Chapter 6

Inverse problems and mapping inversion

6.1 Introduction

The concepts of "inverse problem" and "mapping inversion" are often used interchangeably in the machine learning literature, although they denote different things. The aim of this chapter is: to introduce the area of (Bayesian) inverse problem theory; to compare it with general Bayesian analysis and in particular with latent variable models; and to differentiate it from the problems of mapping inversion and mapping approximation.

Section 6.2 defines inverse problem theory, explains the reasons for non-uniqueness of the solution and reviews Bayesian inverse problem theory, including the topics of the choice of prior distributions, stability and regularisation. It also describes several examples of inverse problems in some detail to clarify the theory and its interpretation. Section 6.3 compares Bayesian inverse problem theory with general Bayesian analysis and in particular with latent variable models. Section 6.4 defines (statistical) mapping inversion, mapping approximation and universal mapping approximators.

6.2 Inverse problem theory

6.2.1 Introduction and definitions

Inverse calculations involve making inferences about models of physical systems from data[1]. The scientific procedure to study a physical system can be divided into three parts:

1. *Parameterisation of the system*: discovery of a minimal set of model parameters[2] whose values completely characterise the system.

2. *Forward modelling*: discovery of the physical laws allowing, for given values of the parameters, predictions of some observable or data parameters to be made.

3. *Inverse modelling*: use of actual measurements of the observed parameters to infer the values of the model parameters. This inference problem is termed the **inverse problem**.

The model parameters conform the model space $\mathcal{M}$, the observable parameters conform the data space $\mathcal{D}$ and the union of both parameter sets conforms the parameter space $\mathcal{X} = \mathcal{D} \times \mathcal{M}$. See section 6.2.3.1 for a further interpretation of the model parameters.

Usually the forward problem is a well-defined single-valued relationship (i.e., a function in the mathematical sense) so that given the values of the model parameters the values of the measured parameters are uniquely

[1] Tarantola (1987) claims that inverse problem theory in the wide sense has been developed by people working with geophysical data, because geophysicists try to understand the Earth's interior but can only use data collected at the Earth's surface. However, inverse problems appear in many other areas of physics and engineering, some of which are briefly reviewed in section 6.2.4.

[2] The term *parameters* is used in inverse problem theory to mean both the variables and the parameters of a model, as these terms are usually understood in machine learning. Throughout this chapter, we will keep the notation and naming convention which is standard in inverse problem theory. In section 6.3 we discuss the point of view of probabilistic models.

identified. This is often due to causality in the physical system. But often this forward mapping is many-to-one, so that the inverse problem is one-to-many: given values of the observed parameters, there is more than one model (possibly an infinite number) that corresponds to them.

Thus, if $\mathbf{g} : \mathcal{M} \to \mathcal{D}$ is the forward mapping, then $\mathbf{d} = \mathbf{g}(\mathbf{m})$ is unique given $\mathbf{m}$, but its inverse $\mathbf{g}^{-1}(\mathbf{d})$ can take several values for some observed $\mathbf{d} \in \mathcal{D}$.

The example in section 6.2.4.1 illustrates this abstract formulation.

6.2.1.1 Types of inverse problems

Inverse problems can be classified as:

Continuous Most inverse problems are of this type. The model to be estimated is a continuous function in several variables. For example, the mass density distribution inside the Earth as a function of the space coordinates.

Discrete There is a finite (actually numerable) number of model parameters to be estimated. Sometimes the problem itself is discrete in nature, e.g. the location of the epicentre in the example 6.2.4.1, which is parameterised by the epicentre coordinates X and Y. But most times, the problem was originally continuous and was discretised for computational reasons. For example, one can express the mass density distribution inside the Earth as a parameterised function in spherical coordinates (perhaps obtained as the truncation of an infinite parameterised series) or as a discrete grid (if the sampling length is small enough).

In this chapter we deal only with discrete inverse problems. Tarantola (1987) discusses both discrete and continuous inverse problems.

6.2.1.2 Why the nonuniqueness?

Nonuniqueness arises for several reasons:

- Intrinsic lack of data: for example, consider the problem of estimating the density distribution of matter inside the Earth from knowledge of the gravitational field at its surface. Gauss' theorem shows that there are infinitely many different distributions of matter density that give rise to identical exterior gravitational fields. In this case, it is necessary to have additional information (such as a priori assumptions on the density distribution) or additional data (such as seismic observations).
- Uncertainty of knowledge: the observed values always have experimental uncertainty and the physical theories of the forward problem are always approximations of the reality.
- Finiteness of observed data: continuous inverse problems have an infinite number of degrees of freedom. However, in a realistic experiment the amount of data is finite and therefore the problem is underdetermined.

6.2.1.3 Stability and ill-posedness of inverse problems

In the Hadamard sense, a well-posed problem must satisfy certain conditions of existence, uniqueness and continuity. Ill-posed problems can be numerically unstable, i.e., sensitive to small errors in the data (arbitrarily small changes in the data may lead to arbitrarily large changes in the solution).

Nonlinearity has been shown to be a source of ill-posedness (Snieder and Trampert, 1999), but linearised inverse problems can often be ill-posed too due to the fact that realistic data is finite. Therefore, inverse problems in general might not have a solution in the strict sense, or if there is a solution, it might not be unique or might not depend continuously on the data. To cope with this problem, stabilising procedures such as regularisation methods are often used (Tikhonov and Arsenin, 1977; Engl et al., 1996). Bayesian inversion is, in principle, always well-posed (see section 6.2.3.5). Mapping inversion (section 6.4) is also a numerically unstable problem but, again, probabilistic methods such as the one we develop in chapter 7 are well-posed.

6.2.2 Non-probabilistic inverse problem theory

For some inverse problems, such as the reconstruction of the mass density of a one-dimensional string from measurements of all eigenfrequencies of vibration of the string, an exact theory for inversion is available (Snieder and Trampert, 1999). Although these exact nonlinear inversion techniques are mathematically elegant, they are of limited applicability because:

- They are only applicable to idealistic situations which usually do not hold in practice. That is, the physical models for which an exact inversion method exists are only crude approximations of reality.
- They are numerically unstable.
- The discretisation of the problem caused by the fact that the data are only available in a finite amount makes the problem underdetermined.

Non-probabilistic inversion methods attempt to invert the mathematical equation of the forward mapping (for example, solving a linear system of equations by using the pseudoinverse). These methods cannot deal with data uncertainty and redundancy in a natural way, and we do not deal with such methods here. A more general formulation of inverse problems is obtained using probability theory.

6.2.3 Bayesian inverse problem theory

The standard reference for the Bayesian view of (geophysical) inversion is Tarantola (1987), whose notation we use in this section; the standard reference for the frequentist inverse theory is Parker (1994); other references are Scales and Smith (1998) and Snieder and Trampert (1999).

In the Bayesian approach to inverse problems, we use physical information about the problem, plus possibly uninformative prior distributions, to construct the following two models:

- A joint prior distribution $\rho(\mathbf{d}, \mathbf{m})$ in the parameter space $\mathcal{X} = \mathcal{D} \times \mathcal{M}$. This prior distribution is usually factorised as $\rho_{\mathcal{D}}(\mathbf{d})\rho_{\mathcal{M}}(\mathbf{m})$, because by definition the a priori information on the model parameters is independent of the observations. However, it may happen that part of this prior information was obtained from a preliminary analysis of the observations, in which case $\rho(\mathbf{d}, \mathbf{m})$ might not be factorisable. If no prior information is available, then an uninformative prior may be used (see section 6.2.3.2).
- Using information obtained from physical theories we solve the forward problem, deriving a deterministic forward mapping $\mathbf{d} = \mathbf{g}(\mathbf{m})$. If a noise model f (typically normal) is applied, a conditional distribution $\theta(\mathbf{d}|\mathbf{m}) = f(\mathbf{d} - \mathbf{g}(\mathbf{m}))$ may be derived. For greater generality, the information about the resolution of the forward problem is described by a joint density function $\theta(\mathbf{d}, \mathbf{m})$. However, usually $\theta(\mathbf{d}, \mathbf{m}) = \theta(\mathbf{d}|\mathbf{m})\mu_{\mathcal{M}}(\mathbf{m})$, where $\mu_{\mathcal{M}}(\mathbf{m})$ describes the state of null information on model parameters.

Tarantola (1987) postulates that the a posteriori state of information is given by the *conjunction* of the two states of information: the prior distribution on the $\mathcal{D} \times \mathcal{M}$ space and the information about the physical correlations between $\mathbf{d}$ and $\mathbf{m}$. The conjunction is defined as

$$\sigma(\mathbf{d}, \mathbf{m}) \stackrel{\text{def}}{=} \frac{\rho(\mathbf{d}, \mathbf{m})\theta(\mathbf{d}, \mathbf{m})}{\mu(\mathbf{d}, \mathbf{m})} \tag{6.1}$$

where $\mu(\mathbf{d}, \mathbf{m})$ is a distribution representing the state of null information (section 6.2.3.2). Thus, all available information is assimilated into the posterior distribution of the model given the observed data, computed by marginalising the "joint posterior distribution" σ (assuming factorised priors $\rho(\mathbf{d}, \mathbf{m})$ and $\mu(\mathbf{d}, \mathbf{m})$):

$$\sigma_{\mathcal{M}}(\mathbf{m}) = \int_{\mathcal{D}} \sigma(\mathbf{d}, \mathbf{m})\, d\mathbf{d} = \rho_{\mathcal{M}}(\mathbf{m})L(\mathbf{m}) \tag{6.2}$$

where the likelihood function L, which measures the data fit, is defined as:

$$L(\mathbf{m}) \stackrel{\text{def}}{=} \int_{\mathcal{D}} \frac{\rho_{\mathcal{D}}(\mathbf{d})\theta(\mathbf{d}|\mathbf{m})}{\mu_{\mathcal{D}}(\mathbf{d})}\, d\mathbf{d}.$$

Thus, the "solution" of the Bayesian inversion method is the posterior distribution $\sigma_{\mathcal{M}}(\mathbf{m})$, which is unique (although it may be multimodal and even not normalisable, depending on the problem). Usually a maximum a posteriori (MAP) approach is adopted, so that we take the model maximising the posterior probability σ: $\mathbf{m}_{\text{MAP}} \stackrel{\text{def}}{=} \max_{\mathbf{m}\in\mathcal{M}} \sigma_{\mathcal{M}}(\mathbf{m})$.

Likewise, the posterior distribution in the data space is calculated as

$$\sigma_{\mathcal{D}}(\mathbf{d}) = \int_{\mathcal{M}} \sigma(\mathbf{d}, \mathbf{m})\, d\mathbf{m} = \frac{\rho_{\mathcal{D}}(\mathbf{d})}{\mu_{\mathcal{D}}(\mathbf{d})} \int_{\mathcal{M}} \theta(\mathbf{d}|\mathbf{m})\rho_{\mathcal{M}}(\mathbf{m})\, d\mathbf{m}$$

which allows to estimate posterior values of the data parameters (*recalculated data*).

In practice, all uncertainties are described by stationary Gaussian distributions:

- likelihood $L(\mathbf{m}) \sim \mathcal{N}(\mathbf{g}(\mathbf{m}), \mathbf{C}_\mathcal{D})$
- prior $\rho_\mathcal{M}(\mathbf{m}) \sim \mathcal{N}(\mathbf{m}_{\text{prior}}, \mathbf{C}_\mathcal{M})$.

A more straightforward approach that still encapsulates all the relevant features (uninformative priors and an uncertain forward problem) is simply to obtain the posterior distribution of the model given the observed data as

$$p(\mathbf{m}|\mathbf{d}) = \frac{p(\mathbf{d}|\mathbf{m})p(\mathbf{m})}{p(\mathbf{d})} \propto p(\mathbf{d}|\mathbf{m})p(\mathbf{m}). \tag{6.3}$$

This equation should be more familiar to statistical learning researchers.

6.2.3.1 Interpretation of the model parameters

Although the treatment of section 6.2.3 is perfectly general, it is convenient to classify the model parameters into one of two types:

- Parameters that describe the *configuration* or *state* of the physical system and completely characterise it. In this case, they could be called *state variables* as in dynamical system theory. We represent them as a vector $\mathbf{s}$. Examples of such parameters are the location of the epicentre in example 6.2.4.1 or the absorption coefficient distribution of a medium in CAT (example 6.2.4.3). These parameters are independent, in principle, of any measurements taken of the system (such as a particular projection in CAT or a measurement of the arrival time of the seismic wave in example 6.2.4.1).
- Parameters that describe the *experimental conditions* in which a particular measurement of the system was taken. Thus, for each measurement $\mathbf{d}_n$ we have a vector $\mathbf{c}_n$ indicating the conditions in which it was taken. For example, in 2D CAT (example 6.2.4.3) one measurement is obtained from a given X-ray source at plane coordinates x, y and at an angle θ; thus $\mathbf{c}_n = (x_n, y_n, \theta_n)$ and the measurement $\mathbf{d}_n$ is the transmittance. In example 6.2.4.1, one measurement is taken at the location (x_n, y_n) of station n; and so on. If there are N measurements, then the model parameters are $\{\mathbf{c}_n\}_{n=1}^N$ (in addition to the $\mathbf{s}$ model parameters) and one can postulate prior distributions for them to indicate uncertainties in their determination. However, usually one assumes that there is no uncertainty involved in the conditions of the measurement and takes these distributions as Dirac deltas. Of course, the measured value $\mathbf{d}_n$ can still have a proper distribution reflecting uncertainty in the actual measurement. In this way, the estimation problem is simplified, because all $\{\mathbf{c}_n\}_{n=1}^N$ model parameters are considered constant, and only the $\mathbf{s}$ model parameters are estimated.

From a Bayesian standpoint, there is no formal difference between both kinds of model parameters, state $\mathbf{s}$ and experimental conditions $\mathbf{c}$—or between model parameters $\mathbf{m}$ and data parameters $\mathbf{d}$, for that matter—because probability distributions are considered for all variables and parameters of the problem.

Thus, if there are N measurements, the forward mapping is $\mathbf{d} = \mathbf{g}(\mathbf{m})$ with $\mathbf{d} = (\mathbf{d}_1, \ldots, \mathbf{d}_N)$ and $\mathbf{m}$ including both kinds of parameters (state variables and experimental conditions): $\mathbf{m} = (\mathbf{s}, \mathbf{c}_1, \ldots, \mathbf{c}_N)$. Usually the measurements are taken independently, so that

$$\rho_\mathcal{D}(\mathbf{d}) = \prod_{n=1}^N \rho_{\mathcal{D},n}(\mathbf{d}_n) \qquad \mu_\mathcal{D}(\mathbf{d}) = \prod_{n=1}^N \mu_{\mathcal{D},n}(\mathbf{d}_n)$$

and the forward mapping decomposes into N equations $\mathbf{d}_n = \mathbf{g}_n(\mathbf{s}, \mathbf{c}_n)$. Thus $\theta(\mathbf{d}|\mathbf{m}) = \prod_{n=1}^N \theta_n(\mathbf{d}_n|\mathbf{s}, \mathbf{c}_n) = \prod_{n=1}^N f(\mathbf{d}_n - \mathbf{g}_n(\mathbf{s}, \mathbf{c}_n))$ and the likelihood function factorises as $L(\mathbf{m}) = \prod_{n=1}^N L_n(\mathbf{m})$ with

$$L_n(\mathbf{m}) \stackrel{\text{def}}{=} \int_{\mathcal{D}_n} \frac{\rho_{\mathcal{D},n}(\mathbf{d}_n)\theta_n(\mathbf{d}_n|\mathbf{m}, \mathbf{c}_n)}{\mu_{\mathcal{D},n}(\mathbf{d}_n)}\, d\mathbf{d}_n.$$

6.2.3.2 Choice of prior distributions

The controversial matter in the Bayesian approach is, of course, the construction of prior distributions. Usual ways to do this are (Jaynes, 1968; Kass and Wasserman, 1996):

- Define a measure of information, such as the entropy, and determine the distribution that optimises it (e.g. maximum entropy).

- Define properties that the noninformative prior should have, such as invariance to certain transformations (Jeffreys' prior). For example, for a given definition of the physical parameters $\mathbf{x}$, it is possible to find a unique density function $\mu(\mathbf{x})$ which is form invariant under the transformation groups which leave the fundamental equations of physics invariant.

- The previous choices, usually called "objective" or "noninformative," are constructed by some formal rule, but it is also possible to use priors based on subjective knowledge.

In any case, the null information distributions are obtained in each particular case, depending on the coordinate systems involved, etc. However, the choice of a noninformative distribution for a continuous, multidimensional space remains a delicate problem. Bernardo and Smith (1994, pp. 357–367) discuss this issue.

6.2.3.3 Bayesian linear inversion theory

Assuming that all uncertainties are Gaussian, if the forward operator is linear, then the posterior distribution σ will also be Gaussian. This is equivalent to factor analysis, which is a latent variable model where the prior distribution in latent space is Gaussian, the mapping from latent onto data space is linear and the noise model in data space is Gaussian.

Linear inversion theory is well developed and involves standard linear algebra techniques: pseudoinverse, singular value decomposition and (weighted) least squares problems. Tarantola (1987) gives a detailed exposition.

6.2.3.4 Bayesian nonlinear inversion theory

Almost all work in nonlinear inversion theory, particularly in geophysics, is based on linearising the problem using physical information. Usual linearisation techniques include the Born approximation (also called the single-scattering approximation), Fermat's principle and Rayleigh's principle (Snieder and Trampert, 1999).

6.2.3.5 Stability

In the Bayesian approach to inverse problems, it is not necessary in principle to invert any operators to construct the solution to the inverse problem, i.e., the posterior probability σ. Thus, from the Bayesian point of view, no inverse problem is ill-posed (Gouveia and Scales, 1998).

6.2.3.6 Confidence sets

Once a MAP model has been selected from the posterior distribution σ, confidence sets or other measures of resolution can be extracted from $\sigma(\mathbf{m}_{\mathrm{MAP}})$. Due to the mathematical complexity of this posterior distribution, only approximate techniques are possible, including the following ones:

- The forward operator $\mathbf{g}$ is linearised about the selected model $\mathbf{m}_{\mathrm{MAP}}$, so that the posterior becomes normal: $\sigma(\mathbf{m}) \sim \mathcal{N}(\mathbf{m}_{\mathrm{MAP}}, \mathbf{C}'_{\mathcal{M}})$. The posterior covariance matrix $\mathbf{C}'_{\mathcal{M}}$ is obtained as $\mathbf{C}'_{\mathcal{M}} = (\mathbf{G}^T \mathbf{C}_{\mathcal{D}}^{-1} \mathbf{G} + \mathbf{C}_{\mathcal{M}}^{-1})^{-1}$, where $\mathbf{G}$ is the derivative[3] of $\mathbf{g}$ with respect to the model parameters evaluated at $\mathbf{m}_{\mathrm{MAP}}$. This has the same form as the posterior covariance matrix in latent space of a factor analysis, as in eq. (2.59), where $\mathbf{G}$ would be the factor loadings matrix $\mathbf{\Lambda}$.

- Sampling the posterior distribution with Markov chain Monte Carlo methods (Mosegaard and Tarantola, 1995).

6.2.3.7 Occam's inversion

In Occam's inversion (Constable et al., 1987), the goal is to construct the smoothest model consistent with the data. This is not to say that one believes a priori that models are really smooth, but rather that a more conservative interpretation of the data should be made by eliminating features of the model that are not required to fit the data. To this effect, they define two measures:

[3]The linearised mapping $\mathbf{g}(\mathbf{m}_{\mathrm{MAP}}) + \mathbf{G}(\mathbf{m} - \mathbf{m}_{\mathrm{MAP}})$ is usually called Fréchet derivative in inverse problem theory, and is the linear mapping tangent to $\mathbf{g}$ at $\mathbf{m}_{\mathrm{MAP}}$.

- A measure of data fit (irrespective of any Bayesian interpretation of the models):

$$d(\mathbf{m},\mathbf{d}) \stackrel{\text{def}}{=} (\mathbf{g}(\mathbf{m})-\mathbf{d})^T\mathbf{C}_{\mathcal{D}}^{-1}(\mathbf{g}(\mathbf{m})-\mathbf{d}),$$

  that is, the Mahalanobis distance between $\mathbf{g}(\mathbf{m})$ and $\mathbf{d}$ with matrix $\mathbf{C}_{\mathcal{D}}^{-1}$.

- A measure of model smoothness: $\|\mathbf{Rm}\|$, where $\mathbf{R}$ is a Tikhonov roughening operator (Tikhonov and Arsenin, 1977), e.g. a discrete second-difference operator, such as

$$\mathbf{R} = \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & -2 \end{pmatrix}. \tag{6.4}$$

Then, Occam's inversion finds a model being both smooth and fitting well the data by solving the optimisation problem:

$$\min_{\mathbf{m}\in\mathcal{M}} \|\mathbf{Rm}\| \text{ subject to } d(\mathbf{m},\mathbf{d}) \le \epsilon$$

for some tolerance ϵ. Practically, due to the distance d being a quadratic form, this can be conveniently implemented as a weighted least-squares problem with a Lagrange multiplier to control the tradeoff between model smoothness and data fit: for fixed λ, solve the weighted, regularised least-squares problem

$$\min_{\mathbf{m}\in\mathcal{M}} (\mathbf{g}(\mathbf{m})-\mathbf{d})^T\mathbf{C}_{\mathcal{D}}^{-1}(\mathbf{g}(\mathbf{m})-\mathbf{d}) + \lambda(\mathbf{m}-\mathbf{m}_{\text{prior}})^T\mathbf{R}^T\mathbf{R}(\mathbf{m}-\mathbf{m}_{\text{prior}}). \tag{6.5}$$

Then, increase λ until $(\mathbf{g}(\mathbf{m})-\mathbf{d})^T\mathbf{C}_{\mathcal{D}}^{-1}(\mathbf{g}(\mathbf{m})-\mathbf{d}) > \epsilon$.

Clearly, Occam's inversion is a particular case of Bayesian inversion, in which the uncertainty distributions are taken as Gaussians (with the appropriate covariance matrix) and the prior distribution over the models is used as a smoothness regularisation term by taking $\mathbf{C}_{\mathcal{M}}^{-1} = \lambda\mathbf{R}^T\mathbf{R}$. However, Bayesian inversion is more general than Occam's inversion in that the prior distributions allow to introduce physical knowledge into the problem. Gouveia and Scales (1997) compare Bayes' and Occam's inversion in a seismic data problem.

6.2.3.8 Locally independent inverse problems

In the general statement of inverse problems, the data parameters $\mathbf{d}$ depend on all the model parameters $\mathbf{m}$ which in turn are a continuous function of some independent variables, such as the spatial coordinates $\mathbf{x}$. Thus $\mathbf{m} = \mathbf{m}(\mathbf{x})$ and $\mathbf{d} = \mathbf{g}(\mathbf{m})$. A single datum parameter depends on the whole function $\mathbf{m}(\cdot)$, even if that datum was measured at point $\mathbf{x}$ only.

Sometimes we can assume locally independent problems, so that a datum measured at point $\mathbf{x}$ depends only on the value of $\mathbf{m}(\mathbf{x})$, not on the whole function $\mathbf{m}$ for all $\mathbf{x}$. If we have N measurements $\{\mathbf{d}_n\}_{n=1}^N$ at points $\{\mathbf{x}_n\}_{n=1}^N$ and we discretise the problem, so that we have one model parameter $\mathbf{m}_n$ at point $\mathbf{x}_n$, for $n = 1,\dots,N$, then:

$$\theta(\mathbf{d}|\mathbf{m}) = \prod_{n=1}^N \vartheta(\mathbf{d}_n|\mathbf{m}_n) \Longrightarrow \theta(\mathbf{d},\mathbf{m}) \propto \rho_{\mathcal{M}}(\mathbf{m}) \prod_{n=1}^N \vartheta(\mathbf{d}_n|\mathbf{m}_n) \tag{6.6}$$

where the distribution ϑ is the same for all parameters because the function $\mathbf{g}$ is now the same for all values of $\mathbf{m}$. This is equivalent to inverting the mapping $\mathbf{x} \to \mathbf{m}(\mathbf{x}) \stackrel{\mathbf{g}}{\to} \mathbf{d}(\mathbf{m}(\mathbf{x}))$ at data values $\mathbf{d}_1,\dots,\mathbf{d}_N$ and obtaining values $\mathbf{m}_1 = \mathbf{g}^{-1}(\mathbf{d}_1),\dots,\mathbf{m}_N = \mathbf{g}^{-1}(\mathbf{d}_N)$. This approach is followed in the example of section 6.2.4.2. We deal with problems of this kind in section 6.4.1 and give examples. However, this simplification cannot be applied generally. For example, for the CAT problem (section 6.2.4.3) a measurement depends on all the points that they ray travels through.

If we also assume an independent prior distribution for the parameters, $\rho_{\mathcal{M}}(\mathbf{m}) = \prod_{n=1}^N \varrho_{\mathcal{M}}(\mathbf{m}_n)$, then the complete inverse problem factorises into N independent problems:

$$\theta(\mathbf{d}|\mathbf{m}) \propto \prod_{n=1}^N \varrho_{\mathcal{M}}(\mathbf{m}_n)\vartheta(\mathbf{d}_n|\mathbf{m}_n).$$

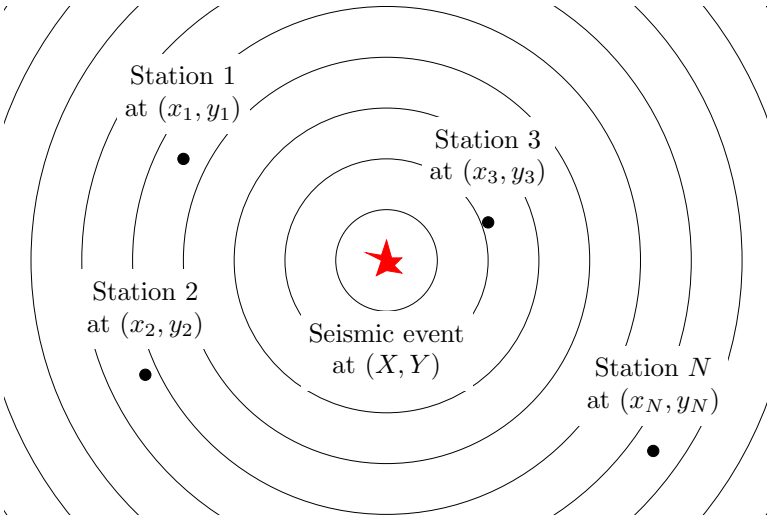

Figure 6.1: A seismic event takes place at time $\tau = 0$ at location (X, Y) and the seismic waves produced are recorded by several seismic stations of Cartesian coordinates $\{(x_n, y_n)\}_{n=1}^N$ at times $\{d_n\}_{n=1}^N$. Determining the location of the epicentre from the wave arrival times is an inverse problem.

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6.2.4 Examples of inverse problems

To clarify the concepts exposed, we briefly review some examples of inverse problems, some of which have a rich literature.

6.2.4.1 Locating the epicentre of a seismic event

We consider the simplified problem[4] of estimating the epicentral coordinates of a seismic event (e.g. a nuclear explosion), depicted in fig. 6.1. The event takes place at time $\tau = 0$ at an unknown location (X, Y) on the surface of the Earth (considered flat). The seismic waves produced by the explosion are recorded in a network of N seismic stations of Cartesian coordinates $\{(x_n, y_n)\}_{n=1}^N$, so that $\mathbf{d}_n = d_n$ is the observed arrival time of the seismic wave at station n. The waves travel at a velocity v in all directions.

The model parameters to be determined from the data parameters $\{d_n\}_{n=1}^N$ are:

- State parameters: the coordinates of the epicentre (X, Y).
- Experimental condition parameters: the coordinates of each station (x_n, y_n), the time of the event τ and the wave velocity v.

Thus $\mathbf{m} = (\mathbf{s}, \mathbf{c}_1, \ldots, \mathbf{c}_N) = (X, Y, \tau, v, x_1, y_1, \ldots, x_N, y_N)$. Assuming that the station coordinates, the time of the event and the wave velocity are perfectly known, we can drop them and avoid defining prior distributions for them, so that $\mathbf{m} = (X, Y)$.

Given (X, Y), the arrival times of the seismic wave at the stations can be computed exactly as $\mathbf{d}_n = \mathbf{g}_n(X, Y) = \frac{1}{v}\sqrt{(x_n - X)^2 + (y_n - Y)^2}$ for $n = 1, \ldots, N$, which solves the forward problem. Determining the epicentre coordinates (X, Y) from the arrival times at the different stations is the inverse problem, whose complete solution is given by Tarantola (1987).

6.2.4.2 Retrieval of scatterometer wind fields

A satellite can measure the amount of backscatter generated by small ripples on the ocean surface, in turn produced by oceanic wind fields. The satellite scatterometer consists of a line of cells, each capable to detect backscatter at the location to which it is pointing. At a given position in space of the satellite, each cell records a *local measurement*. A *field* is defined as a spatially connected set of local measurements obtained from a swathe, swept by the satellite along its orbit. For example, for the ESA satellite ERS-1, which follows a polar

[4] This example is adapted from problem 1.1 of Tarantola (1987, pp. 85–91).

orbit, the swathe contains 19 cells and is approximately 500 km wide. Each cell samples an area of around 50×50 km, with some overlap between samples.

The *backscatter* $\boldsymbol{\sigma}^0$ is a three-dimensional vector because each cell is sampled from three different directions by the fore, mid and aft beams, respectively. The near-surface *wind vector* $\mathbf{u}$ is a two-dimensional, quasicontinuous function of the oceanic spatial coordinates (although see comments about the wind continuity in section 7.9.6). Both $\boldsymbol{\sigma}^0$ and $\mathbf{u}$ contain noise, although the noise in $\boldsymbol{\sigma}^0$ is dominated by that of $\mathbf{u}$. A backscatter field is written as $\boldsymbol{\Sigma}^0 = (\boldsymbol{\sigma}_i^0)$ and a wind field as $\mathbf{U} = (\mathbf{u}_i)$.

The forward problem is to obtain $\boldsymbol{\sigma}^0$ from $\mathbf{u}$ and is single-valued and relatively easy to solve. The inverse problem, to obtain the wind field from the backscatter, is one-to-many and no realistic physically-based local inverse model is possible. The aim of the inversion is to produce a wind field $\mathbf{U}$ that can be used in data assimilation for numerical weather prediction (NWP) models. The most common method for inversion is to use lookup tables and interpolation. Following the standard Bayesian approach of inverse problem theory described in section 6.2.3, Cornford and colleagues[5] (Cornford et al., 1999a; Nabney et al., 2000; Evans et al., 2000) model the conditional distribution $p(\boldsymbol{\Sigma}^0|\mathbf{U})$ and the prior distribution of the wind fields $p(\mathbf{U})$. The prior is taken as a zero-mean normal, $p(\mathbf{U}) \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_\mathbf{U})$. The conditional distribution of the backscatter field $\boldsymbol{\Sigma}^0$ given the wind field $\mathbf{U}$ can be factorised into the individual distributions at each point in the region (i.e., at each cell) as $p(\boldsymbol{\Sigma}^0|\mathbf{U}) = \prod_i p(\boldsymbol{\sigma}_i^0|\mathbf{u}_i)$ because theoretically there is a single-valued mapping $\mathbf{u} \to \boldsymbol{\sigma}^0$. However, rather than using a physical forward model to obtain a noise model $p(\boldsymbol{\sigma}^0|\mathbf{u})$, which is difficult, they use Bayes' theorem to obtain $p(\boldsymbol{\sigma}^0|\mathbf{u}) \propto p(\mathbf{u}|\boldsymbol{\sigma}^0)/p(\mathbf{u})$, the factor $p(\boldsymbol{\sigma}^0)$ being constant for a given data, and they model $p(\mathbf{u}|\boldsymbol{\sigma}^0)$ as a mixture density network (Bishop, 1994), which is basically a universal approximator for conditional densities (see section 7.11.3). Applying Bayes' theorem again, the posterior distribution is

$$p(\mathbf{U}|\boldsymbol{\Sigma}^0) \propto p(\mathbf{U}) \prod_i \frac{p(\mathbf{u}_i|\boldsymbol{\sigma}_i^0)}{p(\mathbf{u}_i)}.$$

Given a backscatter field $\boldsymbol{\Sigma}^0$, the corresponding wind field is determined by MAP: a mode of $p(\mathbf{U}|\boldsymbol{\Sigma}^0)$ is found using a conjugate gradients method.

The fact that this inverse problem can be factorised into independent mapping inversion problems (see section 6.4.1) and the quasicontinuous dependence of the wind on the space coordinates make this problem amenable to the technique described in chapter 7.

6.2.4.3 Computerised tomography

The aim of computerised tomography (Herman, 1980) is to reconstruct the spatially varying absorption coefficients within a medium (e.g. the human body) from measurements of intensity decays of X-rays sent through the medium. Typically, X-rays are sent between a point source and a point receiver which counts the number of photons not absorbed by the medium, thus giving an indication of the integrated attenuation coefficient along that particular ray path (fig. 6.2). Repeating the measurement for many different ray paths, conveniently sampling the medium, the spatial structure of the attenuation coefficient can be inferred and so an image of the medium can be obtained.

The transmittance ρ_n (the probability of a photon of being transmitted) along the nth ray is given by:

$$\rho_n \stackrel{\text{def}}{=} \exp\left(-\int_{R_n} \mathbf{m}(\mathbf{x}(s_n))\, ds_n\right)$$

where:

- $\mathbf{m}(\mathbf{x})$ is the linear attenuation coefficient at point $\mathbf{x}$ and corresponds to the probability per unit length of path of a photon arriving at $\mathbf{x}$ being absorbed.
- R_n is the ray path, identified by the coordinates of the X-ray source and its shooting angle (ray paths of X-rays through an animal body can be assimilated to straight lines with an excellent approximation).
- ds_n is the element of length along the ray path.
- $\mathbf{x}(s_n)$ is the current point considered in the line integral along the ray (in Cartesian or spherical coordinates).

[5] Papers and software can be found in the NEUROSAT project web page at `http://www.ncrg.aston.ac.uk/Projects/NEUROSAT`.

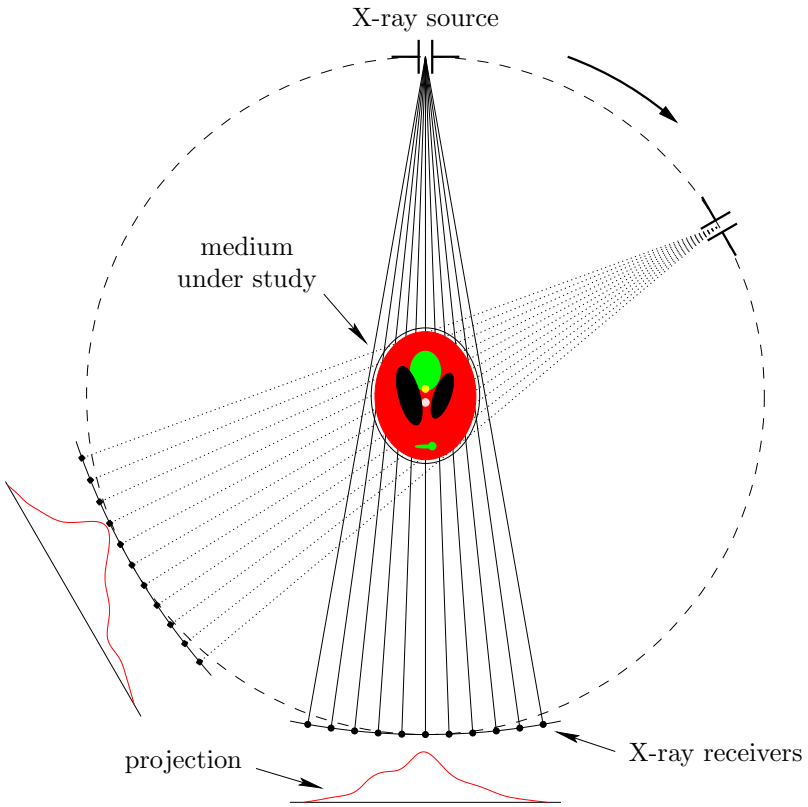

Figure 6.2: Setup for 2D X-ray tomography. A source sends a beam of X-rays through the object under study. Each individual X-ray is attenuated differently according to its path through the object. The X-rays are measured by an array of receivers, thus providing with a projection of the object. By rotating the source or having several sources surrounding the object we obtain several projections. Reconstructing the object density from these projections is the inverse problem of tomography.

Defining the data

$$d_n \stackrel{\text{def}}{=} -\ln \rho_n = \int_{R_n} \mathbf{m}(\mathbf{x}(s_n))\, ds_n \tag{6.7}$$

gives a linear relation between the data d_n and the unknown function $\mathbf{m}(\mathbf{x})$. Eq. (6.7) is the Radon transform of the function $\mathbf{m}(\mathbf{x})$, so that the tomography problem is the problem of inverting the Radon transform.

Thus, here the model parameters are the attenuation $\mathbf{m}(\mathbf{x})$ in the continuous case, or $\mathbf{m} = (m_{ijk})$ in a discretised version, and the observed parameters are the measured log-transmittance d_n. Given $\mathbf{m}(\mathbf{x})$, the forward problem is solved by the linear equation (6.7).

Similar problems appear in non-destructive testing and in geophysics. For example, in *geophysical acoustic tomography* the aim is to compute the acoustic structure of a region inside the Earth from seismic measurements. This allows, for example, to detect gas or oil deposits or to determine the radius of the Earth's metallic core. Acoustic waves are generated by sources at different positions inside a borehole and the travel times of the first wave front to receivers located in other boreholes around the region under study are recorded. The main difference with X-ray tomography is that the ray paths are not straight (they depend on the medium structure and are diffracted and reflected at boundaries), which makes the forward problem nonlinear. Acoustic tomography is an inverse scattering problem, in which one wants to determine the shape or the location of an obstacle from measurements of waves scattered by the obstacle.

Unlike example 6.2.4.2, this inverse problem does not factorise into independent mapping inversion problems and thus is not approachable by the technique of chapter 7.

6.3 Inverse problems vs Bayesian analysis in general

In Bayesian analysis in general, a parametric model is a function $p(\mathbf{x}; \boldsymbol{\Theta})$ where $\mathbf{x}$ are the variables of interest in the problem and $\boldsymbol{\Theta}$ the parameters, which identify the model. One is interested in inferences about both

Bayesian inverse problem theory	Latent variable models
Data space $\mathcal{D}$	Observed or data space $\mathcal{T}$
Model space $\mathcal{M}$	Latent space $\mathcal{X}$
Prior distribution of models $\rho_{\mathcal{M}}(\mathbf{m})$	Prior distribution in latent space $p(\mathbf{x})$
Forward mapping $\mathbf{g} : \mathcal{M} \to \mathcal{D}$	Mapping from latent space onto data space $\mathbf{f} : \mathcal{X} \to \mathcal{T}$
Uncertainty in the forward mapping $\theta(\mathbf{d}\|\mathbf{m}) = f(\mathbf{d} - \mathbf{g}(\mathbf{m}))$	Noise model $p(\mathbf{t}\|\mathbf{x}) = p(\mathbf{t}\|\mathbf{f}(\mathbf{x}))$

Table 6.1: Formal correspondence between continuous latent variable models and Bayesian inverse problem theory.

the parameters and the data, e.g. prediction via conditional distributions $p(x_2|x_1)$, etc. Bayesian inference is often approximated by fixing the parameters to a certain value given a sample $\{\mathbf{x}_n\}_{n=1}^N$ of the data, e.g. via maximum a posteriori (MAP) estimation:

$$\mathbf{\Theta}_{\text{MAP}} \stackrel{\text{def}}{=} \arg\max_{\mathbf{\Theta}} p(\mathbf{\Theta}|\mathbf{x}) = \arg\max_{\mathbf{\Theta}} p(\mathbf{x}|\mathbf{\Theta})p(\mathbf{\Theta}). \tag{6.8}$$

The model parameters $\mathbf{m}$ and the observed parameters $\mathbf{d}$ of inverse problem theory correspond to the parameters $\mathbf{\Theta}$ and the problem variables $\mathbf{x}$, respectively, of the Bayesian analysis in general. Bayesian inference about the model parameters $\mathbf{m}$, as shown in section 6.2.3, coincides with equation 6.8. But the emphasis is solely in inferences about the parameter estimates, i.e., how to find a single value of the model parameters that hopefully approximates well the physical reality. Thus, inverse problem theory is a *one-shot inversion problem*: use as much data as required to find a single value $\mathbf{m}_{\text{MAP}}$. Even if a second inversion is performed, we would expect the new inverse value of the model parameters to be close to the previous one—assuming that the system has not changed, i.e., assuming it is stationary or considering it in a fixed moment of time.

6.3.1 Inverse problems vs latent variable models

As an interesting example of the differences in interpretation between inverse problem theory and general Bayesian inference, let us consider continuous latent variable models as defined in chapter 2. As mentioned before, estimating the parameters of any probabilistic model can be seen as an inverse problem. But even when these parameters have been estimated and fixed, there is a formal parallelism between latent variable models and Bayesian inverse problem theory (in fact, all the estimation formulas for factor analysis mirror those of linear inverse problem theory). In latent variable models, we observe the data variables $\mathbf{t} \in \mathcal{T}$ and postulate a low-dimensional space $\mathcal{X}$ with a prior distribution $p(\mathbf{x})$, a mapping from latent space onto data space $\mathbf{f} : \mathcal{X} \to \mathcal{T}$ and a noise model in data space $p(\mathbf{t}|\mathbf{x}) = p(\mathbf{t}|\mathbf{f}(\mathbf{x}))$. Thus, the *model* here means the whole combined choice of the prior distribution in latent space, $p(\mathbf{x})$, the noise model, $p(\mathbf{t}|\mathbf{x})$, and the mapping from latent onto data space, $\mathbf{f}$, as well as the dimensionality of the latent space, L. And all these elements are equipped with parameters (collectively written as $\mathbf{\Theta}$) that are estimated from a sample in data space, $\{\mathbf{t}_n\}_{n=1}^N$. Table 6.1 summarises the formal correspondence between continuous latent variable models and Bayesian inverse problem theory.

The choice of model parameters to describe a system in inverse problem theory is not unique in general, and a particular choice of model parameters is a *parameterisation* of the system, or a *coordinate system*. Two different parameterisations are equivalent if they are related by a bijection. Physical knowledge of the inverse problem helps to choose the right parameterisation and the right forward model. However, what really matters is the combination of both the prior over the models and the forward mapping, $\rho_{\mathcal{M}}(\mathbf{m})\theta(\mathbf{d}|\mathbf{m})$, because this gives the solution to the Bayesian inversion. The same happens in latent variable models: what matters is the density in observed space $p(\mathbf{t})$, which is the only observable of the problem, rather than the particular conceptualisation (latent space plus prior plus mapping) that we choose. Thus, we are reasonably free to choose a simple prior in latent space if we can have a universal approximator as mapping $\mathbf{f}$, so that a large class of $p(\mathbf{t})$ can be constructed. Of course, this does not preclude using specific functional forms of the mapping and distributions if the knowledge about the problem suggests so.

We said earlier that inverse problem theory is a one-shot problem in that given a data set one inverts the forward mapping once to obtain a unique model. In continuous latent variable models, the latent variables are interpreted as *state variables*, which can take any value in their domain and that determine the observed

variables of the system (up to noise). That is, when the system is in the state $\mathbf{x}$, the observed data is $\mathbf{f}(\mathbf{x})$ (plus the noise). The model remains the same (same parameters $\boldsymbol{\Theta}$, same prior distribution, etc.) but the marginal distribution of the latent and observed variables $p(\mathbf{x}, \mathbf{t})$ can be used to make inferences about $\mathbf{t}$ given $\mathbf{x}$ (forward problem, related to the deterministic and now estimated mapping $\mathbf{f} : \mathcal{X} \to \mathcal{T}$) and about $\mathbf{x}$ given $\mathbf{t}$ (inverse problem, or dimensionality reduction), for different values of $\mathbf{x}$ and $\mathbf{t}$. Thus, once the latent variable model has been fixed (which requires estimating any parameters it may contain, given a sample in data space) it may be applied any number of times to different observed data and give completely different posterior distributions in latent space, $p(\mathbf{x}|\mathbf{t})$—unlike in inverse problem theory, where different data sets are expected to correspond to the same model.

The particular case of independent component analysis (ICA), discussed in section 2.6.3, cannot be considered as an inverse problem because we do not have a forward model to invert. Even though we are looking for the inverse of the mixing matrix $\boldsymbol{\Lambda}$ (so that we can obtain the sources $\mathbf{x}$ given the sensor outputs $\mathbf{t}$), $\boldsymbol{\Lambda}$ is unknown. ICA finds a particular linear transformation $\mathbf{A}$ and a nonlinear function f that make the sources independent, but we do not either invert a function (the linear transformation $\boldsymbol{\Lambda}$) or estimate an inverse from input-output data ($\{\mathbf{x}_n, \mathbf{t}_n\}_{n=1}^N$).

6.4 Mapping inversion

Consider a function[6] $\mathbf{f}$ between sets $\mathcal{X}$ and $\mathcal{Y}$ (usually subsets of $\mathbb{R}^D$):

$$\begin{array}{rccc} \mathbf{f}: & \mathcal{X} & \longrightarrow & \mathcal{Y} \\ & \mathbf{x} & \mapsto & \mathbf{y} = \mathbf{f}(\mathbf{x}). \end{array}$$

Mapping inversion is the problem of computing the inverse $\mathbf{x}$ of any $\mathbf{y} \in \mathcal{Y}$:

$$\begin{array}{rccc} \mathbf{f}^{-1}: & \mathcal{Y} & \longrightarrow & \mathcal{X} \\ & \mathbf{y} & \mapsto & \mathbf{x} = \mathbf{f}^{-1}(\mathbf{y}). \end{array}$$

$\mathbf{f}^{-1}$ may not be a well-defined function: for some $\mathbf{y} \in \mathcal{Y}$, it may not exist or may not be unique. When $\mathbf{f}^{-1}$ is to be determined from a training set of pairs $\{(\mathbf{y}_n, \mathbf{x}_n)\}_{n=1}^N$, perhaps obtained by sampling $\mathcal{X}$ and applying a known function $\mathbf{f}$, the problem is indistinguishable from **mapping approximation** from data: *given a collection of input-output pairs, construct a mapping that best transforms the inputs into the outputs.*

A **universal mapping approximator** (UMA) for a given class of functions $\mathcal{F}$ from $\mathbb{R}^L$ to $\mathbb{R}^D$ is a set $\mathcal{U}$ of functions which contains functions arbitrarily close (in the squared Euclidean distance sense, for definiteness) to any function in $\mathcal{F}$, i.e., any function in $\mathcal{F}$ can be approximated as accurately as desired by a function in $\mathcal{U}$. For example, the class of multilayer perceptrons with one or more layers of hidden units with sigmoidal activation function or the class of Gaussian radial basis function networks are universal approximators for continuous functions in a compact set of $\mathbb{R}^D$ (see Scarselli and Tsoi, 1998 for a review). The functions in $\mathcal{U}$ will usually be parametric and the optimal parameter values can be found using a learning algorithm. There are important issues in statistical mapping approximation, like the existence of local minima of the error function, the reachability of the global minimum and the generalisation to unseen data. But for our purposes in this last part of the thesis what matters is that several kinds of UMAs exist, in particular the multilayer perceptron (MLP), for which practical training algorithms exist, like backpropagation.

A multivalued mapping assigns several images to the same domain point and is therefore not a function in the mathematical sense. Among other cases, multivalued mappings arise when computing the inverse of an injective mapping (i.e., a mapping that maps different domain points onto a same image point)—a very common situation. That is, if the direct or forward mapping verifies $\mathbf{f}(\mathbf{x}_1) = \mathbf{f}(\mathbf{x}_2) = \mathbf{y}$ then both $\mathbf{x}_1$ and $\mathbf{x}_2$ are inverse values of $\mathbf{y}$: $\mathbf{f}^{-1}(\mathbf{y}) \supseteq \{\mathbf{x}_1, \mathbf{x}_2\}$. UMAs work well with univalued mappings but not with multivalued mappings. In chapter 7 we give a method for reconstruction of missing data that applies as a particular case to multivalued mappings, and we compare it to UMAs as well as other approaches for mapping approximation like vector quantisation (section 7.11.4) and conditional modelling (section 7.11.3).

6.4.1 Inverse problems vs mapping inversion

Mapping inversion is a different problem from that of inverse problem theory: in inverse problem theory, one is interested in obtaining a unique inverse point $\mathbf{x}$ which represents a model of a physical system—of which

[6] We use the term *function* in its strict mathematical sense: a correspondence that, given an element $\mathbf{x} \in \mathcal{X}$, assigns to it one and only one element $\mathbf{y} \in \mathcal{Y}$. We use the term *mapping* for a correspondence which may be multivalued (one-to-many).

we observed the values $\mathbf{y} \in \mathcal{Y}$. In mapping inversion, we want to obtain an inverse mapping $\mathbf{f}^{-1}$ that we can use many times to invert different values $\mathbf{y} \in \mathcal{Y}$.

In section 6.2.3.8 we saw that the Bayesian inverse problem theory could be recast to solve such a mapping inversion problem. We rewrite eq. (6.6) with a simplification of the notation and decompose the model parameters $\mathbf{m}$ into parameters of *state* $\mathbf{s}$ and *experimental conditions* $\mathbf{c}_n$, $\mathbf{m} = (\mathbf{s}, \mathbf{c}_1, \ldots, \mathbf{c}_N)$:

$$p(\mathbf{s}, \mathbf{c}_1, \ldots, \mathbf{c}_N | \mathbf{d}_1, \ldots, \mathbf{d}_N) \propto p(\mathbf{s}, \mathbf{c}_1, \ldots, \mathbf{c}_N) \prod_{n=1}^{N} p(\mathbf{d}_n | \mathbf{s}, \mathbf{c}_n)$$

where $p(\mathbf{d}_n | \mathbf{s}, \mathbf{c}_n) = f(\mathbf{d}_n - \mathbf{g}(\mathbf{c}_n; \mathbf{s}))$ and $\mathbf{g}$ is the known forward mapping. This can be interpreted as a function $\mathbf{g}$ which maps $\mathbf{c}_n$ into $\mathbf{d}_n$ and has trainable parameters $\mathbf{s}$. However, $\{\mathbf{c}_n\}_{n=1}^N$ are *unknown parameters themselves, not data*. We are interested in constructing an inverse mapping $\mathbf{g}^{-1}$ given a data set consisting of pairs of values $\{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$ so that $\mathbf{y}_n = \mathbf{g}(\mathbf{x}_n)$ for a mapping $\mathbf{g}$ (not necessarily known). Clearly, in these terms the distinction between inverse and forward mapping disappears and the problem, as before, becomes a problem of mapping approximation.

Practitioners of inverse problem theory may object that by considering the forward mapping unknown we are throwing away all the physical information. But the theorems about universal approximation of mappings and about universal approximation of probability density functions support the fact that, given enough data, we can obtain (ideally) a good approximation of the joint density of the observed data and thus capture the information about the forward mapping too. This has the added flexibility of making inferences about any group of variables given any other group of variables by constructing the appropriate conditional distribution from the joint density—which includes both the forward and inverse mappings.

Two well-known examples of mapping inversion problems with one-to-many inverse mappings (often referred to as inverse problems in the literature) are the **inverse kinematics problem of manipulators** (the robot arm problem) (Atkeson, 1989) and the **acoustic-to-articulatory mapping problem** of speech (Schroeter and Sondhi, 1994). We describe them and apply to them our own algorithm later in this thesis.

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