Taming uncertainty in geophysical inversion

Malcolm Sambridge*
Research School of Earth Sciences
Australian National University
Malcolm.Sambridge@anu.edu.au

Rhys Hawkins
Research School of Earth Sciences
Australian National University
Rhys.Hawkins@anu.edu.au

Jan Dettmer
Research School of Earth Sciences
Australian National University
Jan.Dettmer@anu.edu.au

SUMMARY

The concept of uncertainty in geophysical inversion is often confined to quantification of errors in parameters estimated from some data. A broader definition is to include uncertainty arising from the assumptions made in posing the inverse problem in the first place. These may include assumptions about the physics of the relationship between observations and unknowns, the class of parameterisation assumed for the unknowns, and guesses about the statistical character of random noise contaminating the data. Typically these assumptions are required to arrive at a tractable mathematical problem to solve using geophysical inversion methods. In this paper we outline an inversion approach that allows a broader definition of uncertainty which includes each of these classes of assumption. Including uncertainty in the model parametrization or in the nature of the noise statistics can lead to more realistic inversion results, but not always with increased error bars on the model parameters. For example, relaxing rigid assumptions in the nature of the parametrisation, even in simple problems can result in smaller and more realistic model error estimation. Using the data to decide between different classes of parameterization, physical assumptions or observational noise process is often called `model choice' in statistics, an area that is often overlooked in the geosciences. Over the past 5 years the trans-dimensional inversion approach has increasingly found applications across a variety of inference problems in the geosciences, with new applications appearing regularly.

Key words: Inversion, uncertainty, geophysical imaging, seismology.

INTRODUCTION

In less than a decade the age of big data has impacted on every corner of science and engineering. Advances in digital data acquisition together with cost reductions have resulted in a rapid growth in sensor numbers and resolution to the point where we collect, process and transmit data at rates never before seen in history. The large Hadron Collider at CERN produces 15 petabytes of data every year, while a single sequenced genome can amount to 140 gigabytes (Marx, 2013). Digital camera sensors can now collect still and video images with up to three orders of magnitude more pixels than they did a decade ago and at a fraction of the cost. Low cost image sensors have allowed billions of people to generate high resolution video, while also creating a flood of security cameras, digital images from satellites, telescopes and airborne drones (Baraniuk, 2011). The rapid growth in data is not restricted to the physical and medical sciences and is perhaps even greater in the social sciences where, for example, behavioural studies that were once based on costly surveys of 1000 participants have been replaced with automated text analysis of 100 million social media posts a day (King, 2011). Gantz, (2010) estimates the global rate of data collection to be increasing at 58% per year, which in 2010 alone amounted to 1250 billion gigabytes, more bytes than the estimated number of stars in the universe. Since 2007 we have been generating more bits of data per year than can be stored in all of the world's storage devices (Gantz, 2010).

This *data deluge* is profoundly changing the way science is done in fields from astronomy, chemistry, biology, and medicine, to physics, engineering and the geosciences. Industry and governments have become focused on the challenges of `big data' like never before with commensurate investments at scale. By 2016 the concept has received so much exposure that academics and likely peer reviewers may have begun to suffer big data fatigue. While attention of data scientists is often focused on issues of data storage, management, accessibility, reproducibility and interoperability the data science age has also refocused much needed attention of how information is extracted from observations in a meaningful way. In the geosciences this issue has always been an evolving research challenge even when data sets were small and hand processed, and many still are! This is largely because of the complexity of the relationship between geophysical observables collected on the Earth's surface and its properties at depth or back in time. The indirect nature of our observations means there is always an inverse problem in robustly extracting information about quantities that we do not directly measure. For example, seismic, MT, potential field or Airborne EM observations taken at (or above) the surface, never uniquely constrain their corresponding physical properties at depth. For more than four decades geophysicists have made substantial contributions to the understanding of inverse problems in which models of physical properties are sought that match observations.

Pioneering work on linear inverse problems in the 1960s arose out of the need to understand how to use new surface observables from seismology to constrain radial variations in geophysical properties at depth within the Earth. Data were few in number and attention was focused on the mathematical structure of the inverse problem and the ways in which reliable information could be recovered. This resulted in a series of important papers beginning with Backus & Gilbert (1967, 1968, 1970). Since that time the geosciences, like many other fields, have moved into the data rich environment with increasing availability of computational power. Considerable progress has been made over 30 years utilizing the class of linear (typically least squares) parameter estimation algorithms, which are common to many areas of the physical sciences, Aster et al., (2005). As data precision and abundance increases together with theoretical and computational advances, linear analysis tools are becoming increasingly outmoded. In most cases the dependence of the geophysical observables on the parameters describing the model is non-linear, so that the outcomes can be conditioned by the assumptions made for the initial model. Over the last 30 years there has been considerable progress in the solution of highly nonlinear inverse problems involving a limited number of parameters so that thorough exploration can be made of the character of models, e.g.. Sambridge and Mosegaard (2002). In contrast there has been meagre progress with large scale problems with many unknowns that make heavy computational demands, although this situation is undergoing change. Today the geophysical `inverse modeller', as they have become known, must grapple with non-uniqueness, data noise, model uncertainty, and high computational complexity while drawing meaningful conclusions as to what lies beneath.

In this paper we discuss a relatively new approach to inverse problems that is only recently becoming popular in the geosciences known as trans-dimensional inversion. This is an extension of Bayesian sampling which seeks to generate ensembles of solutions generated probabilistically and consistent with the data and any prior information available. Bayesian sampling techniques have been a workhorse approach in computational statistics for several decades, Brooks et al (2011). The trans-D variant is more recent, Geyer and Møller (1994), Green (1995), and may be used to address issues of uncertainty, not just in the model parameters themselves, but also and quite uniquely in the assumptions upon which the inversion is based in the first place, Malinverno (2002). This approach shows much promise for Earth imaging problems in a range of situations, and new geoscience applications are appearing regularly. For a review see Sambridge et al. (2013).

METHOD AND RESULTS

All inversion approaches require choices to be made by the practitioner whether they be in the nature of the model parameterisation, the way the subsurface is represented, the level of approximations used in the physics, e.g. assuming a 1-D, 2-D or 3-D earth, or the size and nature of the noise contaminating the observations. Such assumptions are made at the outset and kept fixed during any single solution process. We hope these choices do not influence our conclusions and if there is sufficient time, we may repeat an inversion and test a few alternatives. With a trans-D approach the data is used to not only constrain the model parameters but also decide between the previously fixed assumptions employed in the inversion. In practice each alternative, or even a continuum of choices, may be incorporated into the inference process and the data used to quantitatively estimate the level of support available for each choice as a percentage. In this way information on Earth model parameters and their uncertainty is recovered without dependence on any one assumption or choice, and indeed no winner is selected, but rather the inference process allows all assumptions to contribute in proportion to their support from the data itself.

The name `trans-dimensional' arises because often each particular inversion assumption can be represented as a different mathematical model, e.g. in terms of the class of parameterise, or the number of unknowns. Probabilistic Bayesian sampling can be performed across each class with an algorithm transitioning between parameter spaces of different dimension. A simple example is shown in FIGURE 1 using a simple regression dataset of Sambridge et al. (2006). Here the data are being fit by polynomials with

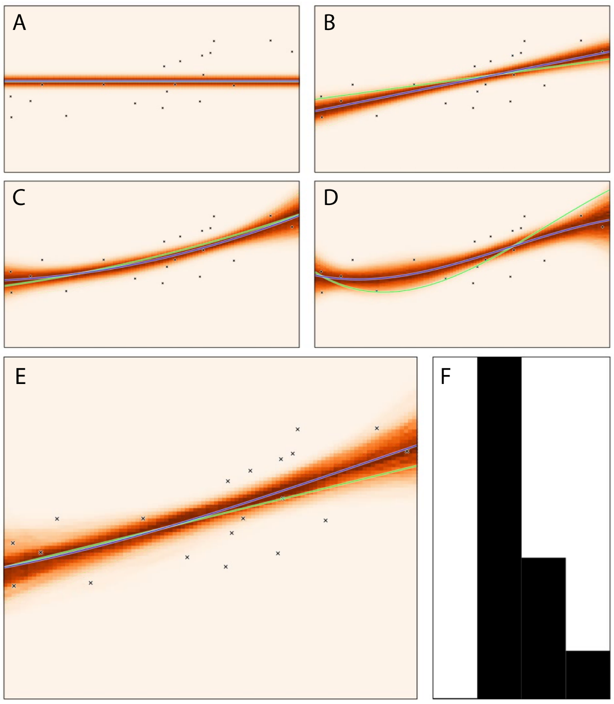

Figure 1: Example of fixed dimension and trans-D Bayesian probabilistic sampling in a regression problem. Panel A shows the density of linear curves produced by Bayesian sampling assuming a zeroth order polynomial fits the scattered data. Panels B-D show similar results assuming first, second and third order polynomials are appropriate. Panel E shows trans-D sampling where the assumptions are relaxed and sampling occurs across all four parameter classes. In the trans-D sampling not all polynomial order are visited equally, but rather the data decodes which is preferred. Panel F shows the frequency of visits as a four bar histogram. The data prefer a linear function over the zeroth and higher order polynomials which is the correct parameterization in this case.

different numbers of dimensions using Bayesian sampling is compared to trans-D sampling which is a single algorithm visiting all four possible model parametrizations. The trans-D algorithm uses the data to decide which order polynomials are supported and in what frequency. Here the trans-D sampler visits the linear function about 87% of the time, while there is 11% support for the quadratic, and less than 4% support for the cubic, and the zeroth order is in effect ruled out by the data with less than 1% support as shown in panel D.

This simple example shows that the trans-D is not biased by the assumptions in the fixed order polynomial cases but instead provides evidence about which is better and in turn produces a comprehensive picture of uncertainty on the regression function provided by the data. Note that introducing more unknowns will always result in a better fitting optimal polynomial in case D compared to, C, B or A, however this does not mean that the Bayesian trans-D sampling will favour the parameter space with more unknowns. In fact the most support by the data lies in the first order polynomial. This is an example of the parsimonious nature of trans-D sampling.

Although this is a very simple example, it demonstrates the fundamental feature of trans-D sampling which is to visit multiple classes of parameter space, which can be defined by the model parameterisation or other types of assumption e.g. on the physics of the forward model or the assumptions about noise in the data. This approach broadens the class of question that can be handled in an inference process and means that uncertainty may be quantified in a way that reflects all assumptions or model classes, e.g. as seen in the spread of admissible solutions shown in FIGURE 1E & 1F.

CONCLUSIONS

Over the last decade the authors, their colleagues and many others have extended the range of areas where trans-D sampling has been applied, in particular to much larger and more complex geophysical imaging problems. These include seismic travel time and waveform tomography (Bodin and Sambridge, (2009), Bodin et al, 2012a, Hawkins & Sambridge (2015); geophysical imaging of the crust with seismic, ground based and airborne EM, Piana-Agostinetti and Malinverno (2010), Brodie, and Sambridge, (2012), Bodin et al., (2012b); Local earthquake tomography, Piana-Agostinetti et al. (2015); Geoacoustic acoustic imaging of sea-bed and near surface properties, Dettmer and Dosso (2010), Dettmer et al. (2012a&b), Steininger et al. (2014) and more recently seismic and Tsunami source studies, Dettmer et al. (2014). Trans-D approaches have also begun to make a mark in exploration geophysics. Applications have appeared in inversion of marine CSEM data, Ray and Key (2012), inversion of controlled-source electromagnetic data, Gehrmann et al. (2015), and full waveform elastic inversion of marine seismic data Ray et al. (2016).

Further afield this approach has been applied in Hydrology, Minsley (2011), signal processing, Kolb and Lekić (2014), environmental monitoring for exploration, Warner et al. (2015), inversion of geoid data for viscosity, Rudolph et al. (2016), various problems in Geochemistry including estimating thermal properties of the Lithosphere, Gallagher et al. (2009, 2011), plate tectonic reconstructions, Iaffaldano et al. (2012), and a variety of Earth Science regression problems, similar to that in FIGURE 1, such as paleo sea-level reconstruction, Lambeck et al. (2014), and even to estimating the variable rotation of the Earth's solid inner core, Tkalčić et al. (2013) and paleomagnetic time series analysis, Ingham et al. (2014). The versatility and power of the methodology have given it wide appeal and are leading to increasing numbers of novel applications.

ACKNOWLEDGMENTS

Many colleagues have contributed to the authors' studies and understanding of trans-D inversion over the past decade including Roberto Benavente, Thomas Bodin, Ross Brodie, Phil Cummins, Stan Dosso, Kerry Gallagher, Charles Holland, Anya Reading, Hrvoje Tkalčić, Giampiero Iaffaldano, Alberto Malinverno, Burke Minsley, Nick Rawlinson, Gavin Steininger, and Stephen Sagar.

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