Exploration of data space through trans-dimensional sampling: A case study of 4D seismics

Nicola Piana Agostinetti¹, Maria Kotsi², and Alison Malcolm³

¹University of Milano-Bicocca ²PanGeo Subsea Inc ³Memorial University of Newfoundland

November 28, 2022

Abstract

We present a novel methodology for exploring 4D seismic data in the context of monitoring subsurface resources. Data-space exploration is a key activity in scientific research, but it has long been overlooked in favour of model-space investigations. Our methodology performs a data-space exploration that aims to define structures in the covariance matrix of the observational errors. It is based on Bayesian inferences, where the posterior probability distribution is reconstructed through trans-dimensional (trans-D) Markov chain Monte Carlo sampling. The trans-D approach applied to data-structures (termed "partitions") of the covariance matrix allows the number of partitions to freely vary in a fixed range during the McMC sampling. Due to the trans-D approach, our methodology retrieves data-structures that are fully data-driven and not imposed by the user.

We applied our methodology to 4D seismic data, generally used to extract information about the variations in the subsurface. In our study, we make use of real data that we collected in the laboratory, which allows us to simulate different acquisition geometries and different reservoir conditions. Our approach is able to define and discriminate different sources of noise in 4D seismic data, enabling a data-driven evaluation of the quality (so-called "repeatability") of the 4D seismic survey. We find that: (1) trans-D sampling can be effective in defining data-driven data-space structures; (2) our methodology can be used to discriminate between different families of data-structures created from different noise sources. Coupling our methodology to standard model-space investigations, we can validate physical hypothesis on the monitored geo-resources.

Exploration of data space through trans-dimensional sampling: A case study of 4D seismics

Nicola Piana Agostinetti

³ ZED Depth Exploration Data GmbH, Vienna, Austria

Maria Kotsi

- ⁴ PanGeo Subsea Inc
- ⁵ Earth Sciences Department, Memorial University of Newfoundland, St John's,
- 6 NL, Canada

Alison Malcolm

- 7 Earth Sciences Department, Memorial University of Newfoundland, St John's,
- ⁸ NL, Canada

PanGeo Subsea Inc

Earth Sciences Department, Memorial University of Newfoundland, St John's, NL, Canada

ZED Depth Exploration Data GmbH, Vienna, Austria

Abstract.

We present a novel methodology for exploring 4D seismic data in the con-10 text of monitoring subsurface resources. Data-space exploration is a key activ-11 ity in scientific research, but it has long been overlooked in favour of model-12 space investigations. Our methodology performs a data-space exploration that 13 aims to define structures in the covariance matrix of the observational errors. 14 It is based on Bayesian inferences, where the posterior probability distribution 15 is reconstructed through trans-dimensional (trans-D) Markov chain Monte Carlo 16 sampling. The trans-D approach applied to data-structures (termed "partitions") 17 of the covariance matrix allows the number of partitions to freely vary in a fixed 18 range during the McMC sampling. Due to the trans-D approach, our method-19 ology retrieves data-structures that are fully data-driven and not imposed by the 20 user. 21

We applied our methodology to 4D seismic data, generally used to extract in-22 formation about the variations in the subsurface. In our study, we make use of 23 real data that we collected in the laboratory, which allows us to simulate dif-24 ferent acquisition geometries and different reservoir conditions. Our approach 25 is able to define and discriminate different sources of noise in 4D seismic data, 26 enabling a data-driven evaluation of the quality (so-called "repeatability") of the 27 4D seismic survey. We find that: (1) trans-D sampling can be effective in defin-28 ing data-driven data-space structures; (2) our methodology can be used to dis-29 criminate between different families of data-structures created from different noise 30

DRAFT

- ³¹ sources. Coupling our methodology to standard model-space investigations, we
- ³² can validate physical hypothesis on the monitored geo-resources.

1. Introduction

In their investigations of the Earth system, geo-scientists have to deal with two complemen-33 tary spaces: data space and model space. The *model space* is generally defined as the space 34 of the investigated parameters. For a given parameterization of the system, each point of the 35 model space defines a possible model of the system, represented by a combination of values 36 of the model parameters. To make inferences on the model parameters, we need to take mea-37 surements of relevant geo-observables. The data space contains all the possible combinations 38 of such observations [Tarantola, 2005] and the measured data points form a local subset of the 39 data space with its own structure. While there is a vast literature about methodologies for in-40 vestigating the model space [Sambridge and Mosegaard, 2002, e.g.], few attempts have been 41 made at a systematic exploration of the data space. Exploration of the data space is an ordinary 42 activity for geo-scientists, and includes, for example, data preparation, quality controls (QC)s 43 for data selection and estimation of data errors. Some of those activities, for example the data 44 selection, could have a strong impact on the data space, modifying, for example, the data struc-45 ture. Generally, such activities rely on the *expert-opinion* of the geoscientists and are carried 46 out ahead of the main geophysical investigations that are related to the model space. 47

There are two main reasons for considering a systematic exploration of the data space. First, the ever growing amount of geo-data available to geo-scientists needs to be tackled with more automated workflows; expert opinion is generally a time-consuming process. Second, more interestingly, expert opinion, as a human activity, implies the separation of data into categories (i.e. a discrete number of outputs) rather than a more general continuous evaluation of probability. For example, in data selection activities, the expert can select and, then exclude, part of

DRAFT

the data based on their experience, using a two category model (in/out, good/bad). Conversely, a more automated workflow, developed in a statistical framework, can associate a probability value to each data point, avoiding the need to remove any of them from the analysis.

In recent years, some studies have reported cases of systematic exploration of the data space, 57 even if such analyses take often a marginal role in the scientific studies themselves. In particu-58 lar, there are some examples [Bodin et al., 2012a; Dettmer and Dosso, 2012; Xiang et al., 2018] 59 where Bayesian inference is applied to a geophysical inverse problem for defining both phys-60 ical parameters (i.e. investigating the model space) and the errors associated to the data (i.e. 61 exploring the data space), the so called *Hierarchical Bayes* approach [Malinverno and Briggs, 62 2004]. In Hierarchical Bayes algorithms, the uncertainties related to the data are assumed to 63 be poorly known and need to be estimated during the process. This approach usually assumes a 64 fixed number of parameters which represent the unknown part of the data space. In most applications of the Hierarchical Bayes approach, the absolute value of the data errors is considered 66 an unknown in the problem that needs to be inferred [Bodin et al., 2012a]. Sometimes, in cases 67 where the structure of the data errors is known (i.e. we know which data points are measured 68 with more precision with respect to other points), a scaling factor of the data error is used as the 69 unknown [Piana Agostinetti and Malinverno, 2018]. In more complex cases, the Hierarchical 70 Bayes approach is adopted to somehow define a function of the data uncertainties, so called 71 "data structures" or "states" hereinafter, which include: estimating an auto regressive model of 72 the data errors [i.e. a form of error correlation, *Dettmer and Dosso*, 2012], and estimating an 73 increasing linear model for the data errors as a function of the geometrical distance between 74 measurement points [e.g. Galetti et al., 2016]. In all of these cases however, the number of pa-75 rameters representing the data structure is fixed a-priori (usually one or two parameters, rarely 76

DRAFT

May 1, 2021, 10:27am

X - 6 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

more than three). By contrast, Steininger et al. [2013] and Xiang et al. [2018], extend Hierar-77 chical Bayes approach to make inferences on the data space by considering data structures that 78 are represented by a variable number of parameters. Xiang et al. [2018] make use of a transdi-79 mensional (trans-D) sampler [Sambridge et al., 2006, 2013] for sampling models belonging to 80 two different states: in one state, one unknown defines an autoregressive model of the first order 81 for the data errors, i.e. assume uncorrelated errors, while in a second state, two unknowns are 82 used to define an autoregressive model of the second order, i.e. exponential correlation between 83 data uncertainties. Using this ability to jump from one state to the other, the algorithm is able 84 to indicate the "predominant" auto-regressive model associated to the data errors. As far as we 85 know, Steininger et al. [2013] and Xiang et al. [2018] are the first applications of a trans-D 86 algorithm in Geophysics, for sampling different states representing different error models, even 87 if they are limited to a transition between states represented by one and two parameters.

In this study, we move a step forward in the development of algorithms for data space ex-89 ploration. We make use of a trans-D sampler for exploring different "states" (represented by 90 a different number of variables), where each state reproduces a partition of the data space (i.e. 91 a data structure). The number of states to be explored is no longer strictly limited [e.g. two 92 states, like in *Xiang et al.*, 2018], and the number of variables representing each state can vary 93 between a user-defined minimum and maximum. The algorithm is developed in a Bayesian 94 framework, used to define the posterior probability of the data structures. Data space structures 95 are expressed in terms of partitions of the covariance matrix of the errors, which allow us to 96 define regions of the data space where measured data are in agreement with a given working 97 hypothesis. The algorithm is applied to the data analysis workflow used for time-lapse seismics 98 (also called 4D seismics), a technology used primarily by oil&gas companies for monitoring 99

DRAFT

their reservoirs. The 4D seismic data consist of time-repeated active seismic surveys that need to be investigated for detecting noise/distortions and focusing the subsequent geophysical inversion on the portion of active seismic data where temporal changes have occurred. The algorithm is applied on laboratory data that mimic active seismic surveys and the results are discussed in light of the potential of the algorithm for statistically separating signals with different origins.

1.1. 4D seismics: key-concepts and present-day challenges

The term 4D seismics indicates the data workflow adopted by oil&gas companies for monitor-105 ing their reservoirs through the repetition, after a few years, of active seismic surveys. The 4D 106 seismic workflow consists of three main phases: acquisition, processing and interpretation. 4D 107 seismics is generally performed for off-shore reservoirs, but the first successes were obtained 108 on-shore [e.g. Porter-Hirsche and Hirsche, 1998; Davis et al., 2003]. This technology is also 109 used for monitoring CO₂ underground storage sites [Lumley, 2010; Cheng et al., 2010; Yang 110 et al., 2014; Roach et al., 2015]. Briefly, a first active seismic survey, the so-called baseline 111 survey, is performed just before starting production to image the untouched resources. After 112 some time and while the reservoir is under production, the active seismic survey is repeated, the 113 so-called *monitor survey*. If the seismic acquisition and data processing are exactly the same 114 as those used for the baseline survey, the differences between the images can be uniquely at-115 tribute to changes in the physical properties of the reservoir due to its exploitation. Through the 116 analysis of such differences, scientists can make informed decisions about the next phases of 117 exploitation of the reservoir. 118

An important question is: how can we get relevant information from 4D seismics? Production related effects on images obtained from the monitor survey can be obscured by distortions induced by the lack of repeatability of the data acquisition and processing. This is one of the

X - 8 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

main technical barriers for getting the correct information from 4D seismics [Koster et al., 122 2000]. The concept of *repeatability* between two or more seismic surveys indicates the degree 123 to which the data-sets can be considered to be generated from the same operational and com-124 putational workflows. Measures of repeatability between two seismic surveys generally include 125 Normalized Root Mean Square (NRMS) and trace correlation [also called *predictability Kragh* 126 and Christie, 2002]. Increasing and evaluating the repeatability of 4D seismics have been the 127 focus of a number of studies in the last decades [Landro, 1999; Houck, 2007; Pevzner et al., 128 2011], with the main efforts going into increasing acquisition quality, i.e. hardware solutions. 129 Statistical approaches to 4D data analysis have been limited to the interpretation phase [e.g. 130 applying Machine Learning algorithms to porosity inversion Dramsch, 2019]. 131

1.2. Methodological framework: Bayesian inference, Markov chain Monte Carlo and trans-dimensional algorithms

¹³² Various geophysical inverse problems have been solved following a probabilistic Bayesian
 ¹³³ framework [*Tarantola*, 2005, 2006]. Bayes' theorem

$$p(\mathbf{m} \mid \mathbf{d}) = \frac{p(\mathbf{m})p(\mathbf{d} \mid \mathbf{m})}{p(\mathbf{d})}$$
(1)

¹³⁴ connects (probabilistic) prior information $p(\mathbf{m})$ about some subsurface properties (*m*) and data ¹³⁵ measured (*d*), generally at the surface, to extract new information about such properties (the so-¹³⁶ called *posterior probability distribution* $p(\mathbf{m} | \mathbf{d})$ or PPD), through an (assumed) known error ¹³⁷ statistics [the Likelihood $p(\mathbf{d} | \mathbf{m})$, or $L(\mathbf{m})$ hereinafter, *Bayes*, 1763]. Thus, in contrast with ¹³⁸ other approaches, the solution of geophysical inverse problems is given in the form of a proba-¹³⁹ bility distribution over the investigated parameters, and not as a single value for each parameter ¹⁴⁰ (i.e. a single model). In simple cases, Bayes' theorem can give an analytic solution to geophys-

D R A F T May 1, 2021, 10:27am D R A F T

ical inverse problems [Tarantola, 1987]. However, numerical methods have been widely used 141 in more complex cases. In particular, Markov chain Monte Carlo (McMC) sampling has been 142 found to be well suited for sampling a chain of Earth models with a probability proportional to 143 the PPD and, thus, to make inferences on relevant parameters based on such sampled models 144 [Sambridge and Mosegaard, 2002]. Here, we follow the approach presented in Mosegaard and 145 *Tarantola* [1995] and we develop a sampler of the prior probability distribution which can be 146 "switched" to sample models with a probability that follows the PPD. After collecting a relevant 147 number of models from the PPD, we compute numerical estimators of the investigated parame-148 ters directly from the sampled models. For example, the mean value of the parameter m, can be 149 estimated as 150

$$\hat{m} = \frac{1}{N_s} \sum_{j}^{N_s} m^j, \tag{2}$$

where N_s is the number of samples computed during the McMC sampling and m^j is the value of parameter *m* for the *j*-th model sampled. Following the approach in *Mosegaard and Tarantola* [1995], we define the probability of accepting a new model along the Markov chain as:

$$\alpha = \min[1, L(\mathbf{m}_{cand})/L(\mathbf{m}_{cur})], \qquad (3)$$

where \mathbf{m}_{cand} , the candidate model, and \mathbf{m}_{cur} , the current model, are two consecutive Earth models along the Markov chain and $L(\mathbf{m})$ is the likelihood of the model given the observed data. In other words, the candidate is always accepted if $L(\mathbf{m}_{cand}) \ge L(\mathbf{m}_{cur})$. If $L(\mathbf{m}_{cand}) < L(\mathbf{m}_{cur})$, the random walk moves to the candidate model with probability equal to $L(\mathbf{m}_{cand})/L(\mathbf{m}_{cur})$. The last point, $L(\mathbf{m}_{cand}) < L(\mathbf{m}_{cur})$, guarantees that the McMC sampler will not get stuck in a local

D R A F T May 1, 2021, 10:27am D R A F T

maximum of the likelihood function, because models which worsen the fit to the data may still
 be accepted.

Two fundamental points in Bayesian inferences are the initial states of knowledge about the 161 investigated parameters, the so-called *priors*, which can take a closed analytical form, or be 162 represented by a set of rules (e.g. one parameter has to be smaller than a second parameter, like 163 in P- and S- waves velocities in rocks). More interestingly, the statistics of the data uncertainties 164 should be known at a certain level. Such statistics is used to compute the likelihood value of an 165 Earth model. Simplified statistics can be adopted (e.g. a diagonal covariance matrix in Gaussian 166 distributed errors) but has been proven to give un-realistic results in some cases [Birnie et al., 167 2020]. Both of these assumptions have to hold to make inferences on physical parameters and, 168 given Equation 1, the solution to the geophysical inverse problem may change under different 169 assumptions. 170

An efficient design of the McMC sampler is fundamental for achieving robust results (in terms 171 of number of samples extracted from the PPD) in a limited amount of time. Several different 172 recipes have been designed in the past for proposing a *candidate model*, i.e. a new point in 173 the model space, as a perturbation of the *current model*, i.e the last visited point in the model 174 space [Bodin et al., 2012b]. In fact, if the sampling is too limited to the neighbourhood of the 175 current model, McMC will converge too slowly toward the global maximum of the likelihood 176 function. Conversely, too strong a perturbation of the current model will likely lead to poorly 177 fitting candidate models, most of which will be rejected. In recent years, one ingredient that 178 has been added to many implementations of the McMC sampler is the possibility of sampling a 179 candidate model which has a different number of variables than the current model [Malinverno, 180 2002; Sambridge et al., 2006]. In practise, we relax the hard constraint of a fixed number 181

DRAFT

May 1, 2021, 10:27am

¹⁸² of variables in the models, allowing it to vary between fixed minimum and maximum values. ¹⁸³ This new generation of McMC samplers are collectively called trans-dimensional samplers [e.g. ¹⁸⁴ *Sambridge et al.*, 2013] and are based on the pioneering works of *Geyer and Møller* [1994] and ¹⁸⁵ *Green* [1995]. For trans-dimensional samplers, Equation 3 holds under specific assumptions on ¹⁸⁶ the model space transformation and its Jacobian matrix [see Appendix B in *Piana Agostinetti* ¹⁸⁷ *and Malinverno*, 2010, for details].

2. Data

We consider a simple time-lapse scenario that consists of an overburden layer and a reservoir. 188 To better mimic a real world application, we use a scaling factor of 10000 such that a frequency 189 of 200 kHz represents a frequency of 20 Hz, and a dimension of 1 mm represents 10 m. To 190 build this experiment in the lab we take two Plexiglas blocks with dimensions $310 \times 154 \times 77$ 191 mm, and attach them together (Figure 1). The first Plexiglas block represents the overburden 192 layer with elastic properties of $V_p = 2780$ m/s, $V_s = 1480$ m/s, and $\rho = 1.19$ g/cm³. This 193 overburden layer remains unchanged between the two surveys. To build the reservoir layer we 194 remove a rectangular cube from the second block, allowing us to insert different fluids into our 195 'reservoir'. 196

¹⁹⁷ For the baseline survey, we keep the second block empty, representing a gas-filled reservoir. ¹⁹⁸ In this case, the elastic properties of the air are $V_p = 332$ m/s, $V_s = N/A$, and $\rho \sim 0$ g/cm³. For ¹⁹⁹ the monitor survey, we fill the block with water, miming a scenario where the gas in the reservoir ²⁰⁰ has been replaced with brine. The elastic properties of the water are $V_p = 1500$ m/s, $V_s = N/A$, ²⁰¹ $\rho \sim 1$ g/cm³. Figure 1 shows the experimental setup for the data acquisition. For the source ²⁰² we use a P-wave transducer with a single-cycle sine wavelet at 200 kHz, generated through ²⁰³ the function generator (top left corner of Figure 1). This P-wave transducer has a diameter of

DRAFT May 1, 2021, 10:27am DRAFT

X - 12 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

10 mm. For the receivers, we use a laser vibrometer that measures the particle velocity along 204 the direction of the laser beam (perpendicular to the surface), and sends it to the oscilloscope 205 to be saved. The laser measures the signal at 160 points along the tape, giving us a total of 206 160 receivers with a sampling distance of 0.5 mm. The nearest offset in this case is 10 mm. 207 Figure 1 top right corner shows the signal reading at the nearest offset for the baseline case. 208 Throughout the data acquisition the P-wave transducer is glued to the Plexiglas box, and the 209 laser is attached to a stage that stably moves it along the tape. This allows for a controlled and 210 repeatable time-lapse experiment. Summarising, the experimental set-up allows us to record 211 160 "wiggles" for each of the two different reservoir-states, composing two "shot-gathers". For 212 the first 100 wiggles in each shot-gather, clear arrivals from the surface and the reservoir can 213 be separated. These shot-gathers compose a homogeneous, discrete (x, t)-space, where x is the 214 wiggle offset, and t is the recording time (Figure 2). In general, we use the first shot-gather from 215 the first reservoir-state experiment as the "baseline survey" (Figure 2a). We combine the wiggles 216 for the two experiments to simulate different monitoring scenarios. For example, in Figure 2b, 217 we mimic: (a) the misplacement of some sensors (wiggles between 15 and 25), replacing the 218 correct baseline wiggles with wiggles from the baseline survey but with a four-wiggles shift; 219 and (b) the presence of changes in the reservoir (wiggles 60 to 90), replacing wiggles from the 220 baseline with wiggles from the second reservoir-state experiment. Point-wise measurements of 221 the squared difference between baseline and monitor surveys can be larger for misplacement 222 sensors than for reservoir alteration (Figure 2c), making the discrimination between the two 223 effects quite challenging. 224

To test our methodology, we used one in five wiggles for the first 100 wiggles, thus, we collect 20 "traces" for each survey, $N_w = 20$. Downsampling the number of wiggles allows

DRAFT

²²⁷ us to have enough data for simulating the misplacement of the receiver in the monitor survey. ²²⁸ In the following, we continue to call "wiggles" the recording for a single detector position as ²²⁹ a function of time in each shot-gather, and we call "traces" the wiggles selected to compose ²³⁰ the baseline and monitor surveys. Each trace is composed of $N_s = 1251$ samples. Thus, our ²³¹ (x, t)-space is composed of $N_w \cdot N_s = 25020$ data-points.

2.1. Error statistics

To rigorously compare the monitor and baseline survey we need to know how the errors are 232 statistically distributed in the two data-sets, i.e. the error covariance matrix. Computing the 233 rank of such a large $(N_w \cdot N_s) \times (N_w \cdot N_s)$ matrix could be intractable. To avoid this, we estimate 234 the covariance matrix from the data themselves with the following assumptions. First, we do 235 not consider inter-trace correlation, so our model of the covariance matrix is block-diagonal, 236 one block for each trace. Note that this assumption means that near-by traces are not correlated, 237 which could be un-realistic under some scenarios, e.g. weather conditions, acquisition systems 238 and so on. Second, we assume the same error statistics for the baseline and monitor surveys. 239 Again, this assumption could be partially false for, e.g., surveys acquired with a large (10s of 240 years) time-gap. However, under our assumptions, we can estimate a tractable error covariance 241 matrix $C^*_{e,ii}$ which can be decomposed following the approach developed in Malinverno and 242 Briggs [2004], with an adequate correlation model [Kolb and Lekić, 2014]. 243

Given the nature of our data, i.e. band-limited waveforms, our covariance matrices are semipositive definite Toeplitz matrices and they can be decomposed as:

$$\mathbf{C}_{\mathbf{e}\,\mathbf{i}\mathbf{i}}^* = \mathbf{S}\mathbf{R}\mathbf{S} \tag{4}$$

where:

DRAFT

May 1, 2021, 10:27am

$$\mathbf{S} = \begin{pmatrix} \sigma_{1,1} & 0 & 0 & \dots & 0 \\ 0 & \sigma_{2,1} & 0 & \dots & 0 \\ 0 & 0 & \sigma_{3,1} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sigma_{N_s,N_w} \end{pmatrix}$$
(5)

represents the diagonal matrix containing the standard deviation of each data point b_{ij} in the

²⁴⁸ baseline [*Malinverno and Briggs*, 2004].

With the assumption of independent traces, the correlation matrix \mathbf{R} can be represented as a 249 block-diagonal matrix with N_w blocks, each of dimension: $N_s \times N_s$. The block \mathbf{R}_i represents 250 the error correlation within the *j*-th trace and can be estimated from the data [*Piana Agostinetti* 251 and Malinverno, 2018; Piana Agostinetti and Martini, 2019]. However, such data-derived cor-252 relation matrices \mathbf{R}_i are often not positive definite and need to be approximated, e.g., with the 253 singular value decomposition, to use them for estimating the covariance matrix and computing 254 the likelihood $L(\mathbf{m}_{cand})$. In this study, we make use of a correlation model that results in posi-255 tive definite matrices and guarantees stable matrix inversion [Kolb and Lekić, 2014]. Thus, our 256 blocks \mathbf{R}_i assume the form: 257

$$\mathbf{R}_{j} = R_{ik,j} = e^{-\lambda_{j}|t_{i}-t_{k}|} \cos\left(\lambda_{j}\omega_{j}|t_{i}-t_{k}|\right)$$
(6)

where t_k and t_i are the time of the b_{kj} and b_{ij} samples, respectively, while λ_j and ω_j are estimated from the data in the *j*-th trace. In Figure 3, we illustrate the computation of σ_{ij} , λ_j and ω_j . In Figure 3a, we show how we estimate the standard deviation of each point in each trace. For the *j*th trace (red), we consider all traces between *j*-5 and *j*+5 and we compute a stack of these traces (Figure 3b). From the stack, we compute a residual for each trace considered (Figure 3c) and the residuals are autocorrelated. The autocorrelation functions are stacked to obtain an average

DRAFT May 1, 2021, 10:27am DRAFT

²⁶⁴ autocorrelation (orange line in Figure 3d). This function is used to estimate λ_j and ω_j (green line ²⁶⁵ in Figure 3d), through a 2-parameter grid search. Our model for the autocorrelation function ²⁶⁶ fits the empirical function well before $10\mu s$ and somewhat over-estimates sample correlation at ²⁶⁷ longer periods, thus it should be considered a conservative model.

3. Exploration of the data-space through trans-dimensional sampling: methodology

Exploring the data space of 4D seismics implies the separation of multiple sources for the 268 "4D signal" (i.e. the signal arising when monitor and baseline surveys differ). Here we consider 269 a simplified case using three signal sources: ambient random noise (*noise*, hereinafter), sensor 270 misplacement (*perturbation*) and physical changes in the reservoir (*target signal*). With perfect 271 survey repetition (no sensor misplacement) and no change in the reservoir, the unique source 272 of 4D signal is the noise. Assuming an empirically estimated noise model, we can define our 273 working hypothesis: in the case of a unique source of 4D signal from the noise, the fit of the 274 monitor survey with respect to the baseline survey should close to the number of data-points 275 $N_w \times N_s$, where the fit is statistically represented by:

$$\phi^* = \left(\mathbf{e}_{\mathbf{i}\mathbf{j}}^{\mathrm{T}} \left(2 \times \mathbf{C}_{\mathbf{e},\mathbf{i}\mathbf{j}}^* \right)^{-1} \mathbf{e}_{\mathbf{i}\mathbf{j}} \right),\tag{7}$$

²⁷⁷ which is used to compute the likelihood of the monitoring to the baseline survey:

$$L^* = \prod_{i=1}^{N_w} \frac{1}{[(2\pi)^{N_s} | 2 \times \mathbf{C}^*_{\mathbf{e}, \mathbf{ij}} |]^{1/2}} \exp\left(-\frac{1}{2}\phi\right),\tag{8}$$

and we assume Gaussian distributed noise with the error model defined in Section 2.1. Here, the covariance matrix $C_{e,ij}^*$ is directly estimated from the data through their autocorrelation and

D R A F T May 1, 2021, 10:27am D R A F T

X - 16 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

their standard deviation. It is interesting to note that the likelihood computation is what we need to advance our McMC sampling, following Equation 3.

When there signals in the 4D data caused by different sources, we can adopt a Hierarchical 282 Bayes approach to define a different configuration for the covariance matrix so that the new 283 covariance matrix will again closely fit our error model and the working hypothesis defined by 284 Equation 8. As detailed in *Bodin et al.* [2012a], modifications to the covariance matrix obtained 285 through a Hierarchical Bayes algorithm not only represent improved estimates of the data un-286 certainties, but also include any additional source of uncertainty arising from, e.g., un-realistic 287 modelling or, as in our case, incorrect assumptions. In fact, the likelihood function above does 288 represent the differences in the two surveys in case of noise only (our assumption), and the 289 covariance matrix needs to be modified appropriately when this hypothesis is violated. In the 290 case of sensor mis-placement (i.e. when errors occur in the geometry of the monitor survey), 291 the modification of the covariance matrix should be the same for all the points belonging to 292 the misplaced traces. Conversely, when changes in the reservoir occur, the covariance matrix 293 needs to be modified only for those seismic phases generated at the top of the reservoir for some 294 consecutive traces (in our simplified data, from the top and the bottom in field measurements). 295 Summarising, we will try to define a different structure for the covariance matrix so that the 296 modified covariance matrix will approximate our error model. 297

3.1. Partition of the error covariance matrix

Here we define a new structure of the covariance matrix as an unambiguous correspondence between a partition of the data and a partition of the covariance matrix, so that separating regions of the data space separates distortions in the covariance. Given the properties of the covariance

DRAFT

matrix and assigning a relevant weight to each sampled point (x,t), we can create a modified covariance matrix such as

$$\mathbf{C}_{\mathbf{e},\mathbf{ij}}(\mathbf{m}) = \mathbf{W}(\mathbf{m}) \times 2 \times \mathbf{C}_{\mathbf{e},\mathbf{ij}}^* \times \mathbf{W}(\mathbf{m})$$
(9)

303 where

$$\mathbf{W}_{ii}(\mathbf{m}) = 10^{w_{ij}(\mathbf{m})},\tag{10}$$

and w_{ij} is a weight associated to sample point (x,t), derived by the model sampled during the 304 McMC process. Note that our assumptions on the original covariance matrix (block-diagonal 305 matrix generated from a modelled correlation function) are not necessary for generating $C_{e,ij}$. 306 Thus, the following discussion can be generalized to any covariance matrix. The goal now is to 307 generate sensitive weights for all points, to be able to separate the portion of the monitor survey 308 where the signal follows the likelihood in Equation 8, from the signal where other distortions 309 are present. Given the nature of the distortions considered here, we can assume that, in the 310 case of the misplacement of a single sensor, all the weights associated to the corresponding 311 trace have to be modified by the same amount. This means that, for a given j, the weights w_{ii} 312 would be the same for one entire block along the diagonal of the covariance matrix, associated 313 to the misplaced trace. Conversely, in case of a change in the reservoir, all weights associated 314 to the same seismic phase need to be homogeneously modified. Thus, w_{ii} would be the same 315 for the same time interval across different traces (assuming an almost flat interface generating 316 phases arriving almost at the same time at the receivers, as in Figure 2a at about 70μ s). This 317 second kind of distortion strongly impacts the covariance matrix, equivalently modifying many 318 blocks along its diagonal. Having homogeneous weights for different portions of the covariance 319

X - 18 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

matrix, we can create a partition of the covariance matrix based on the corresponding partition of the (x, y)-space associated to the relevant distortion. Giving the nature of our algorithm, i.e. a new way for elaborating partitions of the data, it could be categorized as a member of the family of clustering algorithms, where the number of cluster is not pre-specified by the user or chosen during or after the data analysis, but it is self-defined by the data themselves [e.g. *Mechelen et al.*, 2018].

326 3.1.1. Model parameterization

We model our partition of the covariance matrix as rectangular partitions of the data-space 327 (Figure 4). Our model is represented by a variable number of rectangular patches (so-called 328 *cells*) that cover the data-space, where each patch has an associated constant weight. In detail, 329 our model **m** is composed of a scalar *n* and five *n*-vectors, $\mathbf{m} = (n, \mathbf{c}_n, \mathbf{r}_n, \mathbf{t}_n, \mathbf{s}_n, \pi_n)$, where *n* is 330 the number of cells, c_n the vector of position of cell centres along the x-axis, r_n the vector of 331 cell radii along the x-axis, t_n the vector of the time-position of the cell centres along the time 332 axis, s_n the vector of the time-width of the cells, and π_n the vector of the cell weights. Keeping 333 the model definition in mind, we can assume that the relevant weight for each point in the data 334 space is the sum of the weights of the cells that extend to cover that particular point: 335

$$w_{ij}(\mathbf{m}) = 0 \quad \text{if} \quad x_{ij} \notin C_m \forall m = 1, ..., n$$

$$(11)$$

$$w_{ij}(\mathbf{m}) = \sum_{m=1}^{n} \pi_m \quad \text{if} \quad x_{ij} \in C_m$$
(12)

where C_m represents the time-space extension of the cell associated to the *m*-th nucleus, i.e.:

$$x_{ij} \in C_m \Leftrightarrow \begin{cases} c_m - 1/2 \cdot r_m < x_i < c_m + 1/2 \cdot r_m, \\ t_m - 1/2 \cdot s_m < x_j < t_m + 1/2 \cdot s_m \end{cases}$$
(13)

Having defined the weight for each data point as a function of the partitioning model of the data space, we now have most of the elements for sampling the model space according to

our McMC strategy. In fact, the weights define the likelihood of the model from Equation 8 substituting $C_{e,ij}$ for $C^*_{e,ij}$, i.e.:

$$L(\mathbf{m}) = p(\mathbf{d} \mid \mathbf{m}) = \prod_{i=1}^{N_w} \frac{1}{[(2\pi)^{N_s} |\mathbf{C}_{\mathbf{e}, \mathbf{ij}}|]^{1/2}} \exp\left(-\frac{1}{2}\phi\right),\tag{14}$$

where:

$$\phi = \left(\mathbf{e}_{ij}^{\mathrm{T}} \mathbf{C}_{\mathbf{e},ij}^{-1} \mathbf{e}_{ij}\right). \tag{15}$$

The novelty of our approach resides in the fact that, differently from standard McMC schemes, here the dependence of the likelihood function on the model is solely expressed in the covariance matrix and not in the residuals **e** [e.g. *Malinverno*, 2002].

³³⁹ Our choice of rectangular cells is optimal for the case of vertical and horizontal anomalies, ³⁴⁰ because the trans-D sampler can easily mimic this kind of distortions with a limited number of ³⁴¹ cells. However, all models sampled from the PPD will have vertical and horizontal boundaries, ³⁴² thus generating a somewhat "blocky" PPD. For more complex, i.e. dipping, anomalies, more ³⁴³ general functions such as "anisotropic Gaussian kernels [*Belhadj et al.*, 2018] can be adopted.

3.2. Priors

To make Bayesian inferences about the data partitions we define appropriate prior probability 344 distributions on the model parameters. We make use of uniform probability distributions be-345 tween minimum and maximum values for all investigated parameters. Minimum and maximum 346 values are reported in Table 2. Uniform priors have several advantages from a computational 347 point of view, and keep the number of pieces of prior information to a minimum (two values per 348 parameter). We do not impose any constraints on the radius and time-window parameters for 349 cell centres approaching the boundary of the (x,t) space, i.e. some cells could span outside the 350 (x,t) space (this is the reason why some cells seem to have their centres not exactly in the middle 351

DRAFT

X - 20 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

of the cells in Figure 4). While this assumption can introduce some combinations of parameters with very limited impact on the likelihood function (e.g. when c_m is close to one or close to N_W and r_m is small), the /it parsimonious behaviour of our trans-D approach guarantees that useless cells are removed from the model at some point, thus avoiding keeping too many cells.

3.3. Candidate selection

We now need to define how to progress in our McMC sampling, i.e. how to propose a new candidate model to be compared to the current one, the so called *recipe*. Defining an efficient recipe, in terms of convergence to the global maximum of the likelihood function and ability to explore a (potentially) multi-modal distribution, is fundamental for keeping the required computational resources reasonable.

Our recipe comprises seven moves, each of which represents a different way of perturbing the current model. During the definition of the candidate model only one of the moves is performed. Moves are selected with different probability. In detail, we define the following moves:

1. perturb the time-position t_n of a randomly picked cell nucleus (this move has a probability of 0.15 to be selected);

- 2. perturb the space-position c_n of a randomly picked cell nucleus (0.15)
- 367 3. perturb the time-extension s_n of a randomly picked cell nucleus (0.15);
- 4. perturb the space-extension r_n of a randomly picked cell nucleus (0.15);
- 5. perturb the weight π_n of a randomly picked cell (0.2);
- $_{370}$ 6. birth of a new cell: one cell is ad dded to the model (0.1);
- $_{371}$ 7. death of a cell: one cell is removed from the model (0.1).

DRAFT

Perturbation of the parameters in moves [1]-[5] are made according to the scheme in Ap-372 pendix A in Piana Agostinetti and Malinverno [2010]. Following this scheme, the nor-373 mal proposal distributions for sampling the uniform priors have the following variances σ_i^2 : 374 $\sigma_1^2 = \sigma_3^2 = 8 \times 10^{-3}$ for moves [1] and [3]; $\sigma_2^2 = \sigma_4^2 = 0.0025$ for moves [2] and [4]; 375 $\sigma_5^2 = 10^{-6}$ for move [5]. Moves [6] and [7] are called trans-dimensional moves because they 376 imply the changing of the number of variables associated to the candidate model with respect 377 to the current model. Such moves are defined as in Appendix B in Piana Agostinetti and Ma-378 *linverno* [2010], so that the determinant of their Jacobian matrix is equal to 1. We follow the 379 approach developed in *Mosegaard and Tarantola* [1995] for moves [6] and [7]. Thus, we make 380 use of a sampler that walks across the prior distributions (the so-called sampling from the priors 381 approach), and we accept or reject the candidate model with the probability in Equation 3. It 382 is worth noticing that sampling from the priors can be quite inefficient if the data contain a lot 383 of information about the investigated parameters, and thus the PPD likely differs from the prior 384 probability distribution. On the contrary, if there is limited information contained in the data, 385 sampling from the priors is a convenient sampling strategy, as it removes the need to define a 386 proposal distribution [as in, e.g., Bodin et al., 2012a]. 387

4. Results

4.1. Simple cases: Misplaced sensors or changes in the physical properties of the rocks

In this section we consider three simple tests. As a first illustration of the algorithm, we construct a monitor survey which mimics the mis-placement of some sensors (Figure 5). The baseline survey is composed of twenty traces (Wiggle numbers: 5, 10, 15, ..., 100) from the first experimental set-up (Plexiglas/air). For the monitor survey, we use the same traces as in the baseline survey, and substitute five traces (Wiggle numbers: 50, 55, ..., 70) with shifted

X - 22 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

traces (Wiggle numbers: 54, 59, 64,..., 74, all positions have been shifted by the same amount) 393 from the same Plexiglas's/air experimental set-up. In this way, the amplitude of the arrivals 394 do not have relevant changes, but we introduce a temporal shift. It is worth noticing that the 395 number of traces used, the number of shifted traces, and the shift amplitude have been selected 396 to keep a reasonable number of traces in the inversion (20 wiggles out of 100 available) while 397 having enough space to introduce a significant shift in the traces (four wiggles). The results are 398 obtained by running 5 parallel McMC samplings. Each chain is composed of 2×10^6 models, 399 half of which are discarded as part of the burn-in phase [Somogyvari and Reich, 2019]. For each 400 chain, we used 20 CPUs on a Linux cluster for about 17 hours. The full computation time was 401 about 5x350 core-hours. Computation time is almost constant across all tests presented in this 402 study, due to the same number of traces and the limited number of rectangular cells used by the 403 trans-D sampler. 404

In Figure 5, we show the most relevant information extracted from the PPD, together with the 405 monitor and baseline surveys. The misplaced traces in the monitor survey are marked (yellow box in Figure 5b). For each point in the discrete (x, t)-space, we compute the 1D marginal PPD 407 of w_{ij} and plot its mean posterior value (Figure 5c) and standard deviation (std, Figure 5d). 408 As a rule of thumb, high values of the mean posterior w_{ii} indicate regions where the baseline 409 and monitor surveys differ the most. Low and high values of the std differentiate well- and 410 less- constrained regions, respectively. Our results illustrate how the algorithm works in this 411 simple case. Due to the kind of distortion used, i.e. misplaced sensors, we should attribute 412 almost the same weight to the entire set of misplaced traces. The algorithm accomplishes this 413 task using a limited number of rectangular cells (about 20 cells, see Figure S1), confined in 414 the vertical area of misplaced traces. The std also displays the same pattern with low values 415

DRAFT

⁴¹⁶ indicating a robust result. Due to the realistic nature of our test (traces obtained in laboratory ⁴¹⁷ and not synthetic traces), the results are not "perfect" and there are some anomalies (higher ⁴¹⁸ std for surface arrivals and a vertical stripe in the std plot within the misplaced traces) due to ⁴¹⁹ complexity in the experimental set-up (hardware noise).

The performance of the algorithm (Figure S1) highlights some key-aspects of the sampling. First, we are not overfitting the data because the number of cells in the sampled models is limited, and thus so is the number of inverted parameters. The acceptance probability for trans-D moves is very low, so we need long chain (> 1 million of models) to guarantee the necessary exploration of the data-space. However, after 1 million models, the number of cells used is almost stable between 15 and 30, but not constant, i.e. chains are still sampling models with variable number of dimensions but within a limited range of values.

Our second test is designed to complement the previous one and considers a monitor survey 427 where only changes in the reservoir state are present (Figure 6). In this case, we make use of the 428 same baseline as in the previous test, but in the monitor survey we substitute five traces (Wiggle 429 number: 50 to 70) with the traces recorded at the same position but for the Plexiglas/water 430 experimental set-up. Both posterior mean and std of w_{ij} share the same structure, with a vertical 431 block and a pinched horizontal structure. The main difference in the results, with respect to 432 the previous test, is the presence of a dark (large weights) spot in the location of the change 433 in the reservoir-state, i.e. limited to the arrivals from the top of the reservoir and not including 434 the surface waves (Figure 6c). Also, while the results contain a vertical stripe in the mean 435 posterior w_{ii} in the region of the reservoir changes, as in Figure 5c, the std along the same stripe 436 is very large. Horizontally, the rectangular cells seem to be able to move slightly and the dark 437

DRAFT

May 1, 2021, 10:27am

region in the mean posterior w_{ij} (defining the reservoir changes) propagates across some traces, suggesting a higher vertical than horizontal resolution.

The third test considers the presence of both reservoir-changes and receiver misplacement 440 in two separated regions of the (x, t)-space (Figure 7). In this case, while the baseline is kept 441 the same as in previous tests, the monitor survey is composed as follows: for the misplaced 442 sensors, three traces (wiggle numbers 15, 20 and 25) are replaced with wiggles from the same 443 experimental set-up but with a 4 wiggle shift (so replaced with wiggle numbers: 19, 24 and 29); 444 for the reservoir-changes, we substitute seven traces from 60 to 90, with the wiggles recorded 445 in the same position but with the second experimental set-up. Note that the number of traces 446 representing the two anomalies is different from the previous tests, to keep them separated and 447 to be able to split it into two regions (see next section). 448

The results clearly show that, in the case of not-interacting anomalies, the two kinds of distor-449 tions can be separately identified (Figure 7c). Both anomalies can be seen in the mean posterior 450 of w_{ii} with the same characteristics as in the previous tests. In the analysis of the std there is 451 a clear difference, with respect to the previous tests, in the bright spot defining the reservoir-452 change, but also in the value (lower here) of the vertical stripe defining the misplaced sensors. 453 However, such changes could be attributed to the different numbers of traces composing the 454 anomalies (Figure 7d), indicating that the std is more sensitive to the lateral extension of the 455 anomaly than to the mean posterior value. 456

4.2. Complex case: simultaneous retrieval of misplaced sensor and changes in the physical properties of the rocks

The most interesting case represents the co-existence of both misplaced receivers and reservoir-changes in the same region of (x, t)-space. To test this, the baseline is kept the same

as in previous tests. The monitor survey is composed of the baseline traces with substitutions in 459 three different and contiguous regions. In the first region, called "A", six traces are substituted 460 by shifted wiggles from the same experimental set-up (i.e. mimic misplacement receivers only: 461 wiggles numbers 30, 35, ..., 55 are replaced with 34, 39, ..., 59). Also in the second region 462 "B" we have misplaced traces (three traces, wiggles numbers 60,65 and 70 replaced with 64, 69 463 and 74) but from the second experimental set-up, to simultaneously reproduce both misplaced 464 receivers and reservoir-changes. Finally in the third region "C", we consider reservoir changes 465 only. Four traces (wiggles numbers 75 to 90) are replaced with the wiggles recorded in the same 466 position, but from the second experimental set-up. The minimum region dimension is three 467 traces, but the "misplaced sensors" anomaly covers nine traces, while the "reservoir-changes" 468 anomaly covers seven traces (Figures 8 and 9). 469

As expected, the outcomes from a complex case are more challenging to describe. The mean 470 posterior of w_{ij} still clearly defines the reservoir changes as a dark (large values) elongated 471 region that covers exactly the expected traces (Figure 8 and Figure 9b). However, recognizing 472 the boundaries between regions "A" and "B", and "B" and "C" is not easy in the mean posterior. 473 In fact the value of the mean posterior of w_{ii} does not change significantly through regions "A" 474 to "C" away the reservoir-changes zone, with fluctuation given by experimental noise and lateral 475 smearing of the reservoir-changes anomaly. It is hard to recognise which traces have only been 476 shifted (from the region between traces number 1 to 5 where the two surveys share the same 477 wiggles) or which traces are both shifted and have a reservoir-change. Knowing the monitor 478 survey composition, we can see that more traces than the ones composing region "C" have been 479 locally perturbed, from the occurrence of the high-weights at localised times (dark region), but 480

DRAFT

May 1, 2021, 10:27am

X - 26 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

we cannot really discriminate which of the traces that also have the reservoir-change signature
 have been displaced.

The results for the posterior std of the w_{ij} furnish some additional insights into the separation of the three regions. In fact, comparing both mean and std shows that the posterior std is generally uniform, but very large in the region where we only have reservoir changes (as seen also in Figure 6). The posterior std is lower and more variable for the region where we have misplaced traces (both with and without simultaneous reservoir changes). In practise, only the simultaneous analysis of both mean and std posterior for w_{ij} can somewhat unequivocally define the three regions.

Finally, the posterior std is very low in the core of the reservoir-changes anomaly, as found in the previous test (compare to Figure 8d), likely caused by the large lateral extent of the anomaly (quite large, seven traces (one third of the total)). Moreover, we observe that the area of the std where we only have misplaced sensors is not uniform as expected, due to the interaction with the reservoir anomaly (anomaly lateral smearing). However, the std is large where the two anomalies interact.

5. Discussion

We propose a new methodology for exploring 4D seismic data and detecting potential noise sources other than random ambient noise, and relevant signals from the alteration of a reservoir. The algorithm has been proven to correctly perform in isolating simple case scenarios (one noise source or one reservoir change, or both present in two different portions of the 4D seismic data). In such cases, our algorithm identifies the different anomalies and their position, and it is able to characterise them in terms of both the amplitude of the posterior weights and their standard deviation. In particular, anomalous signals related to a misplacement of the sensors is identified

D R A F T May 1, 2021, 10:27am D R A F T

as a broad portion of the monitoring survey where the posterior weights are uniformly increased by a limited amount, and their standard deviation is uniform too. Conversely, in the portion of the monitoring survey where the anomaly is related to a reservoir change, the posterior weights are extremely high in a localised 2D patch. Their standard deviation also displays a peculiar pattern, with very low values in the inner portion of the anomaly and very high values along its border. We suggest that the rapid change in the standard deviation is the key-element that can define the shape of the anomaly related to reservoir changes.

In more complex cases, i.e. where both noise sources and reservoir signals coexist, the 510 interpretation of the results is more challenging. Dis-aggregating co-existing changes/mis-511 positioning is not easy (Figure 9), but we observe that reservoir changes are always the most 512 striking and isolated feature. Also in this case, the analysis of the standard deviation of the 513 weights is a critical point for making inferences. In fact, even here the sharp change in the 514 standard deviation defines the border of the anomaly given by reservoir changes. Moreover, 515 the standard deviation also helps to define the area where the mis-placed sensors are present 516 (these regions have a lower standard deviation compared to area where only reservoir changes 517 are present). It is worth noting that the estimation of the standard deviation of the weights is a 518 brand new outcome of our algorithm, given by our statistical approach to data-space exploration. 519 Our results display to some extent the boundaries of our rectangular patches (i.e they seems 520 to have a block-structure). Such blockiness indicates the resolution limits of our model to some 521 extent, and are related to our choice of rectangular partitions. In trans-D algorithms, the effects 522 of the parameterization on the retrieved results is an on-going research field [e.g. *Gao and Lekic*, 523 2018]. Here, we suggest that other choices of partition shape could be more efficient on bigger-524

DRAFT

May 1, 2021, 10:27am

X - 28 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

scale data, such as the *anisotropic kernels*, proposed in *Belhadj et al.* [2018], which could more easily reproduce the true shape of anomalies in field measurements.

Our approach to 4D seismic data analysis could be used to support more complex data work-527 flows adopted in energy industries. In Figure 10, we compare the results of our complex case, 528 with a standard analytic indicator (NRMS) commonly used in data-workflow for 4D seismics. 529 Comparing Figure 10a and 10b, it seems that mis-positioning is the most impactful issue in 530 terms of likelihood between baseline and monitoring surveys, but it is easily separated from 531 reservoir changes, which have the strongest W_{ii} in our case. As seen in Figure 10c, NRMS is 532 clearly higher in the area of sensor misplacement. Such an anomaly masks the signal coming 533 from the "altered conditions in the reservoir". In fact such a signal can be seen as a small am-534 plitude anomaly (i.e. around 40% at trace 16-19, still higher NRMS with respect to trace 1-5 535 where no anomaly is present at all), but it is totally obscured between traces 11 and 15, where 536 the dominant effect is the sensor misplacement. Our approach could be used as a support to 537 standard data-workflow and could save time during subsequent physical modelling of the reser-538 voir (an extremely time-consuming task). Because it makes no preliminary assumption on the 539 reservoir geometry, our approach does not risk bringing an initial bias into the results and thus 540 could furnish more reliable information on the state of the geo-resources. 541

6. Conclusions

In this study, we presented a new methodology for the exploration of the data-space. We followed a trans-D sampling approach to recreate and validate data-structures in the form of partitions of the covariance matrix. We applied the new methodology to 4D seismic data acquired for monitoring the sub-surface. Our results indicate that:

DRAFT

May 1, 2021, 10:27am

the trans-D approach can be applied to data-space exploration for defining unknown data structures and separating data-volumes that are coherent with a-priori physical hypotheses;

⁵⁴⁸ 2. the analysis of the full PPD of the data-structures can be used for classifying different ⁵⁴⁹ sources of 4D signal, like repeatability noise and 4D signal from the geo-resources;

⁵⁵⁰ 3. In comparison with standard measures of repeatability like NRMS, our approach is less ⁵⁵¹ biased by the presence of different sources if 4D signal in the same data-volume and can be ⁵⁵² used to efficiently separate such sources.

In the future, we will further develop our methodology to include different shapes and orientation of the partitions [i.e. not rectangular patches, also called *anisotropic kernels, as in Belhadj et al.*, 2018] for increasing the efficiency of the McMC sampling; and to consider 3D partitions and the comparison of two entire 3D volumes.

7. Acknowledgements

NPA would like to thank Daniele Melini at INGV for assistance with the linux cluster. NPA 557 publications are printed with the financial support of the Austrian Science Fund (FWF), project 558 number: M2218-N29. We are also grateful for support at Memorial provided by Chevron and 559 with grants from the Natural Sciences and Engineering Research Council of Canada Industrial 560 Research Chair Program and InnovateNL (IRCPJ 491051-14). We would also like to thank 561 Kamal Moravej for his help and instructions at the lab in order to collect the data used in this 562 study. Raw data (i.e. waveform used as baseline and monitoring surveys) can be requested to 563 MK via email: mk7251@mun.ca. The Generic Mapping Tools software was used for plotting 564 the figures of this manuscript [Wessel and Smith, 1998]. 565

DRAFT

May 1, 2021, 10:27am

References

⁵⁶⁶ Bayes, T. (1763), An essay towards solving a problem in the doctrine of chances, *Philos. Trans.*

⁵⁶⁷ *R Soc. London*, *53*, 370–418.

- Belhadj, J., T. Romary, A. Gesret, M. Noble, and B. Figliuzzi (2018), New parameteriza-
- tions for bayesian seismic tomography, *Inverse Problems*, *34*(6), 065,007, doi:10.1088/1361 6420/aabce7.
- ⁵⁷¹ Birnie, C., K. Chambers, D. Angus, and A. L. Stork (2020), On the importance of benchmarking
- ⁵⁷² algorithms under realistic noise conditions, *Geophysical Journal International*, 221(1), 504–
 ⁵⁷³ 520, doi:10.1093/gji/ggaa025.
- ⁵⁷⁴ Bodin, T., M. Sambridge, N. Rawlinson, and P. Arroucau (2012a), Transdimensional tomogra-
- ⁵⁷⁵ phy with unknown data noise, *Geophys. J. Int*, doi: 10.1111/j.1365-246X.2012.05414.x.
- ⁵⁷⁶ Bodin, T., M. Sambridge, H. Tkalcic, P. Arroucau, K. Gallagher, and N. Rawlinson (2012b),
- 577 Transdimensional inversion of receiver functions and surface wave dispersion, J. Geophys.
- ⁵⁷⁸ *Res.*, *117*(B02301), doi:10.1029/2011JB008560.
- ⁵⁷⁹ Cheng, A., L. Huang, and J. Rutledge (2010), Time-lapse VSP data processing for monitoring
 ⁵⁸⁰ co2 injection, *The Leading Edge*, 29(2).
- Davis, T. L., M. J. Terell, R. D. Benson, R. Cardona, R. R. Kendall, and R. Winarsky (2003),
- ⁵⁸² Multicomponent seismic characterization and monitoring of the CO2 flood at Weyburn field,
- Saskatchewan, *The Leading Edge*, 22(7), 606–700.
- ⁵⁸⁴ Dettmer, J., and S. E. Dosso (2012), Trans-dimensional matched-field geoacoustic inversion
- with hierarchical error models and interacting Markov chains, J. Acoust. Soc. Am., 132(4),

⁵⁸⁶ 2239–2250.

PIANA AGOSTINETTI ET AL.:	TRANS-DIMENSIONAL DATA SPACE EXPLORATION	X - 31
---------------------------	--	--------

- ⁵⁸⁷ Dramsch, J. S. (2019), Machine learning in 4d seismic data analysis: Deep neural networks in ⁵⁸⁸ geophysics, Ph.D. thesis, Technical University of Denmark, Lyngby, Denmark.
- Galetti, E., A. Curtis, B. Baptie, D. Jenkins, and H. Nicolson (2016), Transdimensional Love-
- wave tomography of the British Isles and shear-velocity structure of the East Irish Sea Basin
- ⁵⁹¹ from ambient-noise interferometry, *Geophysical Journal International*, 208(1), 36–58, doi:
- ⁵⁹² 10.1093/gji/ggw286.
- ⁵⁹³ Gao, C., and V. Lekic (2018), Consequences of parametrization choices in surface wave inver-
- sion: insights from transdimensional Bayesian methods, *Geophysical Journal International*,
- ⁵⁹⁵ 215(2), 1037–1063, doi:10.1093/gji/ggy310.

⁵⁹⁶ Geyer, C. J., and J. Møller (1994), Simulation procedures and likelihood inference for spatial ⁵⁹⁷ point processes, *Scand. J. Stats*, *21*, 359–373.

- ⁵⁹⁸ Green, P. J. (1995), Reversible jump Markov chain Monte Carlo computation and Bayesian ⁵⁹⁹ model determination, *Biometrika*, 82(4), 711–732.
- Houck, R. T. (2007), Time-lapse seismic repeatability How much is enough?, *The Leading* Edge, 26(7), -.
- Kolb, J. M., and V. Lekić (2014), Receiver function deconvolution using transdimensional hierarchical Bayesian inference, *Geophysical Journal International*, *197*(3), 1719–1735, doi:
- 604 10.1093/gji/ggu079.
- Koster, K., P. Gabriels, M. Hartung, J. Verbeek, G. Deinum, and R. Staples (2000), Time-lapse
- seismic surveys in the North Sea and their business impact, *The Leading Edge*, 19(3), 286–
 293, doi:10.1190/1.1438594.
- Kragh, E., and P. Christie (2002), Seismic repeatability, normalized RMS, and predictability,
 The Leading Edge, 21(7), 640–647, doi:10.1190/1.1497316.

DRAFT

X - 32 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

- Landro, M. (1999), Repeatability issues of 3D VSP data, Geophysics, 64(6), -. 610
- Lumley, D. (2010), 4D seismic monitoring of CO₂ sequestration, The Leading Edge, 29(2), 611
- https://doi.org/10.1190/1.3304817. 612
- Malinverno, A. (2002), Parsimonious Bayesian Markov chain Monte Carlo inversion in a non-613
- linear geophysical problem, Geophys. J. Int., 151(3), 675–688. 614
- Malinverno, A., and V. A. Briggs (2004), Expanded uncertainty quantification in in-615 verse problems: Hierarchical Bayes and empirical Bayes, Geophysics, 69(4), 1005-1016, 616 doi:10.1190/1.1778243. 617
- Mechelen, I. V., A.-L. Boulesteix, R. Dangl, N. Dean, I. Guyon, C. Hennig, F. Leisch, and 618
- D. Steinley (2018), Benchmarking in cluster analysis: A white paper. 619
- Mosegaard, K., and A. Tarantola (1995), Monte Carlo sampling of solutions to inverse prob-620 lems, J. Geophys. Res., 100(B7), 12,431-12,447. 62
- Pevzner, R., V. Shulakova, A. Kepic, and M. Urosevic (2011), Repeatability analysis of land 622 time-lapse seismic data: CO2 CRC Otway pilot project case study, Geophysical Prospecting, 623 59(1), -. 624
- Piana Agostinetti, N., and A. Malinverno (2010), Receiver Function inversion by 625 trans-dimensional Monte Carlo sampling, Geophys. J. Int, 181, doi:10.1111/j.1365-626 246X.2010.04530.x. 627
- Piana Agostinetti, N., and A. Malinverno (2018), Assessing uncertainties in high-resolution, 628 multi-frequency receiver function inversion: a comparison with borehole data, *Geophysics*, 629 83(3), KS11–KS22, doi: 10.1190/geo2017-0350.1. 630
- Piana Agostinetti, N., and F. Martini (2019), Sedimentary basins investigation using teleseis-631 mic p-wave time delays, Geophysical Prospecting, 67(6), 1676–1685, doi:10.1111/1365-

DRAFT

632

May 1, 2021, 10:27am

633 2478.12747.

- Porter-Hirsche, J., and K. Hirsche (1998), *Repeatability study of land data acquisition and* processing for time lapse seismic, pp. 9–11, doi:10.1190/1.1820663.
- Roach, L. A. N., D. J. White, and B. Roberts (2015), Assessment of 4d seismic repeatability
- and co2 detection limits using sparse permanent land array at the aquistore co2 storage site, *Geophysics*, 80(2).
- Sambridge, M., and K. Mosegaard (2002), Monte Carlo methods in geophysical inverse prob-
- lems, *Rev. Geophys.*, 40(3), doi:10.1029/2000RG000,089.
- 641 Sambridge, M., K. Gallagher, A. Jackson, and P. Rickwood (2006), Trans-dimensional in-
- verse problems, model comparison and the evidence, *Geophys. J. Int.*, 167(2), 528–542,
- doi:10.1111/j.1365-246X.2006.03155.x.
- Sambridge, M., T. Bodin, K. Gallagher, and H. Tkalcic (2013), Transdimensional inference in
 the geosciences, *Phil. Trans. R. Soc. A*, *371*, 20110547.
- ⁶⁴⁶ Somogyvari, M., and S. Reich (2019), Convergence tests for transdimensional markov chains
- in geoscience imaging, *Math Geosci*, https://doi.org/10.1007/s11004-019-09811-x.
- Steininger, G., J. Dettmer, J. Dosso, and S. Holland (2013), Transdimensional joint inversion of
- seabed scattering and reflection data, J. acoust. Soc. Am., 133, 1347–1357.
- Tarantola, A. (1987), *Inverse problem theory: methods for data fitting and model parameter estimation*, Elsevier Science publishing Co.
- ⁶⁵² Tarantola, A. (2005), Inverse Problem Theory and Methods for Model Parameter Estimation,
- 653 SIAM.
- Tarantola, A. (2006), Popper, Bayes and the inverse problem, *nature physics*, 2.

DRAFT

May 1, 2021, 10:27am

- X 34 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION
- ⁶⁵⁵ Wessel, P., and W. H. F. Smith (1998), New, improved version of the generic mapping tools ⁶⁵⁶ released, *EOS Trans. AGU*, *79*, 579.
- Kiang, E., R. Guo, S. E. Dosso, J. Liu, H. Dong, and Z. Ren (2018), Efficient hierarchical trans-
- dimensional Bayesian inversion of magnetotelluric data, *Geophysical Journal International*,
- ⁶⁵⁹ 213(3), 1751–1767, doi:10.1093/gji/ggy071.
- Yang, D., A. Malcolm, M. Fehler, and L. Huang (2014), Time-lapse walkaway vertical seismic
- profile monitoring for CO_2 injection at the SACROC enhanced oil recovery field: A case
- study, *Geophysics*, 79(2).

	T
Variables	Description
$N_{\scriptscriptstyle W}$	number of traces in the survey
N_s	number of samples per trace
i, k	indices for samples
j	index for a trace
\mathbf{X}_{ij}	space (x_i) and time (x_j) position of the <i>i</i> -th point for the <i>j</i> -th trace
b_{ij}	amplitude of baseline survey at the <i>i</i> -th point for the <i>j</i> -th trace
m_{ij}	amplitude of monitor survey at the <i>i</i> -th point for the <i>j</i> -th trace
$\mathbf{e_{ij}} = (b_{ij} - m_{ij})$	sample-wise difference between baseline and monitor surveys (at the <i>i</i> -th point for the <i>j</i> -th trace)
Terms	Description
	Data
shot-gather	original data from the laboratory, one for each experimental set-up
wiggle	one recording (in time) at a fixed position within one shot- gather
survey	input data for the algorithm: new shot-gather composed of selected wiggles
trace	one recording of the survey
4D signal	differences in the monitoring and baseline surveys
T	Sources of 4D signal
1	riay 1, 2021, 10:27am
target signal	changes in reservoir properties

	Sources of the signal
DRAFT	<u>May 1, 2021, 10:27</u> am D R A F T
target sign	nal changes in reservoir properties
noise	ambient random noise
perturbati	ion sensor misplacement.
Table 1 Description	on of variables and terminology

X - 36 PIANA AGOSTINETTI ET AL.: TRANS-DIMENSIONAL DATA SPACE EXPLORATION

Model parameter	Minimum	Maximum
Number of cells, <i>n</i>	1	200
Cell centre along x-axis, c_n	1	20
Cell radius, r_n	1	10
Cell centre along t-axis, t_n	1	1251
Cell time-window, s_n	1	625
Weight, π_n	0.0	1.0

 Table 2. Uniform prior distributions of model parameters in the m vector.

Figure 1. Experimental setup and photos of the equipment. (a) function generator showing the parameters of the source pulse (b) oscilloscope showing an example of a recorded wiggle. The red spot on the model is the location of the laser receiver, which is moved vertically in controlled increments to generate wiggles at different locations, which are combined into the final shot record.

Figure 2. Example of seismic surveys: (a) Baseline survey using all wiggles generated with air/Plexiglas interface. (b) Monitor survey. Same wiggles as in (a), but: wiggles from 15 to 25 have been replaced with the wiggles from 19 to 29, same interface (simulating misplaced receivers); wiggles from 60 to 89 have been replaced with wiggles recorded in the same position but with a different interface (water/Plexiglas, simulating a change in the physical properties of the reservoir). (c) Squared differences of the two survey, computed for each sample separately. Notably the largest values are associated with "misplaced receivers". See Section 4.1 for the details of this experiment.

Figure 3. Example of data analysis for reconstructing the Covariance matrix of the error associated to trace 155. (a) Zoom of the traces close to trace 155. The yellow box indicates the traces used for estimating the standard deviation and the correlation model needed to compose the Covariance matrix. (b) Stack and standard deviation for the traces in the yellow box in (a). The orange line and the dashed orange lines represent the stack and the standard deviation, respectively. Grey lines report the traces in the yellow box in (a). (c) Residuals between the stack and each single trace in the yellow box in (a). (d) Auto-correlation of the residuals in (c). The orange line shows the average of all autocorrelation curves (grey lines). The green line displays the best-fitting curve, modelled using the function in Eq. 6 [*Kolb and Lekić*, 2014].

ADDITIONAL FIGURES

DRAFT

Figure 4. Example of a model. The rectangles represent the cell, coloured according to their weights. Where cells overlap, weights are summed. Each data point (dots) has an associated weight. Data points outside all cells are associated to a weight $w_{ij} = 0.0$. Yellow circles represent cell nuclei. To make the figure readable, only one of every 15 data-point is plotted.

Figure 5. Results for a simple case: misplacement of receivers. (a) Baseline survey. The grey area denotes where the signal is absent. (b) Monitor survey. See Section 4.1 for details on how the monitor survey is created. (c) Mean posterior weight w_{ij} associated to each data point (*i*-th sample on the *j*-th trace). (d) Posterior standard deviation of w_{ij} . The yellow box indicates the wiggles that changed between the Baseline and Monitor surveys.

Figure 6. Results for a simple case: changes in the physical properties of the reservoir. See Figure 5 for details.

Figure 7. Results for a complex case: misplacement of receivers and changes in the physical properties of the reservoir, separated. See Figure 5 for details.

Figure 8. Results for a complex case: misplacement of receivers and changes in the physical properties of the reservoir, overlapping. See Figure 5 for details. Yellow boxes indicate changes between monitoring and baseline surveys in Figure 5 have been removed for improving readability.

Figure 9. Details of the results for a complex case: misplacement of receivers overlapping changes in the physical properties of the reservoir. (a) Monitor survey. The three letters indicate different area with: [A] misplaced receivers; [B] misplaced sensors and changes in the reservoir, and [C] only changes in reservoir. (b) Mean posterior weight W_{ij} associated with each data point (*i*-th sample at the *j*-th trace). (c) Posterior standard deviation of W_{ij} . See Section 4.2 for details.

Figure 10. (a) Mean posterior weight W_{ij} associated with each data point (*i*-th sample at the *j*-th trace). Posterior standard deviation of W_{ij} is shown as red contour lines. See Section 4.2 for details. (b) Same as in Figure 2c, point-wise L₂ difference between monitoring and baseline surveys. (c) NRMS for each trace of the monitoring survey with respect to baseline survey. NRMS computed as in *Kragh and Christie* [2002]

Figure S1.Details on the trans-D sampling for the simple case: misplacement of receivers. (a) PPD for the number of sectors in the model. (b) Acceptance rate for the seven moves composing the recipe for the trans-D sampling. Outcomes for each move are labelled as: "+1", move has been accepted (candidate model improved the fit); "0", move has been rejected; "-1", move has been accepted, but the candidate does not improve the fit. (c) Variation of the number of cells in the sampled models for all five chains. A blue box indicates the "burn-in" period for which sampled models are not considered. Figure 1.



Figure 2.



Trace

Figure 3.



Time (μs)

Figure 4.



Figure 5.



 w_{ij}

0.6

0.8

1.0

0.4

0.0

0.2

 $\sigma(w_{ij})$ 0.00

0.01 0.02 0.03 0.04 0.05 Figure 6.



80

100

006

0.01

0.00

011

 $\sigma(w_{ij})$

0.02 0.03

016

0.04 0.05

80

100

011

0.6

 w_{ij}

0.4

006

0.2

0.0

016

1.0

0.8

Figure 7.







006 011 016

σ(w_{ij}) 0.00 0.01 0.02 0.03 0.04 0.05 Figure 8.





0

20

40

60

80

100



0.0

0.2

0.4

0.6

0.8

1.0

Traces



0

20

40

60

80

(d)



 $\sigma(w_{ij})$

011

016

0.01 0.00 0.02 0.03 0.04 0.05 Figure 9.







Figure 10.



Time (μs)