order. In this

situation *a*, *b* can be considered as 'being same up to a small error', which is a kind of relation called indifference or similarity, denoted as $a \wr b$. Indifference is a non-transitive and symmetric relation, which was first studied by Campbell (1928), and developed in the notion of a just-noticeable-difference (jnd) by Goodman (1951) and Galanter (1956). By using axioms, Luce (1956) defined this indifference relation in an order structure, called *semiorder*, which can be represented by a relational system of a set of real intervals with a constant size. A more general type of order is called *interval order* (Wiener 1921), which can be used to define the relation of intervals with different sizes. Semiorders and interval orders are commonly used in psychology to characterise a perceived or measured relation of objects (stimuli, alternatives) according to some attribute (e.g. brightness, loudness, preference) when "small differences" in the relevant attribute are not detectable due to a sensory or instrumental threshold (Fishburn 1973b).

A binary relation $\lhd$ on *A* is a semiorder if and only if the following three axioms are satisfied.

(i) $\lhd$ is irreflexive.

(ii) $a \lhd b$ and $c \lhd d \Rightarrow a \lhd d$ or $c \lhd b$, for all $a,b,c,d \in A$.

(iii) $a \lhd b$ and $b \lhd c \Rightarrow a \lhd d$ or $d \lhd c$, for all $a,b,c,d \in A$.

An interval order is a binary relation that satisfies axioms (i) and (ii). It is clear that a semiorder is also an interval order. If neither $a \lhd b$ nor $b \lhd a$, then $a \wr b$, where $\wr$ is an indifference. The intransitive property makes $\wr$ different from the equivalence relation.

It has been proved by Fishburn (1970) that if *A* is a countable set and $\lhd$ is an interval order, then $(A, \lhd)$ can be represented by an ordered set of real intervals in the sense that,

$$a \lhd b \text{ if and only if } \sup J(a) < \inf J(b), \tag{4.29}$$

for any $a,b \in A$ and their corresponding intervals *J*(*a*) and *J*(*b*). Scott and Suppes (1958) and Scott (1964) proved that if $\lhd$ is a semiorder on a finite set *A* then there is a mapping *J* from *A* to real intervals which satisfies equations (4.29) and (4.30).

$$\sup J(a) - \inf J(a) = 1, \text{ for all } a \in A \tag{4.30}$$

4.3.2 Empirical relation with a probability assigned

If the measurand values of a stochastic measurand are considered as random variables, the possible empirical relation, for instance a weak order, between two objects may not be unique. Even if there is no measurement error, it is still possible to observe different empirical relations ($a \prec b$ and $b \prec a$) between a pair of objects. Thus, a probability should be assigned to each empirical relation. A theory of representing an ERS with the relational system of random variables in ordinal measurement was developed by Domotor (1969). Suppose $\langle A, \prec \rangle$ is an ERS of a stochastic measurand, where $\prec$ is a weak order, then $\langle A, \prec \rangle$ is measurable if there exists a random function φ, such that, for all $a, b \in A$,

$$P(a \prec b) = P(\varphi(a) \leq \varphi(b)), \tag{4.31}$$

where P is a probabilistic function, $\varphi(a)$, $\varphi(b)$ are random variables and $P(a \prec b)$ is the probability of observing the occurrence of $a \prec b$. Instead of using semiorder or interval order to replace the empirical relation in the deterministic model (preorder or weak order), Domotor's approach assigns a probability to each empirical relation to enable the compatibility of uncertainties.

The measurement of a measurand with intrinsic uncertainty can be modelled as a random function φ, and equation (4.31) is desired to be satisfied. If the measurement φ satisfies equation (4.31), the empirical relation can be correctly estimated with a probability according to the measurement results.

Moreover, if the probabilistic function P satisfies equation (4.32), two binary empirical relations, W and S, can be naturally defined in terms of equations (4.33) and (4.34), respectively.

$$P(a \prec b) + P(b \prec a) = 1 \tag{4.32}$$

$$aWb \quad \text{if and only if} \quad P(a \prec b) \geq \frac{1}{2} \tag{4.33}$$

$$aSb \quad \text{if and only if} \quad P(a \prec c) \geq P(b \prec c), \text{ for all } c \in A \tag{4.34}$$

Relations W and S are useful for determining the conformity or classification according to measurement results when the uncertainties of the results are significant. The properties of relations W and S (such as weak and strong stochastic transitivity) are studied in detail in the work by Block and Marschak (1960) and Fishburn (1973a).

4.4 Evaluation of empirical relations with interval orders

Every specified measurand has some intrinsic (definitional) uncertainty, since the specification is always incomplete, and thus can be taken as a stochastic measurand. The ERS of the stochastic measurands can be represented by the relational system of real intervals or random variables. Hence, conversely, by treating the measurement results as intervals or random numbers, the empirical relation of the ERS can be estimated.

Measurement results with uncertainty can be expressed in terms of intervals containing the set of true values of a measurand with a stated probability, which are named as *coverage intervals* at a *coverage probability* in JCGM 100 (2008). The concept of coverage interval is similar to a statistical concept called confidence interval. The difference is that confidence interval should be evaluated according to type A uncertainty only, but coverage interval can be evaluated according to the uncertainties of both type A and type B. For a stochastic measurand, it is natural to consider the estimated coverage intervals as the (mathematical) representations of the objects in the ERS. Let $J(a)$, $J(b)$ denote the coverage intervals of a stochastic measurand corresponding to objects $a,\ b \in A$. When $J(a)$ and $J(b)$ intersect with each other (i.e. $J(a) \cap J(b) \neq \emptyset$), neither $\sup J(a) < \inf J(b)$ nor $\sup J(b) < \inf J(a)$. By (4.29), neither $a \lhd b$ nor $b \lhd a$, thus $a \wr b$.

If $J(a)$, $J(b)$ do not intersect, then one interval is strictly smaller than the other. For example, if $\sup J(a) < \inf J(b)$, then, by equation (4.29), $a \lhd b$. Since the coverage intervals are defined subject to a coverage probability, the estimated interval order also has an uncertainty equal to the coverage probability.

For instance, let $J(a)$, $J(b)$, $J(c)$ be the coverage intervals of three objects a, b, c respectively. If, under 95% coverage probability, $J(a)$, $J(b)$, $J(c)$ are distributed as shown in Figure 4.3, the empirical relations can be written as $a \wr b$, $b \wr c$, and $a \lhd c$.

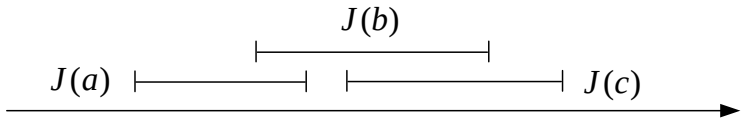


Figure 4.3 The distribution of coverage intervals *A, B, C*

Here $a \lhd c$ means, at a 95% confidence level, that the measurand of a is strictly smaller than the measurand of c. And $a \wr b$ means, at a 95% confidence level, that it cannot be assured whether $a \lhd b$ or $b \lhd a$.

4.5 Evaluation of empirical relations with probabilities assigned

The problem is, when the coverage intervals of the measurand values intersect, instead of saying that the measurands of two objects are 'the same up to a small error', can we give a more meaningful statement by estimating the probability of a certain empirical relation? For instance, in Figure 4.3, what is the probability that the measurand of a is strictly smaller than the measurand of b? To answer the question, it is necessary to treat the values of the measurand as random variables.

Let α, β be the random variables which represent the stochastic measurand of objects $a, b \in A$; α, β are independent of each other. The expected values and standard deviations of α, β can be estimated according to the measurement results of a, b. Finding the empirical relation between a, b with a probability assigned is equivalent to finding the relation of α, β and its probability. To do that, we can create a random variable, $\gamma = \alpha - \beta$. Then

$$P(\alpha < \beta) = P(\gamma < 0), \tag{4.35}$$

$$E(\gamma) = E(\alpha) - E(\beta), \tag{4.36}$$

$$u(\gamma)^2 = u(\alpha)^2 + u(\beta)^2 + 2\mathrm{cov}(\alpha, \beta). \tag{4.37}$$

The covariance, cov(α, β), is zero, since α, β are independent. Thus

$$u(\gamma) = \sqrt{u(\alpha)^2 + u(\beta)^2}. \tag{4.38}$$

If α and β have the same type of distribution, we have

$$P(\gamma < 0) = F_\gamma(0), \tag{4.39}$$

where F_γ is the CDF of γ. It can be obtained according to $E(\gamma)$ and $u(\gamma)$. For instance, if a and b are both normally distributed,

$$F_\gamma(0) = \int_{-\infty}^{0} \frac{1}{u(\gamma)\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\gamma - E(\gamma)}{u(\gamma)} \right)^2 \right). \tag{4.40}$$

If the distributions of α and β are of different types, the situation is more complicated. Let the $g(\alpha)$ be the PDF of α, and $h(\beta)$ be the PDF of β, since two distributions are independent, the JDF, $f(\alpha,\beta)$ is (Chatfield and Collins 1981)

$$f(\alpha,\beta) = h(\alpha)g(\beta). \tag{4.41}$$

The CDF F_γ can be written in terms of an appropriate integral over the JDF (see Figure 4.4) as follows:

$$\begin{aligned} F_\gamma(0) &= \int\int_{\alpha-\beta<0} f(\alpha,\beta)d\alpha\, d\beta \\ &= \int\int_{\alpha-\beta<0} h(\alpha)g(\beta)d\alpha\, d\beta \\ &= \int\int_{\alpha-\beta<0} h(\alpha)g(\beta)d\alpha\, d\beta \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\beta} h(\alpha)d\alpha\, g(\beta)d\beta\,. \end{aligned} \tag{4.42}$$

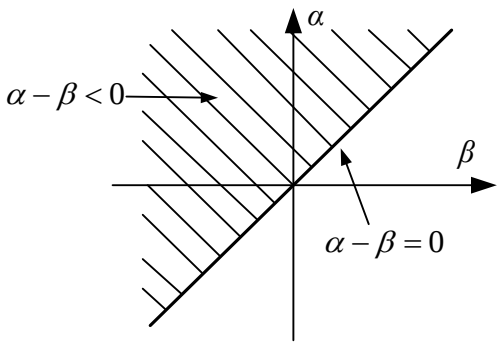


Figure 4.4 Integration of a JDF of two independent random variables, α and β, to evaluate the probability of $\boldsymbol{\alpha - \beta < 0}$

Example 4.1 Let α be a normally distributed variable, $\alpha \sim N(3, 0.09)$, and β be a uniformly distributed variable, $\beta \sim U(2.8, 4)$, then the PDFs of α and β are

$$h(\alpha) = \frac{1}{0.3\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\alpha - 3}{0.3} \right)^2 \right), \tag{4.43}$$

$$g(\beta) = \begin{cases} \left(\dfrac{1}{4 - 2.8} \right) & \text{for } 2.8 \le \beta \le 4 \\ 0 & \text{for } \beta < 2.8 \text{ or } \beta > 0 \end{cases}. \tag{4.44}$$

By equation (4.42), the probability of $\alpha < \beta$ is

$$P(\alpha < \beta) = F_\gamma(0) = \int_{2.8}^{4}\int_{-\infty}^{\beta} \frac{1}{0.3\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\alpha-3}{0.3}\right)^2\right) d\alpha \left(\frac{1}{4-2.8}\right) d\beta \quad . \quad (4.45)$$
$$= 0.7956$$

By equation (4.31), the estimated empirical relation between *a, b* is

$$P(a \prec b) = P(\alpha \le \beta) = 0.7956\,, \quad (4.46)$$

or $a \prec_{0.7956} b.$

If the empirical relation $\prec$ is complete (for all $a \neq b \in A$, either $a \prec b$ or $b \prec a$), equation (4.32) is satisfied. According to the estimated probability, $P(a \prec b)$, a complete binary relation *W* can be obtained according to equation (4.33). This provides a general method to define a binary relation between a pair of measured objects when the uncertainty is involved.

4.6 Conclusions

In this chapter, it has been demonstrated that it is necessary to generalise the deterministic model of indirect measurements to a probabilistic model due to the inevitable measurement error and the intrinsic uncertainty of the measurand. In the probabilistic model, the measurand values are treated as probabilistic distributions. As a result, the empirical relation should be estimated with probability assigned. A comparsion of the deterministic model and the probabilistic model of indirect measurements is given in Table 4.1.

For indirect measurements, a part (normally the major part) of the uncertainty of the measurand value is transformed from the measurement uncertainty of the measured data. A method of deriving the uncertainty of the measurand from the uncertainty of the observations is introduced for the measurand that can be expressed by a known function of the proxy quantities. For linear inverse problems, a method of deriving the covariance matrix of the model according to covariance matrix of the multivariate normal random vector of the data is introduced, and a geometrical understanding of the transformation of the uncertainty is provided based on the range isomorphism theorem. The Bayesian method is introduced for estimating the distribution of the measurand when the function from the proxy quantities to the measurand is unknown. For one-dimensional measurands, the interval order is introduced to define the ordering relations of the estimated coverage intervals of measurand values, and thereby used for estimating empirical relations. For the situation that the coverage intervals

intersect, a new method of estimating the empirical relations with probability assigned is introduced.

The intrinsic uncertainty of a measurand is closely related to the way of specifying the measurand, i.e. the specification of the measurand. The uncertainty of specification is defined in the geometrical product specifications and verification system (GPS) (ISO 17450-2 2002), which is discussed in detail in Chapter 6.

	Deterministic model	Probabilistic model
Measurement Process	A homomorphism φ, and $a \square b \Leftrightarrow \varphi(a) = \varphi(b)$	A random function φ, s.t. $P(a \prec b) = P(\varphi(a) \le \varphi(b))$
Measurand values	Fixed numbers	probabilistic distributions
Measurement results	Fixed numbers	Random variables
Empirical relation	Preorder	Preorder with probability assigned
ERS	A set of objects and their empirical relations corresponding to a measurand	A set of objects and their probabilistic empirical relations corresponding to a measurand
NRS	A set of numbers and their relations	A set of random variables (with specified distribution) and their probabilistic relations
Mathematical model of the IPM	$d = F(m)$	$d = F(m) + \eta$
Fitting criterion (P2)	$FGF = F$	$\|F(m) - d\|_2 \le \varepsilon$
Selection of inverse solution (P5)	$\min T(m)$ $F(\mathrm{m}) = d$ $l \le m \le u$	$\min T(m)$ $\|F(\mathrm{m}) - d\|_2 \le \varepsilon$ $l \le m \le u$

Table 4.1 A comparison between the deterministic model and the probabilistic model of indirect measurements

Chapter 5

A Strategy of Reducing the Influence of Uncertainty in the Evaluation of Empirical Relations

5.1 Introduction

It is well known that the objective of measurement is to obtain the values of the measurand (JCGM 100 2008). But the fact that measurement starts with the observation or introduction of a mostly transitive relation (Ellis 1968, p.54) is often been ignored. According to the representational theory of measurement, the values of the measurand and their numerical relations are used to represent the (measured) objects and their empirical relations (Krantz *et al* 1999). Hence the implicit objective of measurement is to compare the objects and obtain the empirical relations.

Most researchers in metrology are focused on the former objective (i.e. to obtain the values of the measurand), since the latter objective (i.e. to obtain the empirical relation) can be achieved by comparing the measurement results. However, to get the best estimations of the measurand, the calculation can be quite complicated, and the measurement uncertainties can be very large (e.g. larger than 30% of the size of the tolerance). In this chapter, the latter objective is taken as the final objective of measurement, and a strategy of reducing the influence of uncertainty in the evaluation of empirical relations is proposed.

An important reason of obtaining the values of the measurand is to determine the conformity with specifications by comparing the measurement results with the specifications. ISO 14253-1 (2013) together with GUM (JCGM 100 2008) provides a method for determining conformity with specifications when uncertainty is involved. In that method, a *complete measurement result* is expressed as $J(x) = \hat{x} \pm U$, where $\hat{x}$ is the result of a measurement, U is the expanded uncertainty with a stated level of confidence (e.g. 95%). Thus $J(x)$ can be taken as a coverage interval containing the (true) value of the measurand x. The conformity with a specification is determined by the relation of the coverage interval and specification limits (see Figure 5.1).

For an arbitrary measurand, the specification limits can be taken as the measurand values of a special type of objects, called *limit samples*. A limit samples is considered as an object of which the measurand value is equal to a specification limit. The conformity of a measured object with the specification can be determined according to the empirical relations between the measured objects and the limit samples. For example, let p, q be the limit samples corresponding to the lower and upper specification limits respectively. Then an object a is within the specification if and only if $p \precsim a \precsim q$, where $\precsim$ is a weak order. Hence the conformity (or nonconformity) of a measurement result with a specification can be determined by the estimated empirical relation.

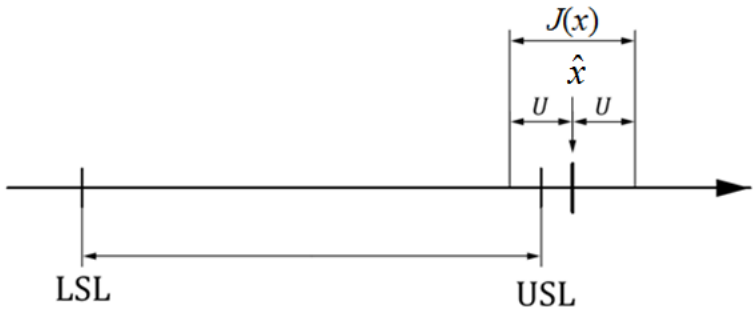


Figure 5.1 A complete measurement result which is neither within nor out of the specification

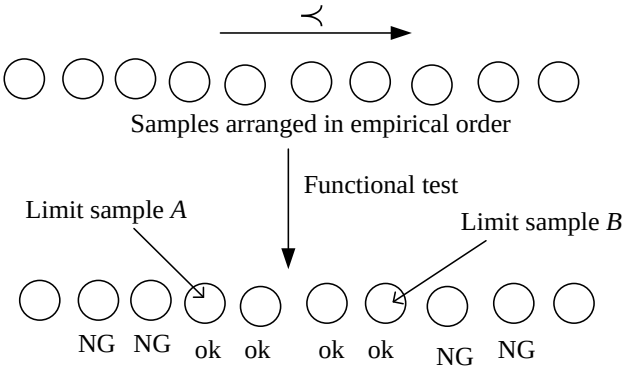


Figure 5.2 Schema of searching the limit samples according to the empirical order and the results of functional test

Evaluation of empirical relations is also important for the design of specifications. To design a specification of a measurand of a workpiece for satisfying certain functional requirement, one usually needs to measure many samples of the workpiece, and order the samples according to their measured values of the measurand. And then, by doing the functional test for some samples according to the obtained order, the samples which marginally satisfy the functional requirement (called limit samples) can be found, so that the specification limits

(e.g. upper and lower specification limits) can be set according to their measurand values. The obtained order is the empirical order which helps for searching the limit samples (see Figure 5.2).

The method of evaluating empirical relations in terms of interval orders is introduced in Section 4.5. In this method, the empirical relation of a stochastic measurand is taken as an interval order, which consists of a strict interval order $\lhd$ and an indifference $\wr$. The ERS $\langle A, \lhd \rangle$ can be represented by the relational system of real intervals, and the coverage intervals of the measurement results can be taken as the representations of the measured objects. Therefore, the empirical relation of the measured objects can be estimated according to the relation of the coverage intervals.

It is obvious that the sizes of coverage intervals (i.e. lengths of the intervals) may affect the interval orders, and thus affect the estimation of the empirical relation. Consider some coverage intervals of an identical size, if this size is large (e.g. 30% of the maximum difference of the measurement results), the adjacent coverage intervals are quite likely to intersect with each other. When two coverage intervals intersect, the empirical relation will be estimated as indifference, thus no transitive relation can be obtained under the coverage probability. So, for estimating empirical relations, the sizes of coverage intervals are preferred to be smaller.

For this reason, the average size of the coverage intervals of a set of measurement results is called as the *resolution of comparison*. A main objective of this chapter is to improve the resolution of comparison by reducing the influence of measurement uncertainty.

5.2 The principle of reducing the influence of uncertainty

5.2.1 Classification of uncertainty components by the sources

The size of coverage intervals are determined by the expanded uncertainties. Hence the resolution of comparison can only be improved by reducing the measurement uncertainty.

Measurement uncertainties can be either classified according to their evaluation methods (statistical or non-statistic) into Type A and Type B, or by the sources of the uncertainties. The latter way classifies uncertainties as the following two types.

- Random uncertainty components: the uncertainties arise from the *random effects*;

- Systematic uncertainty components: the uncertainties arise from incomplete knowledge of the *systematic effects*.

According to GUM (JCGM 100 2008), a random effect is the effect of stochastic or unpredictable variations of *influence quantities* (quantity that is not the measurand but effects the results of the measurement); and a systematic effect is a *recognised* effect of an influence quantity on a measurement result. Both effects could cause some deviation of the measured value from the value of the measurand. Each effect can be taken as a function η in terms of

$$\eta(x, d_i) = x', \tag{5.1}$$

where x is the measurand, d_i is a related influence quantity, x' is a quantity deviated from the measurand due to the random/ systematic effect. For a systematic (random) effect η, the deviation, $(x' - x)$ is the systematic (random) error caused by η.

In practice, it can be difficult to distinguish the two types of effects very clearly. But, since in replicate measurements the systematic error arise from systematic effect remains constant or varies in a predictable manner (JCGM 200 2008), a systematic effect itself is a *deterministic function*. In contrast, a random effect is a random function, and the related d_i is always a random variable.

Moreover, under the repeatability conditions given in GUM ((JCGM 100 2008) B.2.15), some influence quantities of systemic effects, e.g. offset error, are always *fixed* during the measurements of all the objects. These quantities are constants, although the exact values are unknown due to incomplete knowledge. Hence, for a fixed influence quantity d_i, equation (5.1) can be taken as a function of the measurand, denoted as $\eta_{di}(x) = x'$, or simply $\eta(x) = x'$, if it is clear what d_i is.

In many cases, $\eta(x)$ is an increasing function of the measurand. For instance, the effect of imperfect calibration of a gauge can be written as $\eta_c(x) = x + c$, where c is a constant (but unknown) offset error. The effect of the sensitivity of the instrument, which gives rise to the sensitivity error, is in the form of $\eta_a(x) = ax$, where a is unknown constant close to 1. The effect of resolution or digital rounding is in the form of $\eta_b(x) = 10^{-b}\lfloor 10^b x + 0.5 \rfloor$, where b is a integer, $\lfloor\ \rfloor$ is the floor function. The above functions of systematic effects are all (monotonically) increasing. This type of systematic effect is defined as the monotonic effects.

Definition 5.1: For an influence quantity d_i, if it is fixed as a constant in the measurements of all the objects, and its systematic effect η_{di} is an increasing function of the measurand x, then η_{di} is a *monotonic effect.*

That means for any monotonic effect η_{di}, we have

$$x_1 \le x_2 \Rightarrow \eta_{di}(x_1) \le \eta_{di}(x_2), \tag{5.2}$$

where x_1, x_2 are two arbitrary values of the measurand.

The relation between x_1 and x_2 is a representation of the empirical relation between the corresponding objects. Monotonic effects preserve the relation of x_1 and x_2, thus they also preserve empirical relations.

With this definition, systematic effects are classifies into two types: monotonic effects and non-monotonic effects. A monotonic effect may become non-monotonic when the measurement method changes. For example, if the temperature of the objects is an influence quantity, it may be fixed or changing depends on the measurement environment. So to classify the effects, the actual situation of measurement should be fully understood.

Correspondingly, the uncertainty components arise from these effects can be further classified according to their sources as shown in Figure 5.3. For example, monotonic uncertainty components are the uncertainties arise from monotonic effects.

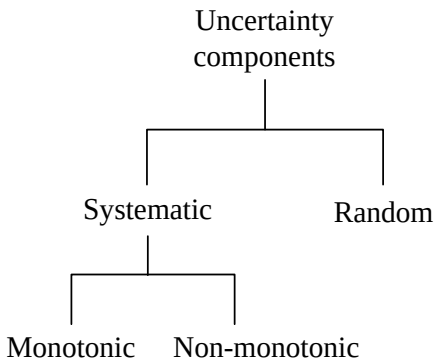


Figure 5.3 Classification of uncertainty components by the sources

5.2.2 Monotonic uncertainty components

To estimate the value of the measurand, all the systematic effects should be corrected from the observed data. But for estimating the empirical relation, it's not necessary to correct the monotonic effects, because, monotonic effects preserve empirical relations. As shown in

equation (5.2), although $\eta(x_1)$ and $\eta(x_2)$ consists the systematic error rise from the monotonic effect, they still reflect the relation of x_1 and x_2. Thus, without correcting the monotonic effects, a quantity, $x' = \eta(x)$, named the *biased measurand*, can be used to estimate the empirical relation.

This is also true when the empirical relation is represented by the interval order of coverage intervals. For example, let η be a monotonic effect, $\eta(x) = ax + b$, where *a, b* are positive real numbers, and let the relation of the coverage intervals $J(x_1)$, $J(x_2)$ and $\eta(x_3)$ of three measurement results be $J(x_3) \wr J(x_2)$, $J(x_2) \lhd J(x_1), J(x_3) \lhd J(x_1)$. As shown in Figure 5.4, $\eta J(x_3) \wr \eta J(x_2)$, $\eta J(x_2) \lhd \eta J(x_1), \eta J(x_3) \lhd \eta J(x_1)$. η does not change the relation of the coverage intervals.

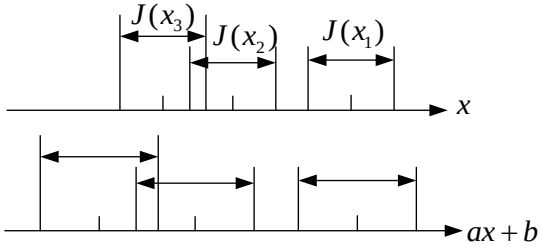


Figure 5.4 The relations of the coverage intervals with and without monotonic effects

Proposition 5.1: Let $J(x_1)$, $J(x_2)$ be the coverage intervals of x_1 and x_2, if $\eta : x \to x'$ is a monotonic effect, then

$$\eta J(x_1) \lhd \eta J(x_2) \Rightarrow J(x_1) \lhd J(x_2).$$

Proof: Let $J(x_1) = [a,b], J(x_2) = [c,d]$, where a, b, c, d are some real constants, by (4.2)

$$J(x_1) \lhd J(x_2) \Leftrightarrow b < c. \tag{5.3}$$

By definition, η is an increasing function, so $\eta J(x_1) = [\eta(a), \eta(b)]$

and $\eta J(x_2) = [\eta(c), \eta(d)]$, hence

$$\eta J(x_1) \lhd \eta J(x_2) \Leftrightarrow \eta(b) < \eta(c). \tag{5.4}$$

Since η is increasing, $b < c$ implies $\eta(b) \le \eta(c)$, and $b \ge c$ implies $\eta(b) \ge \eta(c)$,

and either $b \ge c$ or $b < c$, thus

$$\eta(b) < \eta(c) \Rightarrow b < c. \tag{5.5}$$

By (5.3), (5.4) and (5.5), we obtain

$$\eta J(x_1) \lhd \eta J(x_2) \Leftrightarrow \eta(b) < \eta(c) \Rightarrow b < c \Leftrightarrow J(x_1) \lhd J(x_2).$$

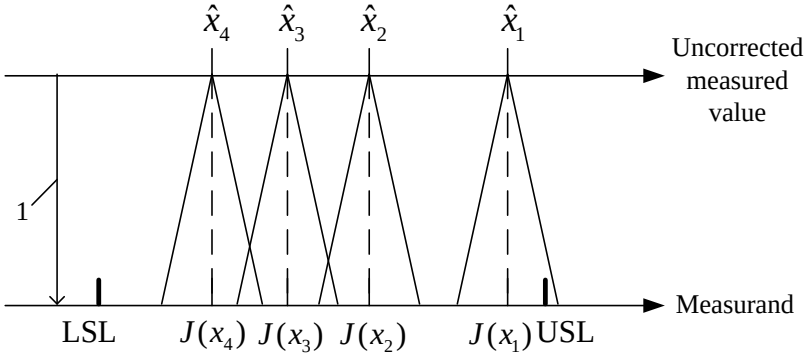
So the proposition is proved. □

That means the interval order of the coverage intervals of the biased measurand can be used to estimate the interval order of the coverage intervals of the measurand, and thus estimate the empirical relation. The coverage intervals of the biased measurand are smaller in size than the coverage intervals of the measurand, because the monotonic uncertainty components are not included in the former coverage intervals. So the resolution of comparison is improved using the coverage intervals of the biased measurand.

It can be proved that $\eta J(x_1) \wr \eta J(x_2)$ does not imply $J(x_1) \wr J(x_2)$, both $J(x_1) \lhd J(x_2)$ and $J(x_2) \lhd J(x_1)$ are possible. But similar to $J(x_1) \wr J(x_2)$, it means no inference on the empirical relation can be given under the coverage probability.

5.3 The strategy

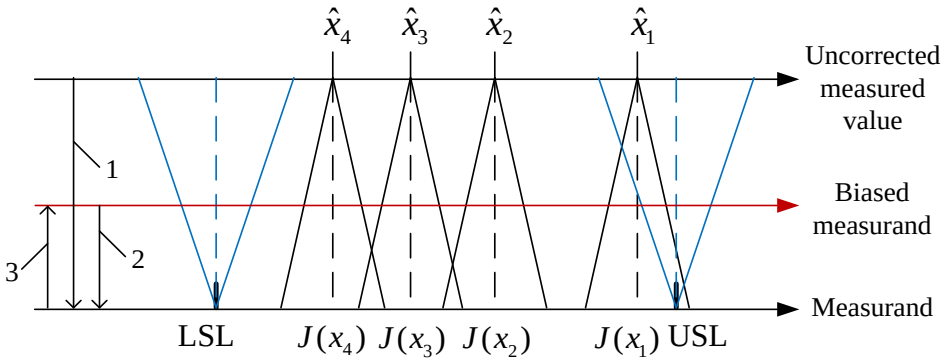
To determine the conformity of measurement results with a specification, one needs to compare the measurement results with the specification limits. Traditionally, the measurement results should be corrected for all the recognised systematic effects before the comparison (see Figure 5.5). Conversely, without correcting the monotonic effects, one can specify a biased measurand x', and estimate the coverage intervals of x' of the limit samples according to the monotonic effects and their uncertainties; and then compare the coverage intervals of the limit samples with the coverage intervals of measurement results (see Figure 5.6).



1: evaluation of the coverage intervals of the measurand

Figure 5.5 The traditional way of determining the conformity with a specification

$\hat{x}_i$ is a measured value without the correction of system effects, $\hat{x}_i$ does not need to be the centre of $J(x_i)$



1: evaluation of the CIs of the measurand
2: correction for the monotonic effects
3: estimation of the coverage intervals of the biased measurand

Figure 5.6 The amended way of determining the conformity with a specification

Figure 5.6 demonstrates the principle of improving the resolution of comparison: due to the order-preserving property of monotonic effects, the biased measurand can be used, instead of the measurand, to estimate the empirical relation, so that the sizes of the coverage intervals to be compared can be reduced. Following this principle, the strategy of estimating empirical relations is summarised as following.

Strategy:

1. Express the measurand in terms of a function of the influence quantities, such as

$$x = f(d_1, d_2, ..., d_n). \tag{5.6}$$

   All the significant errors and corrections should be included in the function.

2. According to the actual situation of the measurement, sort out the influence quantities which are fixed as a constant in the replicate measurements of all the objects.

3. Move the fixed influence quantities to the LHS of the equation (5.6), and get a new equation. Specify a biased measurand x' with the LHS of the new equation, which should consist only of the fixed influence quantities.

4. For each measured object, evaluate the expected value and the expanded uncertainty of the biased measurand with the RHS of the new equation.

5. For the specification limits, take them as the values of the measurand, and use the LHS of the new equation to estimate the expected values and the expanded uncertainties of the biased measurand.
6. Use interval order to describe the relation of all the coverage intervals of the biased measurand, and according the interval order to estimate the empirical relation and decide the conformity with the specification.

This strategy together provides a new method of comparing measurement results and determining conformity with specifications.

5.4 An example

End gauge calibration is an example of uncertainty evaluation given in GUM ((JCGM 100 2008) H.1). Here three end gauges, named *a, b, c,* are of the same specification: 50mm +0.001/−0 mm at 20˚C. They are measured to determine the conformity with the specification and to find out their ordered relation in length.

The end gauges are measured by comparing them with a calibrated standard gauge of the same nominal length. The difference of length *d* is measured by a comparator. As shown in the example in GUM: 2008, with the effect of thermal expansion, the measurand, i.e. length of the end gauges at 20˚C, can be expressed as the following function:

$$l = f(l_S, d, \alpha_S, \theta, \delta\alpha, \delta\theta) = l_S + d - l_S(\delta\alpha \cdot \theta + \alpha_S \cdot \delta\theta) \tag{5.7}$$

where l is the measurand; l_S is the length of the standard gauge given in its calibration certificate; d is the difference of length; α and α_S are the thermal expansion coefficients of the end gauge and the standard gauge respectively, and $\delta\alpha = \alpha - \alpha_S$; θ and θ_S are the deviations in temperature from 20˚C, respectively, of the end gauge and the standard gauge, and $\delta\theta = \theta - \theta_S$.

The arithmetic mean of the readings of the comparator $\bar{d}$ and the actual difference d can be related by the following equation.

$$\bar{d} = d + d_1 + d_2 \tag{5.8}$$

where d_1 and d_2 are quantities describing, respectively, the random and the systematic effects of the comparator. From the above two equations, we obtain

$$l = l_S + \bar{d} - d_1 - d_2 - l_S(\delta\alpha \cdot \theta + \alpha_S \cdot \delta\theta) \tag{5.9}$$

All the expected values, uncertainties and probability distributions of the influence quantities of l are known and given in Table 5.1. For comparing with the classical method, the data given in the example of GUM: 2008 is used. And for simplicity, the degrees of freedom of the Type B uncertainty components are assumed to be infinite.

x_i	Expected/ mean value	$u(x_i)$	Source of uncertainty	Value of standard uncertainty	Probability distribution	$c_i \equiv \partial f / \partial x_i$	Degree of freedom
l_S	50.000623 mm	$u(l_S)$	Monotonic effect	25 nm	Normal	1	∞
$\bar{d}$	215 nm	$u(\bar{d})$	Random effect	5.8 nm	Normal	1	9
d_1	0 nm	$u(d_1)$	Random effect	3.9 nm	Normal	1	∞
d_2	0 nm	$u(d_2)$	Monotonic effect	6.7 nm	Normal	1	∞
α_S	11.5 x10^{-6} $^\circ$C^{-1}	$u(\alpha_S)$	Monotonic effect	1.2x10^{-6} $^\circ$C^{-1}	Rectangular	0	∞
θ	-0.1°C	$u(\theta)$	Non-monotonic effect	0.41°C	Rectangular	0	∞
$\delta\alpha$	0°C^{-1}	$u(\delta\alpha)$	Non-monotonic effect	5.8x10^{-7} $^\circ$C^{-1}	Triangular	$-l_S\theta$	∞
$\delta\theta$	0°C	$u(\delta\theta)$	Non-monotonic effect	0.029°C	Triangular	$-l_S\alpha_S$	∞

Table 5.1 Summary of standard uncertainty components

The values of l_S and α_S are always fixed, since there is only one standard gauge in the measurements. It can be assumed that the systematic error of the comparator, d_2 is fixed during the measurements. $\delta\alpha, \theta$ and $\delta\theta$ are related to systematic effects, but they are not fixed. θ and $\delta\theta$ vary with time; $\delta\alpha$ can be different for different end gauges. So l_S, d_2 and α_S are related to monotonic effects, where α_S is in a nonlinear term, it cannot be moved to the LHS of (5.9) alone. By moving l_S and d_2, we obtain a biased measurand l'.

$$l' = l - l_S + d_2 = \bar{d} - d_1 - l_S(\delta\alpha \cdot \theta + \alpha_S \cdot \delta\theta) \tag{5.10}$$

Since the expected values of d_1, $\delta\alpha$ and $\delta\theta$ are 0, from (5.10), we get

$$E(l') = \bar{d}\,, \tag{5.11}$$

where $E(l')$ is the expected value of l'.

Based on a first-order Taylor series approximation of equation (5.10), the combined standard uncertainty of l' can be evaluation by the following equation (refer to GUM: 2008 for the detail of the evaluation method).

$$\begin{aligned} u_C^2(l') &= u^2(\bar{d}) + u^2(d_1) + (l_S\theta)^2 u(\delta\alpha) + (l_S\alpha_S)^2 u(\delta\theta) \\ &= u^2(\bar{d}) + 299.2\text{nm}^2 \end{aligned} \tag{5.12}$$

Due to the nonlinear of (5.10), the following second-order terms in the Taylor series of (5.10) are significant, which should be added to $u_C^2(l')$.

$$l_S^2 u^2(\delta\alpha) u^2(\theta) + l_S^2 u^2(\alpha_S) u^2(\delta\theta) = 139.8\text{nm}^2 \tag{5.13}$$

So we have

$$u_C^2(l') = u^2(\bar{d}) + 299.2\text{nm}^2 + 139.8\text{nm}^2\,. \tag{5.14}$$

Ten replicate measurements are taken for each end gauge. The values of $\bar{d}$ and $u(\bar{d})$ of the measured gauges are listed as following.

Gauge	$\bar{d}$	$u(\bar{d})$
a	215 nm	5.8 nm
b	91 nm	13.4 nm
c	254 nm	9.3 nm

Table 5.2 Means and standard deviations of the readings of the comparator of the three end gauges

Substitute the data of $\bar{d}$ and $u(\bar{d})$ into (5.11) and (5.14), we obtain the following results.

Gauge	$E(l')$	$u_C(l')$
a	215 nm	22 nm
b	91 nm	25 nm
c	254 nm	23 nm

Table 5.3 Means and combined standard deviations of *l′* of the three end gauges

The result of combined standard uncertainty of gauge *a* (with the same values of all the influence quantity) obtained in GUM: 2008 is $u_C(l) = 34\text{nm}$. Compared to this result, $u_C(l') = 22\text{nm}$ is much smaller.

The effective degree of freedom of $u_C(l')$, $v_{\text{eff}}(l')$ can be obtained from the following Welch-Satterthwaite formula (Welch 1947).

$$v_{\text{eff}}(l') = \frac{u_C^4(y)}{\sum_{i=1}^{n} \frac{u_i^4(y)}{v_i}} = \frac{u_C^4(l')}{\frac{u^4(\bar{d})}{9} + 0 + 0 + 0} = 9\frac{u_C^4(l')}{u^4(\bar{d})} \tag{5.15}$$

The values of $v_{\text{eff}}(l')$ of the three end gauges are all above 100, so the coverage factor can be taken as $k = 2$, providing a coverage probability of approximately 95% (JCGM 100 2008, p 78). The coverage intervals of the three end gauges can be stated as below.

$$J(l')_a = (215 \pm 44)\text{nm}$$
$$J(l')_b = (91 \pm 50)\text{nm}$$
$$J(l')_c = (254 \pm 46)\text{nm}$$

Moreover, the expected values and the standard uncertainties of the upper and lower specification limits (USL & LSL) can be evaluated as following.

$$E(l')_{USL} = E(l - l_S + d_2) = 377\text{nm}$$

$$E(l')_{LSL} = E(l - l_S + d_2) = -623\text{nm}$$

$$u(l')_{USL} = u(l')_{LSL} = (u^2(l_S) + u^2(d_2))^{\frac{1}{2}} = 26\text{nm}$$

Take $k = 2$ as the coverage factor, we have

$$J(l')_{USL} = (377 \pm 52)\text{nm}$$
$$J(l')_{LSL} = (-623 \pm 52)\text{nm}$$

Put the coverage intervals of the three end gauges and the specification limits together. Their relation can be observed from Figure 5.7.

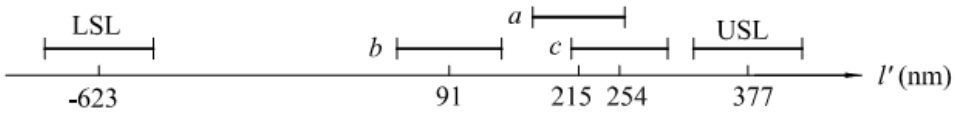


Figure 5.7 The relation of the end gauges and spec. limits (not to scale)

Let p be the limit sample of the LSL, and q be the limit sample of USL. The empirical relation of the end gauges and the limit samples can be stated with interval order as

$$a \wr c,\ p \lhd b \lhd a \lhd q \text{ and } p \lhd b \lhd c \lhd q.$$

The three end gauges are all within the specification.

5.5 Conclusions

In this chapter, a novel strategy of reducing the influence of uncertainty in the evaluation of empirical relations is proposed. Based on the method introduced in Section 4.5, empirical relation is evaluated in terms of interval order by comparing the coverage intervals of the measurement results. This strategy improves the resolution of comparison by reducing the sizes of the coverage intervals to be compared. The measurement uncertainty is classified into random components and systematic components according to GUM (2008). It is demonstrated that the systematic uncertainty components can be further classified into monotonic uncertainty components and non-monotonic components, and the monotonic components can be removed from the measurement uncertainty without affecting the evaluation of empirical relations. The mathematical principle of the strategy is explained, and the steps of implementing the strategy are given in detail. An example is given to demonstrate the application of this strategy.

The strategy proposed in this chapter is designed for estimating the empirical relation of measured objects and determining the conformity with specifications when measurement uncertainty is significant. It provides a method of defining the relation between complete measurement results by taking measurement results as coverage intervals. Moreover, it

allows us to reduce the size of the intervals by ignoring the monotonic uncertainty components, which makes the estimated relation more meaningful without introducing any bias.

This strategy can be quite useful for the following situations: the measurement uncertainty is very significant or too large such that the measurement results are not very meaningful; the specification is given by some standard samples instead of numbers. It is a universal method, and can be applied to many areas of metrology, such as to classify objects into different classes (e.g. A, B, C, D) according to the measurand values.

Chapter 6
An ANOVA Method of Evaluating Specification Uncertainty

6.1 Introduction

Instrinsic uncertainty is an important part of the uncertainty of a measurand. As mentioned in Chapter 4, definitional uncertainty is a common form of intrinsic uncertainty, which is also named as specification uncertainty in ISO 17450-2 (2002). To evaluate the total uncertainty of a measurand accurately, the effect of specification uncertainty should be considered. Hence, it is important to find a proper method of evaulting specification uncertainty.

6.1.1 Specification uncertainty

Specification uncertainty is one of the important uncertainties in the geometrical product specifications and verification system (GPS). It is the uncertainty inherent in a specification when applied to a feature (point/line/plane), which quantifies the ambiguity in the specification (ISO 17450-2 2002). In ISO/TS 17450-2 it is distinguished from measurement uncertainty and defined as the uncertainty that is derived from the incompleteness of the specification.

In industry, most of specifications used in engineering drawings are incomplete. For example, the specification of a shaft, Ø10±0.1 is incomplete, since the association criteria (such as largest two-point diameter, minimum circumscribed cylinder, least square cylinder) is not specified. Due to this incompleteness, the measurement results can be different when the interpretation of the specification varies, even if the measurement uncertainty was zero.

It is important to understand and quantify the effect of the incompleteness of a specification. A specification is designed to achieve some functional requirement. If the interpretation of the specification is largely biased from the original intention of the designer, the functional requirement may not be achieved by the parts controlled by the biased specification. For instance, the difference of the measured values of Ø10±0.1 between two possible interpretations, such as largest two-point diameter and smallest two-point diameter, can be even larger than the tolerance interval (depends on the roundness of the shaft), which means

the measurement results and their conformity (accept or reject) can be totally different when the ambiguity of the specification is too large. Moreover, it is necessary to know how large the ambiguity is, since it is not feasible to make each specification complete. Hence, the ambiguity should be quantified in terms of specification uncertainty, and it should be of the same nature as measurement uncertainty, so that it can be compared with the size of tolerance and the total variation to reveal how large it is. If the specification uncertainty is too large, the specification should be revised to be more complete.

6.1.2 Difficulties of evaluating specification uncertainty

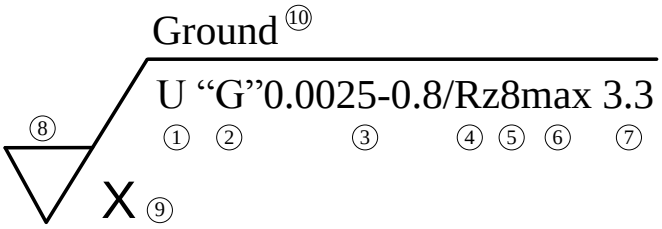
The problem is how to evaluate the specification uncertainty. There is no standard method given in ISO/TS 17450-2 (2002). Only an example is given:

If a specification for a sphere is SØ30±0.1,...The specification uncertainty is derived from the range of values that can be obtained when different association criteria (such as minimum circumscribed sphere, smallest two-point diameter, least squares sphere) are applied to data extracted from an actual workpiece (not perfectly spherical), because the specification does not prescribe which association criterion is to be used.

This implies that specification uncertainty can be evaluated according to the measured values of all the possible interpretations of the (incomplete) specification. One can then, similar to measurement uncertainty, use standard deviation or variance of the measured values to quantify the specification uncertainty. This method is applied in the paper of Lu ((Lu, Jiang, Liu, & Xu, 2008), p.5) to evaluate the specification uncertainty of the diameter of a shaft. However, there is inevitably some measurement uncertainty involved in the measured data, which is also a source of the variance of the measured values. Moreover, the specification uncertainty obtained by this method is relevant to the measured workpiece only. For another workpiece, the evaluated uncertainties can be different. For example, the specification uncertainty of Ø10±0.1 for a shaft with good roundness is small, but for a shaft with poor roundness is much larger. In manufacturing, one normally needs to find out the specification uncertainty with regards to a whole lot of workpieces, thus the variation of the workpieces should also be considered. Therefore, specification uncertainty should be evaluated according to the measured values of a set of workpieces using a measuring equipment base on all the possible interpretations of the specification.

The difficulties of evaluating specification uncertainty consist in (i) listing all the possible interpretations, (ii) removing the effect of measurement uncertainty, and (iii) making it compatible to the variation of workpieces. The method of finding all the possible interpretations is discussed in (Qi *et al* 2013). The aim of this thesis is to propose an easily applicable evaluation method of specification uncertainty, which can solve the second and third difficulties.

6.1.3 Specification of roughness measurement



①Indication of upper (U) or lower (L) specification limit
②Filter type
③Transmission band
④Profile parameter
⑤Evaluation length as the number of sampling length
⑥Comparison rule
⑦Limit value in micrometres
⑧Type of manufacturing process
⑨Surface texture lay
⑩Manufacturing process

Figure 6.1 Control elements in the specification of surface roughness (ISO 1302 2002)

Surface roughness is a good example of the complexity of a complete specification, which shows why specifications are normally incomplete. It is well known that a specification of roughness normally denotes in the form as

$\sqrt{3.0}$ or $\sqrt{\text{Ra } 3.0}$.

But in ISO 1302:2002 (ISO 1302 2002), a complete specification of roughness consists of ten control elements, see figure 6.1. The specifications of roughness given in an engineering drawing are normally incomplete, and it's usually not necessary to specify all the ten control elements. Some of those elements affect the conformity with specification (accept/reject), which are the elements (1), (6) and (7) in figure 6.1; and some of those control the machining process and the appearance of the surface texture, which are (8), (9) and (10), Others, i.e. (2), (3) (4) and (5), affect the measured values. For the measurement of workpieces, only the control elements (2) to (5) could affect the measured values. For the evaluation of

specification uncertainty, all the possible settings of elements (2) to (5) should be considered. This does not imply that the other elements are not important. Actually elements (7) and (8) are compulsory to be specified. When element (1) is not specified, by default, it should be understood as a upper tolerance limit (ISO 1302 2002). 16%-rule is the default setting of element (6) in ISO 1302. And if elements (9), (10) are not specified, it means any surface texture lay and machining process are acceptable.

6.2 Principle of the method

In industry, large amount of parts (workpieces) are manufactured in one batch according to the specifications. The features of these parts are similar, but certainly not the same. Each feature varies among different parts with a certain variation, called *part variation*. This variation can be estimated by the variance of the measured values of some amount (e.g. 32 pieces) of randomly selected samples. But, in the measured values, there are two sources of variations: the variation from different parts and the variation from the measurement error of the measurement system. If the latter is significant, it is not reliable to estimate part variation directly from the variance of measured values. The measurement error of a measurement system can normally arise from two sources: the measuring equipment and the operators or inspector taking the measurement. In measurement system analysis, the variation in measurements caused by the random error of an equipment is named as *repeatability*, and the variation caused by different operators is named as *reproducibility*, they both contribute to the measurement uncertainty (Burdick *et al* 2005). A standardised and commonly used method to study the repeatability and reproducibility is *Gauge R&R* (gauge repeatability & reproducibility). Gauge R&R can be used to distinguish the part variation and the variation from the measurement uncertainty, which is similar to the 2nd difficulty mentioned in Chapter 1, hence the principle of Gauge R&R should be useful for evaluating specification uncertainty.

There are two different statistical approaches to conduct Gauge R&R study. One is called average & range method, the other is *ANOVA* (analysis of variance) *method*. The former is simpler in terms of calculation, but it is not suitable for the situation when some interaction variance (such as the interaction of operators and parts) occurs in the measured values. According to MSA 4th (Down *et al* 2010), the ANOVA-method is preferred; the average & range method should only be used if no PC is available for the calculations.

ANOVA is a statistical tool used to analyse the observed data affected by several *factors*. The observed data varies with each factor, and each factor has different *factor levels*. When the levels of each factor changes, some variance can be observed from the data. ANOVA can be used to partition the observed variance into components attributable to different factors and their interactions (covariances). The processes of conducting ANOVA can be found in the text books of Montgomery (Montgomery 2009). And it can be implemented by statistical software, such as Minitab, SPSS, and Excel.

In Gauge R&R, the parts, the equipment, and the operators are the three factors contribute to the variance of the measured values. To conduct a Gauge R&R study, a set of samples (normally ten or twelve pieces) are randomly selected to be measured by two or three operators with an equipment. Each sample is measured by each operator repetitively two or three times to test the repeatability. So a set of measured values, say 12x3x3, can be obtained. The twelve samples are numbered from 1 to 12, each one corresponding to one factor level of the 'part' factor. Similarly, the three operators are the three levels of the 'operator' factor, and the three repetitive measurements (called trials) are the three levels of the 'equipment' factor. The measured values can be indexed as $d_{i,j,k}$, where *i, j, k* are the indices of the levels of the three factors, and organised in a table (see Table 6.1). With the data (measured values) properly input into the table, the variance of the data can be partitioned into three parts: repeatability, σ_e^2, reproducibility, σ_o^2, and part variation, σ_p^2 by means of ANOVA.

To determine whether the R&R of the measurement system is acceptable, the ratios of R&R to the total variation (%R&R), and to the tolerance (%P/T) are calculated as the following (Burdick *et al* 2005).

$$\%\text{R\&R} = \left(\sqrt{\sigma_e^2 + \sigma_o^2} \Big/ TV\right) \times 100\% \tag{6.1}$$

$$\%\text{P/T} = \left(6 \times \sqrt{\sigma_e^2 + \sigma_o^2} \Big/ \text{tolerance}\right) \times 100\% \tag{6.2}$$

If both ratios are lower than 10%, the measurement system is generally considered to be acceptable. It may be acceptable for some applications, when the ratios are between 10% to 30%. Otherwise, it is considered to be unacceptable (Down *et al* 2010).

Operator	A -			B -			C -		
Sample #	1st Trial	2nd Trial	3rd Trial	1st Trial	2nd Trial	3rd Trial	1st Trial	2nd Trial	3rd Trial
1									
2									
3									
⋮									
12									

Table 6.1 Gauge R&R datasheet

For the situation of evaluating specification uncertainty, as mentioned in the introduction, the data to be analysed should be the measured values of a set of samples corresponding to all the possible interpretations of the specification. So the *part variation* and the *random error of the measuring equipment* are also involved in the total variation of the data. In this evaluation, it is not necessary to consider the effect of different operators, since the data can be collected by a single operator. Instead, another source of variation is contributed by the *different interpretations of the specification*. The effect of different interpretations to the measured values varies from part to part, which is actually similar with the effect of different operators in the sense that both effects are random. So the specification can also be taken as a factor (of the variance of data) with the different interpretations as its factor level. Hence an experiment can be designed similarly with the Gauge R&R study, by replacing the 'operator' factor in Gauge R&R with the 'specification' factor. The sample size of parts and the number of repetitive measurements can be the same as Gauge R&R, which are proved to be enough for statistical inference (Burdick *et al* 2005). And by means of ANOVA, the specification uncertainty can then be partitioned from the total variation of the data. The detail of this evaluation method is discussed in the next chapter.

6.3 A case study in roughness measurement

In this case study, we'll evaluate the specification uncertainty of the following specification on the surface of an iPad metal cover.

$$\sqrt{\text{Ra } 1.2}$$

To demonstrate the evaluation method, assume that the metal cover of the iPad is manufactured according to this specification. The Taylor Hobson PGI (Phase Grating

Interferometer) is used for measuring the roughness in the way of contact stylus measurement.

According to ISO1302:2002, this specification means: the surface to be machined by removing material (e.g. milling); unilateral upper specification limit, maximum roughness average (*Ra*) is 1.2μm. By ISO4288:1998, The default sampling length of *Ra* 1.2 is 0.8mm, the default evaluation length should be five times the sample length (i.e. 4mm), and the cut-off long-wave length shall be chosen equal to the sampling length (ISO 4288 1998). And by ISO3274:1996, the corresponding transmission band shall be 0.0025-0.8mm (ISO 3274 1998). The filter type is not specified, and in ISO 1302:2002, it states that

> 'The standardised filter is the Gaussian filter (ISO 11562). The former standardised filter was the 2RC-filter. In the future, other filter types may be standardised. In the transition period it may be convenient for some companies to indicate the filter type on drawings.'

Hence the Gaussian filter is recommended, but other filter types may also acceptable. According to those ISO standards mentioned above, one can then derive a much more complete specification from the original specification:

$$\sqrt{\text{U0.0025}-0.8/\text{Ra5}\ \ 1.2}$$

To get this derived specification, the inspector needs to have the knowledge and understanding of the four ISO standards, which is actually hard to be guaranteed. There is normally a knowledge gap between the ISO standards and the inspectors. So the ambiguity of an incomplete specification still exists, even if the complete specification can be derived based on some standards.

In this evaluation, it is assumed that the operator has the knowledge of the related standards, and thus the derived specification is obtained. Filter type is the unspecified control element which affects the measured values. There are three options of filter type in the software of PGI: Gaussian, 2CR-PC, and ISO-2CR, which can be taken as the three factor levels of specification. So the specification uncertainty to be evaluated is the variance of the measured values caused by the variation of filter types.

The experiment is designed in the following steps:

1. Mark twelve evenly distributed areas of the size 6x3mm^2 on the surface of the metal cover, and take these areas of surface as twelve samples. The part variation in this case is contributed from the surface inhomogeneity.
2. Set the travelling distance of the stylus of each measurement to be 6mm, and set the transmission band to be 0.0025-0.8mm in the interface of the PGI.
3. Use the PGI to measure the *Ra* of the twelve areas. The measurement of each area shall repeat three times along the same path.
4. For each measurement, set the filter type to be Gaussian, 2CR-PC, and ISO-2CR in sequence to obtain three values of *Ra*.
5. Record and fill the 108 (12x3x3) measured values in Table 6.2.
6. Input the values into the datasheet of SPSS (or some other software), and obtain specification uncertainty from the partitioned variance components (see Table 6.3).

Filters	**Gauss**			**2CR-PC**			**ISO-2CR**		
Sample #	**1st Trial**	**2nd Trial**	**3rd Trial**	**1st Trial**	**2nd Trial**	**3rd Trial**	**1st Trial**	**2nd Trial**	**3rd Trial**
1	0.9621	0.9635	0.9621	0.9627	0.9649	0.9642	0.9732	0.9767	0.9765
2	0.9955	0.9985	1.0015	1.0006	1.0034	1.0058	1.0109	1.0122	1.0146
3	1.0071	1.0092	1.0103	0.9873	0.9897	0.9907	1.0325	1.034	1.035
4	1.0705	1.0717	1.0726	1.0449	1.0456	1.0463	1.0861	1.0873	1.0882
5	1.0373	1.0416	1.0433	1.0404	1.0448	1.047	1.0259	1.0316	1.0358
6	0.9799	0.982	0.9833	0.9856	0.9872	0.9873	1.0032	1.0053	1.0067
7	1.0951	1.0984	1.0998	1.0883	1.0918	1.0934	1.1100	1.1123	1.1126
8	1.0322	1.0336	1.0342	1.0273	1.0296	1.0309	1.0457	1.0480	1.0485
9	1.1127	1.1207	1.1255	1.1202	1.1292	1.135	1.0987	1.1065	1.1115
10	1.0772	1.0816	1.0828	1.0642	1.0687	1.0695	1.0736	1.0777	1.0783
11	1.0441	1.046	1.0463	1.0419	1.0438	1.0443	1.0336	1.035	1.0358
12	1.0611	1.0625	1.0631	1.0468	1.0478	1.0478	1.0386	1.0399	1.0411

Table 6.2 Datasheet of roughness measurements in Ra (μm)

Component	Std. Dev.	Variance	% Contribution
Equipment	0.00278	0.0000077	0.37%
Specification	0.003806	0.0000145	0.70%
Parts	0.043726	0.001912	92.59%
Spec*parts	0.011438	0.0001308	6.33%
Total	0.045443	0.002065	100.00%

Table 6.3 ANOVA results

Table 6.3 shows the results of the variation components contributed from equipment, specification (different filters), different parts, and the interaction of specification and parts in terms of standard deviation, variance, and percentage of contribution in the total variance.

The specification uncertainty is the sum of the variance of specification and covariance of specification and parts. From the results in Table 6.3, it is 0.0001453 in terms of variance, σ_S^2 , and it is 0.012055μm in terms of standard deviation, σ_S . The specification uncertainty can be compared with the total variation and the tolerance by replacing the $\sqrt{\sigma_e^2 + \sigma_o^2}$ in equation (6.1) and (6.2) with σ_S . The results are 26.53% to the total variation, and 6.03% to the tolerance. Compared with the tolerance, it is acceptable, but it is significant and may not be acceptable compared with the total variation.

6.4 Conclusions

In this chapter, an ANOVA method of evaluating specification uncertainty based on the principle of Gauge R&R is proposed. In this method, ANOVA is used to separate specification uncertainty from measurement uncertainty, and the sampling method of Gauge R&R is applied. A case study is given to demonstrate how to use this method to evaluate the specification uncertainty of measuring roughness with PGI (Phase Grating Interferometer) when the filter type is not specified.

This method can be applied not only in roughness measurement but also for any other incomplete specifications. In the case study, the specification has three possible interpretations. In some cases, this number can be higher. For example, if the specification has five control elements, two of them are not specified, and each of the two has five options. Then there are 25 possible interpretations. In this case, the specification uncertainty can still

be calculated in the same ANOVA method, but it will be very time consuming to take so many (12x25x3) measurements to collect the data. Although, it takes fewer measurements to analyse the two control elements separately, it is not correct to combine their uncertainties together to estimate the specification uncertainty, unless they are completely independent.

Chapter 7
A contradiction in the Specifications of Free-form Surface Profiles

7.1 Introduction: the contradiction

Free-form surfaces are the geometrical surface shapes with a gobal complex geometry and have no axes of rotation or other symmetries (Jiang and Whitehouse 2012). A free-form surface profile is the profile that results from the intersection of the real free-form surface by a specified plane.

The specification of a surface profile is defined in ISO 1101 (2005) as a specification of the *form* of a surface profile and its acceptable deviation. The upper and lower specification limits (USL and LSL) are defined as two curves enveloping circles of diameter *t*, the centres of which are situated on the nominal surface profile (see figure 7.1). In the design coordination system (DCS), let l_o, p, q be the functions of the heights of the nominal profile, the LSL and the USL respectively, then $p(x) < l_o(x) < q(x)$ for all $x \in I$, where I is the evaluation interval of the profile. The tolerance zone is the area between p and q. By taking a circular disk with diameter t as the morphological structural element, it can be proved that p and q are respectively the erosion and dilation of l_o. As shown in Figure 7.1, due to the high waviness of the nominal profile, there are sharp valleys on q and sharp peaks on p, and p and q are not equidistance everywhere.

The texture of a surface can be characterised by the *form*, the *waviness*, and the *roughness* of the surface (Anon 2003). The specification of surface profile discussed in this chapter only includes the information of the form and waviness of the surface. For determining the conformity of a surface with a specification of surface profile, only the *form* and the *waviness* of the surface should be measured, the texture in the scale of roughness should be removed from the measurement results by filtering.

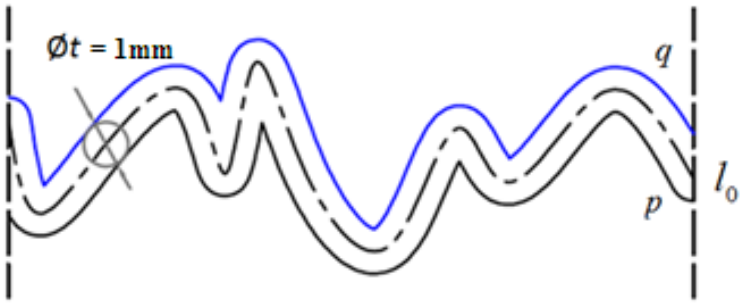


Figure 7.1 The tolerance zone of a free-form surface profile

The measurement methods of the form of free-form surface can be generally classified into two types: contact measurement and non-contact measurement. The non-contact measurement is suitable for areal measurement (3D surface measurement) with higher measuring speed than the contact measurement. However, current optical technologies cannot be scaled small enough to measure deep, nmapping features. The contact measurement with the stylus instruments, such as CMM (coordinate measuring machine), is often used for measuring the surface profile due to its accuracy and traceability. Measurement data of surface profiles can be acquired from the surface either in a point-by-point way (a point each touch) with a touch trigger stylus or continuously (several hundred points per second) with a scanning stylus. Due to the relatively high speed of collecting data points and the ability of measuring complex geometry, the scanning stylus of CMM is quite suitable for measuring the free-form surface profile (Batistic and Stojanovski 2007).

For the specification depicted in Figure 7.1, a default measurement method should be specified in the design stage to avoid the method uncertainty (ISO 17450-2 2002). In Example 3.1, the surface profile is measured by a CMM scanning stylus of a specified size. Assume that this is the specified measurement method. In this method, the surface profile *l* is measured indirectly via the locus of the centre point of the stylus, and the stylus works as a physical dilation filter which transforms *l* to the locus *c*, i.e. $c = D_S(l)$. From the measured locus *c*, the best estimation of the measured surface profile is the real mechanical profile, $\hat{l} = E_S(c) = E_S D_S(l)$. The combination of a dilation operator followed by an erosion operator is a morphological filter called closing (ISO 16610-40 2006), denoted as C_S. Hence we have

$$\hat{l} = C_S(l). \tag{7.1}$$

The measured locus and the estimated profile are in the measurement coordinate system (MCS). To compare an estimated profile with the specification depicted in Figure 7.1, it is essential to arrange them in a common coordinate system. This can be done by a process called localisation, which determines the position and orientation of the design coordinate system (DCS) with respect to the MCS (Li and Gu 2004).

After localisation, a partial order $\precsim$ can be defined between the estimated profile and the specification limits as follows. For any two continuous functions l_1, l_2 in an interval I, $l_1 \precsim l_2$, if and only if $l_1(x) \le l_2(x)$ for all $x \in I$. The conformity of a real surface profile l with the specification is determined by comparing the estimated profile $\hat{l}$ with the specification limits. If $\hat{l}$ is within the tolerance zone, i.e. $p \precsim \hat{l} \precsim q$, l is said to be conformed to the specification.

Consider that if there is a real surface profile l which exactly matches with the USL, i.e. $l = q$, then l is supposed to be marginally within specification. By (7.1) and the extensive property of a closing filter (Serra 1988), we have

$$l \precsim C_S(l) = \hat{l}\,, \tag{7.2}$$

thus the estimated profile is always above the real surface profile. Since $l = q$, (7.2) implies $q \precsim \hat{l}$. That means the measurement result of l can be out of specification. This contradicts with the fact that l is within specification.

The root cause of this contradiction is related with the fact that the measurand (surface profile) is involved in an indirect measurement. Thus the properties of the IPM should be considered.

7.2 The root cause

As an IPM, the mathematical model of the inverse problem involved in the contact measurement is

$$D_S(l) = c\,. \tag{7.3}$$

Thus D_S is the forward mapping. The estimated profile is obtained via an erosion operator E_S, which is a backward mapping. By the properties of morphological filters (Serra 1988),

$$D_S E_S D_S = D_S\,. \tag{7.4}$$

That means E_S is an inner inverse of D_S (see equation (3.33)), which satisfies the desired property P2.

The combination $E_S D_S = C_S$ is *the model resolution* of the inverse problem. As a closing filter, C_S is idempotent ($C_S C_S = C_S$) but not identical ($C_S \neq I$) (ISO 16610-40 2006). Therefore, the estimated profile $\hat{l} = C_S(l)$ is normally not the same as the real surface profile *l*.

The distortion from *l* to $\hat{l}$ is determined by the shape and size of the structuring element of the morphological filter, i.e. the stylus used in the measurement (see Figure 7.2). It can be observed from Figure 7.2 that the distortion is larger when the size of the disk stylus is bigger. According to the catalogue of Renishaw plc (one of the largest global CMM probe suppliers), the diameter of the stylus tips of CMM are commonly in the range of 0.5mm to 12mm, and larger diameter is always recommended for measuring the form of surface to avoid measuring the surface roughness. Hence, for the surface profile with high waviness, such as the profile in Figure 7.1, or the surface profile with sharp valleys, such as the profile (a) in Figure 7.2, the distortion from the real profile to the estimated profile can be significant when the surface profile is measured by a CMM stylus.

The distortion is the effect of the non-identical model resolution. It is not an effect of random error; it is fixed once the measurement method is fixed. Due to the model resolution, the real profile cannot be completely recovered from the measured data. Hence, for an indirect measurement, the model resolution of the IPM is an important property. It determines the capability of recovering the actual measurand.

It should be noticed that a model resolution is mainly determined by the forward mapping of the inverse problem. If the forward mapping *F* is not injective (monic), the inverse solution is not unique, and *F* does not have a left inverse *G* such that $GF = I$. Hence, for any generalised inverse of *F* (inner inverse or quasi-inverse), the model resolution is always not identical when *F* is not injective. Moreover, since the backward mapping is desired to satisfy P2, and thus be a generalised inverse of *F*, the model resolution can always be evaluated using a generalised inverse $F^{\dagger}$ as $F^{\dagger}F$.

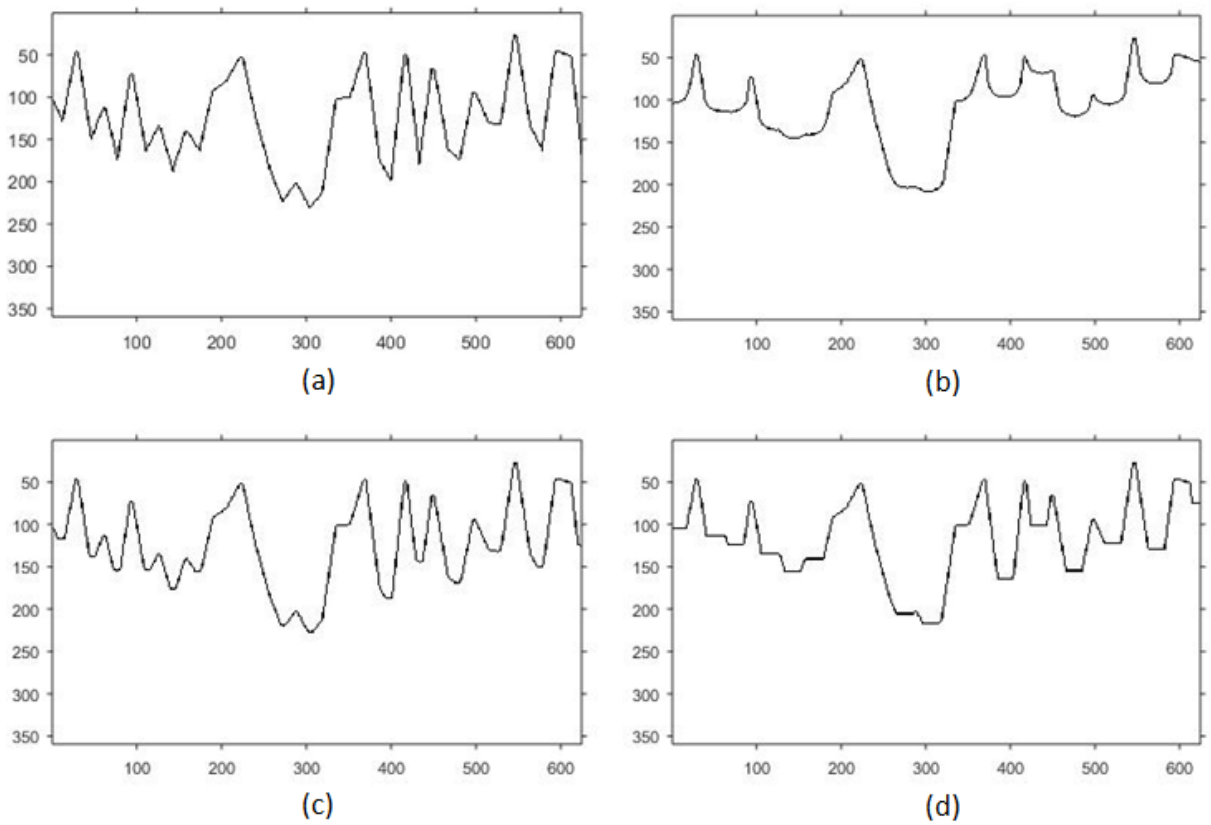


Figure 7.2 Closing filters with different sizes and shapes of structuring elements
(a) the original profile (b) the profile after closing with a 20mm disk
(c) the profile after closing with a 5mm disk (d) the profile after closing with a 20mm horizontal line

For linear inverse problems, the effect of model resolution can be tested with a spike or impulse resolution test, which assesses the recovery of the test model by comparing the corresponding inverse solution (Aster *et al* 2013). A vector which is uniformly zero except a perturbed element is commonly used as a test model, called a spike model.

For example, let matrix **F** be the forward mapping of an inverse problem,

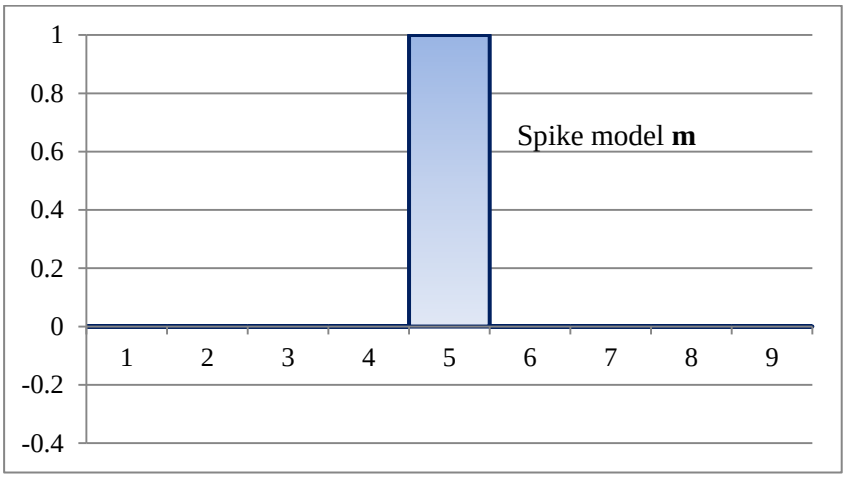
$$\mathbf{F} = \begin{bmatrix} 16 & 94 & 57 & 83 & 61 & 64 & 41 & 98 & 24 \\ 63 & 15 & 36 & 29 & 85 & 48 & 80 & 100 & 44 \\ 21 & 22 & 49 & 53 & 85 & 5 & 16 & 52 & 62 \\ 68 & 57 & 44 & 10 & 55 & 55 & 75 & 66 & 66 \\ 55 & 67 & 93 & 45 & 64 & 34 & 49 & 81 & 65 \\ 78 & 29 & 94 & 30 & 32 & 2 & 42 & 23 & 92 \\ 27 & 52 & 85 & 62 & 8 & 64 & 68 & 67 & 61 \\ 25 & 22 & 10 & 36 & 1 & 55 & 99 & 52 & 6 \end{bmatrix}.$$

Let **m** = [0, 0, 0, 0, 1, 0, 0, 0, 0] be the test (spike) model, the corresponding noise-free data can be predicted as $\mathbf{d}=\mathbf{Fm}$. According to the data **d**, an inverse solution $\hat{\mathbf{m}}$ can be obtained via the Moore-Penrose inverse of **F**,

$$\hat{\mathbf{m}}=\mathbf{F}^{\dagger}\mathbf{d}=\mathbf{F}^{\dagger}\mathbf{Fm}. \tag{7.5}$$

By comparing **m** with $\hat{\mathbf{m}}$, the effect of the model resolution $R_m=\mathbf{F}\mathbf{F}^{\dagger}$ can be observed from Figure 7.3. This effect is sometimes referred as the smoothing effect of model resolution (Aster *et al* 2013).

(a)



(b)

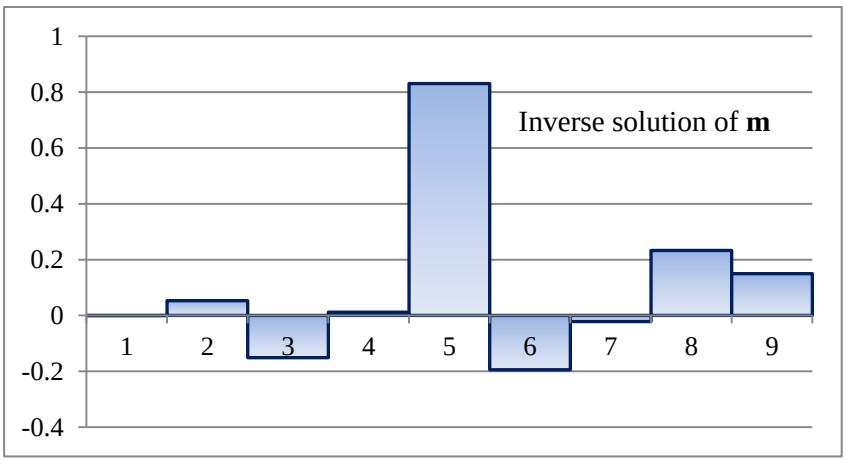


Figure 7.3 The effect of model resolution in a linear inverse problem
(a) the spike model (b) the inverse solution for the spike model without noise

7.3 A desired property of specifications

For an indirect measurement, the model resolution can be predicted according to the mathematical model of the IPM, and the mathematical model can be determined according to

the measurement method. Hence, if there is an expected or default measurement method for the specified measurand, the effect of model resolution on the measurement results can be predicted. Sometimes the expected measurement method for a specification can be found in the related industries standards, or it can be specified in the measurement plan, or directly in the specification. If there are several possible measurement methods, a significant method uncertainty can be caused. Thus a default method should be considered in the design stage, and, if necessary, specified in the measurement plan. With respect to a default measurement method, the effect of model resolution can be predicted, which should be considered at the design stage of the specifications.

It is expected that when the true value of a measurand is in the specification, its measurement result (without measurement error) is also within specification. As demonstrated before, this consistency between measurand value and measurement result can be broken by the effect of model resolution when an IPM is involved in the measurement. To avoid the inconsistency, it should be ensured that if the true value of a measurand x is marginally within specification (i.e. x is equal to a specification limit) the measurement result of x is also within specification. This can be achieved by amending the specification so that the specification limits are immune with the effect of the model resolution. Hence specification limits should be designed to be immune with the effect of the model resolution. This desired property can be formulated into the following statement.

Let p be a specification limit (in terms of a number, vector or function) of a measurand x, if an IPM is involved in the expected measurement method of x, and the model resolution of the IPM is R_m, then p is desired to satisfy

$$R_m(p) = p\,. \tag{7.5}$$

For a specification with USL = q and LSL = p, if p and q are both satisfied with (7.5), then for any object a with its measurand value x_a marginally within specification, i.e. $x_a = p$ or $x_a = q$, we have $R_m(x_a) = x_a$. Thereby, the contradiction described in Section 7.1 can be avoided.

7.4 A correction on the specifications of free-form surface profiles

The problem is how to make sure (7.5) is satisfied. For the measurement of surface profile, since the closing filter C_S is idempotent, if the USL and LSL are in the range of C_S, we have

$C_S(a)=a$, where $a = p$ or q, then (7.5) is satisfied. Therefore, the closing filter can be used to correct the specification limits of surface profiles defined in ISO 1101 (2005). The contradiction can be solved by correcting the USL from q to $C_S(q)$ (see Figure 7.4).

For the LSL p, it can be easily proved that p is the erosion of the nominal profile by a disk of diameter t, denoted as $E_T(l_o)$. By the basic properties of erosion and dilation (Serra 1988), we have $E_S D_S E_S = E_S$, and t is normally bigger than the diameter of the stylus S, so $E_T(l_o)=E_S D_S E_T(l_o)=C_S E_T(l_o)$. That means, $p = C_S(p)$. Hence the LSL is in the range of C_S and does not need to be corrected.

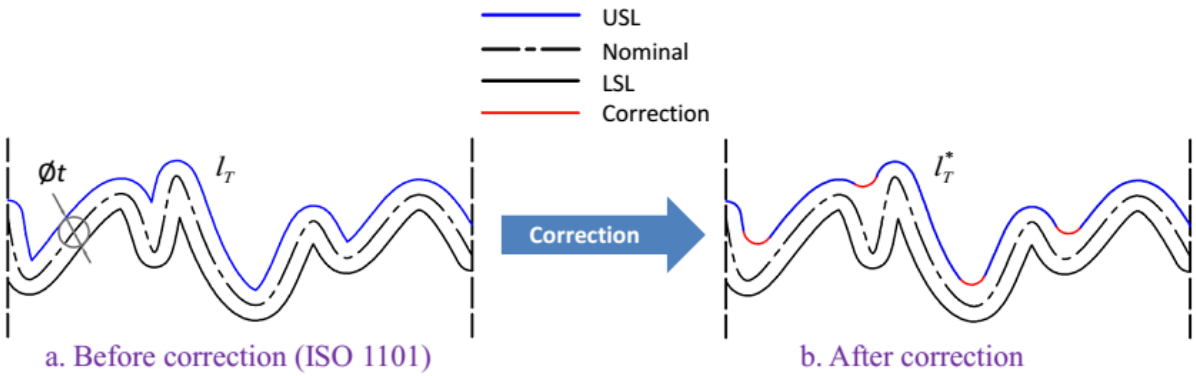


Figure 7.4 A proposed correction on the specification (tolerance zone) of surface profile

This correction can be generalised to all the specifications of measurands that expected to be measured indirectly. For an IPM the backward mapping G is desired to satisfy $FGF = F$, which implies

$$GFGF = GF. \tag{7.6}$$

And since $R_m = GF$, (7.6) implies $R_m R_m = R_m$, thus R_m is idempotent. Similar to the correction of the specification of surface profiles, the USL q and the LSL p of the specifications of indirectly measured quantities can also be corrected as $R_m(p)$ and $R_m(q)$ to avoid the effect of model resolution.

7.5 Conclusions

A contradiction in the specifications of free-form surface profiles is demonstrated in this chapter as an example to show the impact of model resolution on the specifications of the indirectly measured quantities. The contradiction is that if a surface profile exactly matches

the USL of the surface profile, the measurement result can still be out of specification. The contact measurement of surface profiles is treated as an IPM, and the concepts of the IPM are used to explain the root cause of the contradiction. For measurands that are expected to be measured indirectly, a desired property of the specifications is derived according to the model resolution of inverse problems. A correction of the USL of surface profile is proposed to avoid the contradiction, which is generalized for correcting the specifications of indirectly measured quantities.

Chapter 8
Conclusions and Future Work

8.1 Summary of contributions

The main contribution of this research project is the discovery of a general type of inverse problem in metrology with the structural properties related to a Galois connection. This type of inverse problem, named the IPM, is defined in the framework of indirect measurements based on the representational theory of measurement. Some basic structural properties of the IPMs are derived from the desired properties of solving the IPMs, and proved to be closely related to a Galois connection between posets.

The other important contributions associated with the main contribution include:

- The desired properties of solving inverse problems in indirect measurements are listed and investigated in detail.
- Topological stability of the IPMs, in terms of the continuity of a mapping, is defined to generalise the concept of stability in inverse problems for the situation of measurement.
- A probabilistic model of indirect measurements is established, which allows the estimation of empirical relations with probability assigned. The basic methods of estimating empirical relations are introduced.
- A strategy of reducing the effect of measurement uncertainty in the evaluation of empirical relations is developed.
- A method of estimating the specification uncertainty is proposed, which allows the evaluation the intrinsic uncertainty of measurands.
- A contradiction in the specification of free-form surface profile is pointed out, and a correction of the contradiction is proposed.

8.2 Future work

The inverse problem of measurement is a very broad subject. It is impossible to cover all the topics related to this subject in this thesis. The examples and case studies used in this study

are biased in a limited area owing to the author's limited knowledge of inverse problems and mathematical structure. Some interesting topics, which could be investigated further, are revealed in this thesis:

- To test and develop the theory of IPM, more non-linear inverse problems, such as the inverse spectral problem and the inverse scattering problem, should be investigated.
- The condition of a stable indirect measurement is an important topic and more investigation is required.
- Further investigation on the condition of satisfying the desired property P4 (monotonicity of the model resolution *GF*) with some case studies is needed.
- For the methods and strategy of estimating empirical relations, more applications, such as the measurement of surface brightness, can be discussed.
- More specifications of the indirectly measured quantities should be investigated to evaluate the application of the desired property of specification proposed in Chapter 7.

The author hopes that this work can lead to the development of a complete theory of the inverse problem of measurement.

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Appendix A. List of Related Publications

Ding, H., Qi, Q., Scott, P. and Jiang, X. 2015 An ANONA method of evaluating the specification uncertainty in roughness measurement *Laser Metrology and Machine Performance (LAMDAMAP) 2015*

Ding, H., Scott, P. and Jiang, X. 2015 A criterion for comparing measurement results and determining conformity with specifications *Procedia CIRP*

Ding, H., Scott, P. and Jiang, X. 2013 Inverse problems of measurement with application on specification of surface profile *Proceedings of Computing and Engineering Annual Researchers' Conference 2013: CEARC'13* ISBN 9781862181212

Ding, H., Scott, P. J. and Jiang, X. 2013 Relational Structure of Measurement with Application on Specification of Freeform Surface *Proceedings of The 11th International Symposium on Measurement Technology and Intelligent Instruments* ISBN 978-3-86359-138-0

Ding, H. and Scott, P. 2012 Structure of Mathematical Morphology *Proceedings of The Queen's Diamond Jubilee Computing and Engineering Annual Researchers' Conference 2012: CEARC'12* ISBN 978-1-86218-106-9

Qi, Q., Scott, P. J., Jiang, X., Lu, W., & Ding, H. 2013 The Discussion of Uncertainties in Surface Texture during Design , Manufacture and Measurement *Proceedings of The 11th International Symposium on Measurement Technology and Intelligent Instruments* ISBN 978-3-86359-138-0

Appendix B. Selected examples of Programs in Matlab code

The code used in Example 3.9

```
% The following code is used for demonstrating the existence of the Occam's solution of a bounded value linear inverse problem by finding the feasible region of a linear programming problem.%

clear; clc;
% Inputs
n=5;
u=5;
l=0;
c=ones(n,1)*(1/n);
ub=u*ones(n,1);
lb=l*ones(n,1);
ax=(1:n);
% The forward mapping is a 3x5 matrix.
F=round(rand(n-2,n)*100);
NA=null(F);
v=NA(:,1);
p=NA(:,2);
mtrue=rand(n,1)*0.6*(u-l)+ones(n,1)*l+(u-l)*0.2;
d=F*mtrue;
minv=pinv(F)*d;
% plot the true model and its minimum norm solution
figure(1)
plot(ax,ub,'g--',ax,lb,'g--');
hold all;
Lmtrue = plot(ax,mtrue,'k-');
Lminv = plot(ax,minv,'b--');
legend([Lmtrue,Lminv],'true model','estimated model');
axis([1 n l-0.5 u+1.3]);
hold off;
% draw the line corresponding to the upper limit
for i=1:n
    A=v(i);
    B=p(i);
    C=u-minv(i);
```

```
    if  B==0;
        a1u=linspace(-C/A,-C/A,100);
        b1u=linspace(-abs(A)-abs(B)-abs(C),abs(A)+abs(B)+abs(C),100);
    else
        a1u=(-10:0.1:10);
        b1u=(-A.*a1u+C)./B;
    end
% draw the line corresponding to the lower limit
    A=v(i);
    B=p(i);
    C=l-minv(i);
    if  B==0;
        a1l=linspace(-C/A,-C/A,100);
        b1l=linspace(-abs(A)-abs(B)-abs(C),abs(A)+abs(B)+abs(C),100);
    else
        a1l=(-10:0.1:10);
        b1l=(-A.*a1l+C)./B;
    end
    disp(['ploting the ',num2str(i),'th constraint']);
    pause;
    figure(2)
    plot(a1u,b1u,'r-');
    hold all;
    plot(a1l,b1l,'b-');
end
```

The code used in Example 3.10

File name: bvos.m

```
% This is a algorithm for finding the bounded Occam's solutions of a linear
IPM.
% The objective function is
% min c'm, subject to Fm=d, l<=m<=u,
% which is converted to a linear programming problem,
% min/max f(z), subject to lb<= g(z) <=ub,
% where z is a vector of design variables.
% Input the size of matrix F (m by n, m<n),
% upper bound u, and lower bound l of the measurand.

function bvos(m,n,u,l)
```

```
% Let the measurand value be the average of the elements in vector m.
c=ones(n,1)*(1/n);

% Define the vectors of upper bound and lower bound.
ub=u*ones(n,1);
lb=l*ones(n,1);
% Randomly generate a matrix F of the size m-by-n, or specify a matrix F.
F=abs(round(rand(m,n)*100));
% Make sure m<n.
if m>=n
    disp(['Error:m must be smaller than n, since F must be
underdetermined.']);
    return;
end
% Create a true model as a smooth function
tmax=n*1.2;
tmin=0.01;
t=linspace(tmin,tmax,n);
cin=cintrue(t);
mtrue=(u-l)*cin'+lb;
% Calculate the generalized inverse solution using the noise-free data.
d=F*mtrue;
minv=pinv(F)*d;
% Evaluate the measurand value of the true model.
mv=c'*mtrue;
% Plot the true model and its generalized inverse solution
ax=(1:n);
figure(1)
plot(ax,ub,'g--',ax,lb,'g--');
hold all;
Lmtrue = plot(ax,mtrue,'k-');
Lminv = plot(ax,minv,'b--');
axis([1 n l-1 u+1.3]);
hold off;
legend([Lmtrue,Lminv],'true model','estimated model');
% Find out the basis vectors of the null space of F.
NA=null(F);
% Set the matrix A and the vector b to transfer the IPM to a linear
programming problem.
 A=[NA;-NA];
```

```
b=[ub-minv;minv-lb];
% Set a vector f for the objective function of linear programming
f=c'*NA;
% Solve the linear programming problem:
% min f'z, subject to Az <= b
disp(['to evaluate the min solution']);
[z0,~,exitflag] = linprog(f,A,b,[],[]);
% Obtain the minimum solution of the IPM.
mmin=minv+NA*z0;
mv0=c'*mmin;
disp(['the code of exitflag is ',num2str(exitflag)]);
% Solve the linear programming problem:
% min -f'z, subject to Az <= b
disp(['to evaluate the min solution']);
[z1,~,exitflag] = linprog(-f,A,b,[],[]);
% Obtain the maximum solution of the IPM.
mmax=minv+NA*z1;
mv1=c'*mmax;
disp(['the code of exitflag is ',num2str(exitflag)]);
% plot the minimum solution
figure(2)
plot(ax,ub,'g--',ax,lb,'g--');
hold all;
Lmmin = plot(ax,mmin,'b-');
Lmtrue = plot(ax,mtrue,'k--');
axis([1 n l-1 u+1.3]);
legend([Lmmin,Lmtrue],'minimum solution','true model');
hold off;
% Plot the maximum solution
figure(3)
plot(ax,ub,'g--',ax,lb,'g--');
hold all;
Lmmax = plot(ax,mmax,'r-');
Lmtrue = plot(ax,mtrue,'k--');
axis([1 n l-1 u+1.3]);
legend([Lmmax,Lmtrue],'maximum solution','true model');
hold off;
% Display the results of measurand values
disp(['the true measurand value is ',num2str(mv)]);
disp(['the minimum measurand value is ',num2str(mv0)]);
disp(['the maximum measurand value is ',num2str(mv1)]);
```

```
% verify the solutions
e1=norm(F*mmax-d);
e2=norm(F*mmin-d);
disp(['the error from the max solution is ',num2str(e1)]);
disp(['the error from the min solution is ',num2str(e2)]);
```

File name: cintrue.m

```
% This function is used in the bvos algorithm to generate a true model
mtrue.
% Modified from a code given in (Aster et al 2013).%
function cin=cintrue(t)
nt=size(t,2);
off=zeros(3,1);
m=off;
d=off;
% the peak times
off(1)=round(nt/3);
off(2)=round(nt*3/4);
% the peak heights
m(1)=0.8;
m(2)=0.5;
% the peak variances
d(1)=round(nt/14);
d(2)=round(nt/10);
% compute the sum of the described normal curves
cin=zeros(1,nt);
for i=1:2
    cin=cin+m(i)*exp(-(t-off(i)).^2/(2*d(i)^2));
end
```

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