Bayesian geophysical inversion using invertible neural networks

Xin Zhang and Andrew Curtis

School of GeoSciences, University of Edinburgh, United Kingdom

E-mail: *xzhang15@ed.ac.uk*

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SUMMARY

Constraining geophysical models with observed data usually involves solving nonlinear and non-unique inverse problems. Mixture density networks (MDNs) produce an efficient way to estimate Bayesian posterior probability density functions (pdf's) that represent the non-unique solution. However it is difficult to infer correlations between parameters using MDNs, and in turn to draw samples from the posterior pdf. We introduce an alternative to resolve these issues: invertible neural networks (INNs). These are simultaneously trained to represent uncertain forward functions and to solve Bayesian inverse problems. In its usual form, the method becomes less effective in high dimensionality because it uses maximum mean discrepancy (MMD) to train the neural network. We show that this issue can be overcome by maximising the likelihood of the data used for training. We apply the method to two types of imaging problems: 1D surface wave dispersion inversion and 2D travel time tomography, and compare the results to those obtained using Monte Carlo and MDNs. Results show that INNs provide comparable posterior pdfs to those obtained using Monte Carlo, including correlations between parameters, and provide more accurate marginal distributions than MDNs. After training, INNs estimate posterior pdfs in seconds on a typical desktop computer. Hence they can be used to provide efficient solutions for repeated inverse problems using different data sets. And even accounting for training time, our results also show that INNs can be more efficient than Monte Carlo methods for solving single inverse problems.

1 INTRODUCTION

Geoscientists build models of the subsurface in order to understand properties and processes in the Earth's interior. The models are usually parameterized in some way, so to constrain the models we must solve a parameter estimation problem. Data are recorded which provide constraints. However, since the physical relationships between parameters and data usually predict data given the parameters (known as the forward calculation) but not the reverse, the solution must be found using inverse theory.

Geophysical inverse problems usually have non-unique solutions due to noise in the data, to nonlinearity of the physical relationships between model parameters and data, and to fundamentally unconstrained combinations of parameters. Uncertainties in parameter estimates must therefore be quantified in order to interpret inversion results correctly. Unfortunately, estimating uncertainty in nonlinear inverse problems can be computationally expensive, and the cost increases both with the number of parameters, and with the computational cost of the forward calculation. In this study we therefore solve two different types of seismic tomography problems which each have fewer than 100 parameters, and have relatively rapid forward functions (each evaluation takes on the order of seconds). This allows us to evaluate solutions sufficiently accurately to thoroughly test a new method of Geophysical inversion.

Geophysical inverse problems are traditionally solved by linearising (approximating) the nonlinear physics, and using optimization methods which seek a model that minimizes the misfit between observed and predicted data (Aki & Lee 1976; Dziewonski & Woodhouse 1987; Iyer & Hirahara 1993). However, despite their wide applications, linearised procedures cannot produce accurate estimates of uncertainty (Bodin & Sambridge 2009; Smith 2013; Galetti et al. 2015; Zhang et al. 2018). Methods based on nonlinear Bayesian formulations of inverse problems have been introduced to provide more accurate uncertainty estimates, including Monte Carlo sampling methods (Mosegaard & Tarantola 1995; Sambridge 1999; Malinverno et al. 2000; Bodin & Sambridge 2009; Galetti et al. 2015; Zhang et al. 2018) and variational inference (Nawaz & Curtis 2018, 2019; Nawaz et al. 2020; Zhang & Curtis 2020a,b).

Monte Carlo methods generate a set of samples from the posterior probability density function (pdf) which describes the remaining non-uniqueness amongst parameters after information in observed data has been considered (Brooks et al. 2011); those samples can be used thereafter to derive useful statistics which describe that pdf (e.g. mean, standard deviation, etc.). Monte Carlo methods are quite general from a theoretical point of view and can be applied to a range of inverse problems, for example, to surface wave dispersion inversion (Bodin et al. 2012; Shen et al. 2012; Young et al. 2013; Galetti et al. 2017; Zhang et al. 2018, 2020a), travel time tomography (Bodin & Sambridge 2009; Galetti et al. 2015; Piana Agostinetti et al. 2015; Fichtner et al. 2018; Zhang et al. 2020b) and full-waveform inversion (Ray et al. 2016, 2017; Gebraad et al. 2020; Khoshkholgh et al. 2020). However, such solutions are acquired at significant expense, typically requiring days or weeks of computer run time, and hence cannot be applied in scenarios that require rapid solutions such as real-time monitoring (Duputel et al. 2009; Cao et al. 2020), or when many similar inversions must be performed (Käufl et al. 2016).

Variational inference provides a different way to solve Bayesian inference problems. The method seeks an optimal approximation to the posterior pdf within a predefined, expressive family of probability distributions by minimizing the Kullback-Leibler divergence between the approximating pdf and the posterior pdf (Blei et al. 2017). Since the method solves the inference problem using optimization rather than stochastic sampling, it can be more computationally efficient than Monte Carlo methods. Variational methods have been applied to invert for geological facies and petrophysical properties (Nawaz & Curtis 2018, 2019; Nawaz et al. 2020), and for travel time tomography (Zhang & Curtis 2020a) and full waveform inversion (Zhang & Curtis 2020b). However, although variational inference can be relatively efficient, it still typically requires a large compute times to obtain solutions for the latter imaging problems, and therefore may not provide sufficiently rapid solutions for real-time monitoring, nor for cases where many similar inversions are required.

Neural network based methods offer another efficient alternative for certain classes of inverse problems that must be solved many times with new data of similar type. An initial set of Monte Carlo samples is generated from the pdf that describes the *a priori* information (the so-called prior pdf), and data are simulated for each of these samples. Neural networks are flexible mappings which can be trained to emulate any specific inverse mapping from data to parameter space by fitting this set of examples of that mapping (called the training data set; Bishop 2006). Thereafter the trained neural networks interpolate the inverse mapping between the training examples, and can therefore be evaluated efficiently for any new, measured data to provide estimates of corresponding parameter values. Hence they can be applied to applications that require solutions to many different inverse problems within the class of problems represented by the training data. Neural networks were first introduced to Geophysics by Röth & Tarantola (1994) to estimate subsurface velocity from active source seismic waveforms, and have been applied to seismic velocity inversion using earthquake data (Moya & Irikura 2010) and semblance gathers (Araya-Polo et al. 2018). Laloy et al. (2019) introduced vector-to-image transfer networks to solve inverse problems and applied them to transient groundwater flow and ground penetrating radar tomographic problems. Mosser et al. (2020) used so-called generative adversarial networks to re-parameterise geologically correlated Earth structure with a relatively low number of parameters, and inverted for the structure that best fit synthetic seismic waveform data.

The above studies did not provide estimates of uncertainties since for each input data vector their neural networks only predict one parameter vector. Devilee et al. (1999) proposed the first geophysical probabilistic form of neural networks which provide discretised Bayesian posterior pdfs, and used them to invert surface wave dispersion data for crustal thickness maps and their uncertainties across Eurasia. In an alternative formulation, mixture density networks (MDNs) output a probability distribution that is defined by a sum of analytic pdfs called kernels, such as Gaussian distributions, and can be trained to map data to corresponding posterior pdfs (Bishop 2006). MDNs have been applied to surface wave dispersion inversion (Meier et al. 2007a,b; Earp et al. 2020; Cao et al. 2020), 2D travel time tomography (Earp & Curtis 2020), petrophysical inversion (Shahraeeni & Curtis 2011; Shahraeeni et al. 2012), earthquake source parameter estimation (Käufl et al. 2014, 2015), and Earth's radial seismic structure inversion (de Wit et al. 2013). However MDNs become difficult to train in high dimensionality because of numerical instability, and they suffer from mode collapse, that is, some modes of the posterior pdf are missing in the results (Hjorth & Nabney 1999; Rupprecht et al. 2017; Curro & Raquet 2018; Cui et al. 2019; Makansi et al. 2019). Consequently they are less effective at inferring correlations between parameters, so in practice usually very low (often single) dimensional marginal distributions are inferred (Meier et al. 2007a,b; Earp & Curtis 2020; Earp et al. 2020).

To estimate full posterior pdfs, Ardizzone et al. (2018) proposed to use invertible neural networks (INNs) to solve probabilistic inverse problems. INNs provide bijective mappings between inputs (models) and outputs (data), and can be trained to estimate posterior pdfs by introducing additional latent variables in the outputs (data) side. They have been used to solve inverse problems in medicine (Ardizzone et al. 2018), astrophysics (Osborne et al. 2019), optical imaging (Adler et al. 2019; Moran et al. 2018) and morphology (Sahin & Gurevych 2020). In this study we use INNs to solve seismic tomographic inverse problems.

The INN method uses maximum mean discrepancy to measure differences between two distributions, and varies the network parameters so as to minimise this measure during training. However, this measure becomes less effective as the dimensionality increases because of the curse of dimensionality (Ramdas et al. 2015). We show that this issue can be resolved by using a maximum likelihood criterion to train INNs.

In the next section we describe the basic structure of INNs, and how they can be trained to solve Bayesian inference problems. We then apply the method to two types of seismic inverse problems: 1D surface wave dispersion inversion and 2D travel time tomography, and compare the results with those obtained using Markov chain Monte Carlo (McMC) and MDNs. We demonstrate that INNs can provide comparable probabilistic results with those obtained using McMC, including correlations between parameters, whereas MDNs provide far less information about inter-parameter correlations. In one of our examples the computational time of training INNs and MDNs, including generation of the synthetic training data is comparable to one single run of McMC. We thus demonstrate that INNs can provide fast, accurate approximations of posterior pdfs even if the problem is solved only once; they can then produce rapid solutions for subsequent problems within the same problem class.

2 METHODS

2.1 Bayesian inference

Bayesian methods update a *prior* probability density function (pdf) $p(\mathbf{m})$ with new information from data $\mathbf{d}_{obs}$ to produce a probability distribution of model parameters $\mathbf{m}$ post inversion, which is often called a *posterior* pdf and written as $p(\mathbf{m}|\mathbf{d}_{obs})$. According to Bayes' theorem,

$$p(\mathbf{m}|\mathbf{d}_{obs}) = \frac{p(\mathbf{d}_{obs}|\mathbf{m})p(\mathbf{m})}{p(\mathbf{d}_{obs})} \tag{1}$$

where $p(\mathbf{d}_{obs}|\mathbf{m})$ is the *likelihood* which is the probability of observing data $\mathbf{d}_{obs}$ if model $\mathbf{m}$ was true, and $p(\mathbf{d}_{obs})$ is a normalization factor called the *evidence*. The likelihood function is often assumed to follow a Gaussian probability density function around the data predicted synthetically (using known physical relationships) from model $\mathbf{m}$, as this is assumed to be a reasonable approximation to the pdf of uncertainties or errors in measured data. Estimating the posterior distribution given prior information and the likelihood is called Bayesian inference.

2.2 Invertible neural networks

Invertible neural networks (INN) are a class of networks that provide bijective mappings between inputs and outputs. A typical design of an INN contains a serial sequence of reversible blocks, each of which consists of two coupled layers (Dinh et al. 2016; Kingma & Dhariwal 2018). Each block's input vector $\mathbf{u}$ is split into two halves $\mathbf{u}_1$ and $\mathbf{u_2}$, which are transformed by an affine function with coefficients $exp(s_i)$ and t_i to produce the output $[\mathbf{v}_1, \mathbf{v}_2]$:

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{u}_1 \odot exp(s_2(\mathbf{u}_2)) + t_2(\mathbf{u}_2) \\ \mathbf{v}_2 &= \mathbf{u}_2 \odot exp(s_1(\mathbf{u}_1)) + t_1(\mathbf{u}_1) \end{aligned} \tag{2}$$

where $\odot$ represents element-wise multiplication. This process is trivially invertible for any affine functions t and s:

$$\begin{aligned} \mathbf{u}_2 &= (\mathbf{v}_2 - t_1(\mathbf{u}_1)) \odot exp(-s_1(\mathbf{u}_1)) \\ \mathbf{u}_1 &= (\mathbf{v}_1 - t_2(\mathbf{u}_2)) \odot exp(-s_2(\mathbf{u}_2)) \end{aligned} \tag{3}$$

Importantly functions s_i and t_i do not need to be invertible themselves. In this study we use fully connected neural networks or convolutional neural networks to represent trainable functions s_i and t_i. To improve interaction between variables, we add a permutation layer after each reversible block (equation 2), which shuffles outputs of that block in a randomized, but fixed way as in Ardizzone et al. (2018).

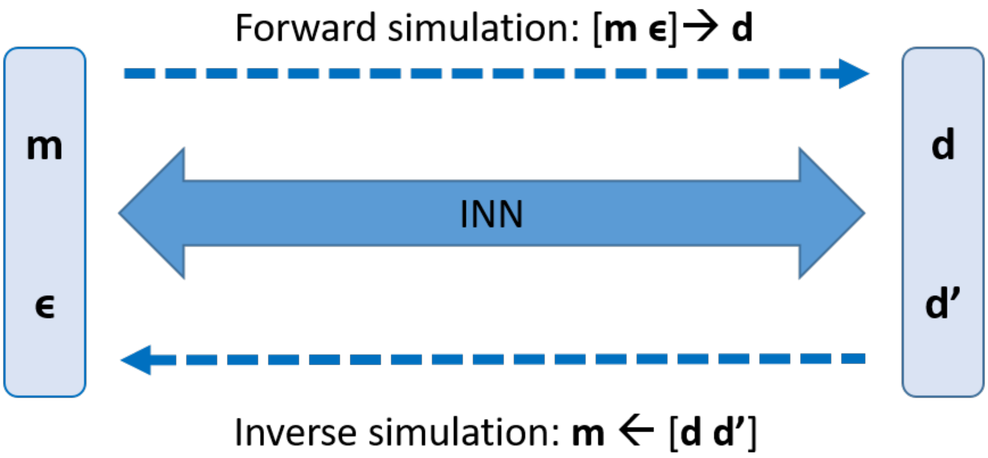

Figure 1. A conceptual figure of invertible neural networks. A latent random variable $\mathbf{d}'$ is added to the outputs to account for uncertainties in the inputs $\mathbf{m}$. The latent variable can follow any probability distribution, and is chosen to follow a standard Gaussian distribution in this study. The posterior distribution of $\mathbf{m}$ can be obtained by sampling $\mathbf{d}'$ for a fixed measurement $\mathbf{d}$ and running the trained neural network backwards. To appropriately account for noise in the data, we include random noise ϵ as additional model parameters.

2.3 Bayesian inference using INNs

INNs provide a natural way to solve inverse problems. For example, training an INN on a well-understood forward process $\mathbf{d} = F(\mathbf{m})$, one can obtain a solution to the inverse problem for free by running the trained network in the reverse direction. However in practice inverse problems often have nonunique solutions. To account for uncertainties in the solution, additional latent variables $\mathbf{d}'$ (Figure 1) can be introduced to the outputs $\mathbf{d}$ (Ardizzone et al. 2018). The networks therefore associate model parameters $\mathbf{m}$ to a unique pair $[\mathbf{d}, \mathbf{d}']$ of measurements and latent variables, written as $[\mathbf{d}, \mathbf{d}'] = f(\mathbf{m}; \theta)$ where θ represents parameters of the neural networks. As in Ardizzone et al. (2018) we train the neural network to approximate the forward process, that is $f(\mathbf{m}; \theta)_d \approx F(\mathbf{m})$ where the subscript d represents the data part of the network output, and meanwhile ensure the latent variable $\mathbf{d}'$ predicted by the network are distributed according to a chosen distribution, for example, a Gaussian distribution. The solution of the inverse problem can be obtained thereafter by running the network backwards given a specific measurement $\mathbf{d}_{obs}$ with latent variable $\mathbf{d}'$ selected randomly from the same Gaussian distribution :

$$
\begin{aligned}
&\mathbf{m} = f^{-1}(\mathbf{d}_{obs}, \mathbf{d}'; \theta) \\
&\mathbf{d}' \sim \mathcal{N}(\mathbf{0}, \mathbf{I})
\end{aligned}
\tag{4}
$$

By taking many samples of $\mathbf{d}'$ for the fixed data set $\mathbf{d}_{obs}$, the trained network transforms the distribution $p(\mathbf{d}')$ to the posterior distribution $p(\mathbf{m}|\mathbf{d}_{obs})$. Define the output distribution of the network in the forward direction to be $q(\mathbf{d}, \mathbf{d}')$:

$$q(\mathbf{d}, \mathbf{d}') = p(\mathbf{m})/|detJ_f(\mathbf{m})| \tag{5}$$

where $p(\mathbf{m})$ is the prior distribution of model $\mathbf{m}$, $J_f(\mathbf{m}) = \frac{\partial f(\mathbf{m};\theta)}{\partial \mathbf{m}}$ is the Jacobian of the forward transform embodied in the network. Given those expressions, the training loss function $\mathcal{L}$ can be expressed as:

$$\mathcal{L} = \|\mathbf{d} - f(\mathbf{m})\| + \alpha \mathrm{MMD}[q(\mathbf{d}, \mathbf{d}'), p(\mathbf{d})p(\mathbf{d}')] \tag{6}$$

where $p(\mathbf{d})$ is the prior distribution of data which is generated by applying the forward function $F(\mathbf{m})$ over the prior distribution $p(\mathbf{m})$, MMD represents the Maximum Mean Discrepency which is a measure of difference between two distributions, and α is the relative weight of the MMD term. MMD can be evaluated using only samples from the two distributions in its arguments. For example, assume X and X' are random variables with distribution p, and that Y and Y' are random variables with distribution q, then MMD can be expressed as:

$$MMD[p, q] = \mathrm{E}_{X,X'}[k(X, X')] - 2\mathrm{E}_{X,Y}[k(X, Y)] + \mathrm{E}_{Y,Y'}[k(Y, Y')] \tag{7}$$

where k is a kernel function. Here we use the Inverse Multiquadratic function $k(x, x') = 1/(1 + \|(x - x')/h\|_2^2)$ as it has heavier tails than a Gaussian kernel and provides meaningful gradients for outliers (Tolstikhin et al. 2017; Ardizzone et al. 2018). MMD equals zero if and only if $p = q$ (Gretton et al. 2012), and it has been shown that when the loss in equation (6) reaches zero, the neural network produces the posterior distribution $p(\mathbf{m}|\mathbf{d})$ (Ardizzone et al. 2018). In practice to facilitate the convergence of training, a loss function on the input side is also included:

$$\mathcal{L} = \|\mathbf{d} - f(\mathbf{m})\| + \alpha \mathrm{MMD}[q(\mathbf{d}, \mathbf{d}'), p(\mathbf{d})p(\mathbf{d}')] + \beta \mathrm{MMD}[q(\mathbf{m}), p(\mathbf{m})] \tag{8}$$

where $q(\mathbf{m}) = p(\mathbf{d})p(\mathbf{d}')/|J_{f^{-1}}(\mathbf{d}, \mathbf{d}')|$ is the input distribution predicted by the neural network acting in the inverse direction and β is the relative weight. Although MMD is an efficient method to discriminate two distributions in low dimensionality, it becomes less efficient (requires many more samples) in high dimensionality (Ramdas et al. 2015). To improve efficiency of the method in high dimensionality we add a maximum likelihood term to the loss function:

$$\begin{aligned}\mathcal{L} =& \|\mathbf{d} - f(\mathbf{m})\| + \alpha \text{MMD}[q(\mathbf{d}, \mathbf{d}'), p(\mathbf{d})p(\mathbf{d}')] + \beta \text{MMD}[q(\mathbf{m}), p(\mathbf{m})] \\ & - \gamma log(p[\mathbf{m} = f^{-1}(\mathbf{d}, \mathbf{d}')]|J_{f^{-1}}(\mathbf{d}, \mathbf{d}')|)\end{aligned} \tag{9}$$

where γ is the relative weight, and $p[\mathbf{m} = f^{-1}(\mathbf{d}, \mathbf{d}')]|J_{f^{-1}}(\mathbf{d}, \mathbf{d}')|$ is the pdf representing the consistency of $(\mathbf{d}, \mathbf{d}')$ and $\mathbf{m}$; this is calculated by feeding $(\mathbf{d}, \mathbf{d}')$ into the network and comparing the result with $\mathbf{m}$. Maximising the likelihood term for all training data $(\mathbf{d}, \mathbf{d}')$ ensures that the network transforms between $p(\mathbf{m})$ and $p(\mathbf{d})p(\mathbf{d}')$. Note that this likelihood term therefore achieves the same goal as the MMD terms alone, but is more effective in high dimensionality.

The method described above only accounts for intrinsic uncertainties caused by non-linearity of underlying physics and neglects uncertainties caused by data noise. This is because theoretically the method requires the loss function in equation 6 to be zero to produce the posterior pdf, which cannot be achieved when there is random noise in the data.To appropriately account for noise in the data such that the estimated posterior pdfs using INNs are consistent with the posterior pdfs in Bayesian inference, we treat random noise as additional model parameters (Figure 1), that is, we assume:

$$\begin{aligned}\mathbf{d} &= F(\mathbf{m}) + \boldsymbol{\epsilon} \\ \boldsymbol{\epsilon} &\sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})\end{aligned} \tag{10}$$

where $\boldsymbol{\Sigma}$ is the covariance matrix of data noise. Note that this idea of treating noise as additional parameters has also been used in training MDNs (Earp et al. 2020). Although in principle we could include a full covariance matrix, in this study we assume Σ to be a diagonal matrix to reduce the number of estimated parameters. Thus the input dimensionality of the network will be:

$$dim(\text{inputs}) = dim(\mathbf{m}) + dim(\mathbf{d}) \tag{11}$$

In this way the estimated posterior pdfs approximate the correct solution for Bayesian inference. Since INNs require the same dimensionality of inputs and outputs, the dimensionality of $\mathbf{d}'$ becomes:

$$
\begin{aligned}
dim(\mathbf{d}') &= dim(\text{outputs}) - dim(\mathbf{d}) \\
&= dim(\text{inputs}) - dim(\mathbf{d}) \\
&= dim(\mathbf{m})
\end{aligned}
\tag{12}
$$

Because the network also needs to capture the distribution of noise parameter $\boldsymbol{\epsilon}$, the dimensionality of $\mathbf{d}'$ may need to be higher than $dim(\mathbf{m})$. In this case zeros can be padded to the inputs side to ensure the same dimensionality.

Note that trained INNs also provide approximating forward functions. For example one can obtain the distribution of data with noise by running the network forward with noise parameter ϵ distributed according to the assumed distribution given a fixed model $\mathbf{m}$. In our case since we assumed Gaussian noise, the same distribution of data can actually be obtained by adding random noise to the synthetic data. However in cases in which noise distributions are not explicitly known, for example noise caused by assumptions in forward modelling, INNs provide a way to generate associated data distributions.

Figure 2 shows a toy example application of the method. The training data (Figure 2a) are generated using a function $y = x^2 + \epsilon$ where $\epsilon \sim \mathcal{N}(0, 0.04)$. We train an INN to predict the posterior pdf $p(x|y)$ as described above. For example, Figure 2b shows the pdf predicted by the trained INN at $y = 0.6$ (orange histogram), which provides an accurate approximation to the results obtained by Markov chain Monte Carlo (blue line). Figure 2c shows the distribution of ϵ (orange histogram) predicted by the network, which matches the true distribution (blue line) as expected. In Figure 2d we show the data distribution predicted by the network when $x = 0.5$, which gives an accurate approximation to the true distribution (blue line). This example shows the potential of INNs to predict accurate posterior pdfs as well as to approximate probabilistic forward functions.

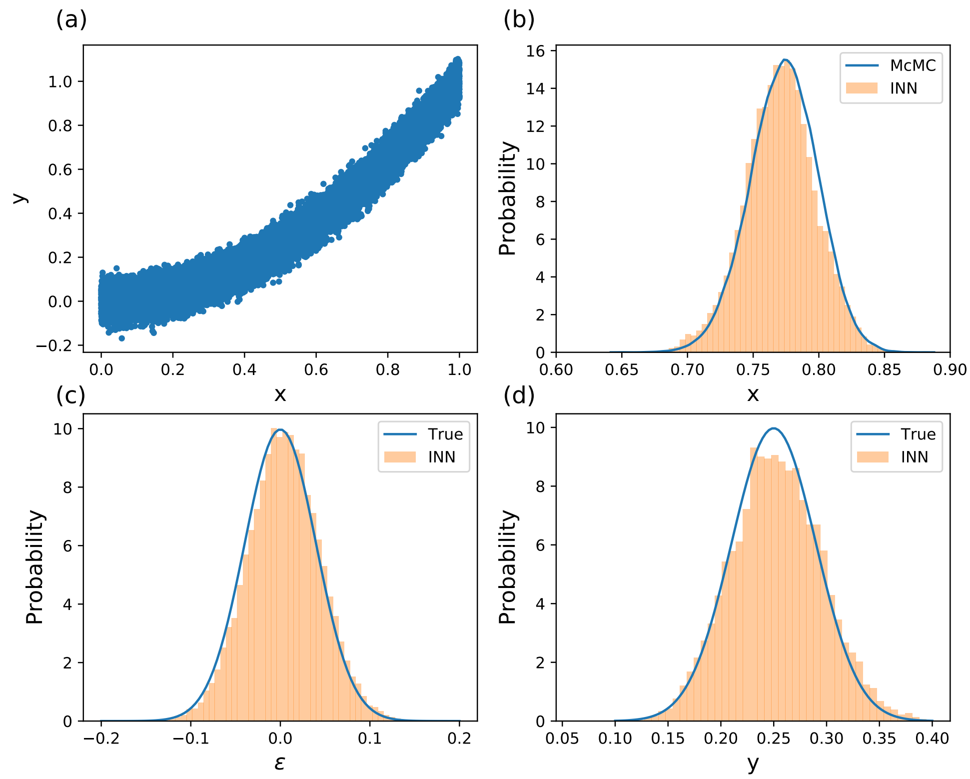

Figure 2. A toy example that uses INNs to predict posterior pdfs. **(a)** Training dataset. **(b)** Posterior pdfs of x and **(c)** noise parameter ϵ obtained using INNs (orange histogram) and McMC (blue line) when $y = 0.6$. **(d)** The distribution of y predicted by INNs (orange histogram) and the true distribution (blue line) when $x = 0.5$.

3 RESULTS

3.1 1D surface wave dispersion inversion

As a first experiment we train an INN to predict posterior pdfs for 1D seismic velocity structure with depth, given surface wave dispersion data. The subsurface is parameterized using ten regular layers with 0.1 km spacings for the shallower part ($< 0.5km$) and 0.2 km spacings for the deeper part ($> 0.5km$) since surface wave dispersion inversions are know to suffer diminishing spatial resolution with depth. For each layer we specify a Uniform prior distribution for the shear wave velocity (Figure 3a), whose velocity range is set to be typical for the near surface (Zhang et al. 2020a). P-wave velocity and density are calculated from the shear velocity using $V_p = 1.16V_s + 1.36$ (Castagna et al. 1985) and $\rho = 1.74V_p^{0.25}$ (Brocher 2005) where V_p and V_s are P and S wave velocity in km/s and ρ is density in g/cm^3. We generate 100,000 models from the prior

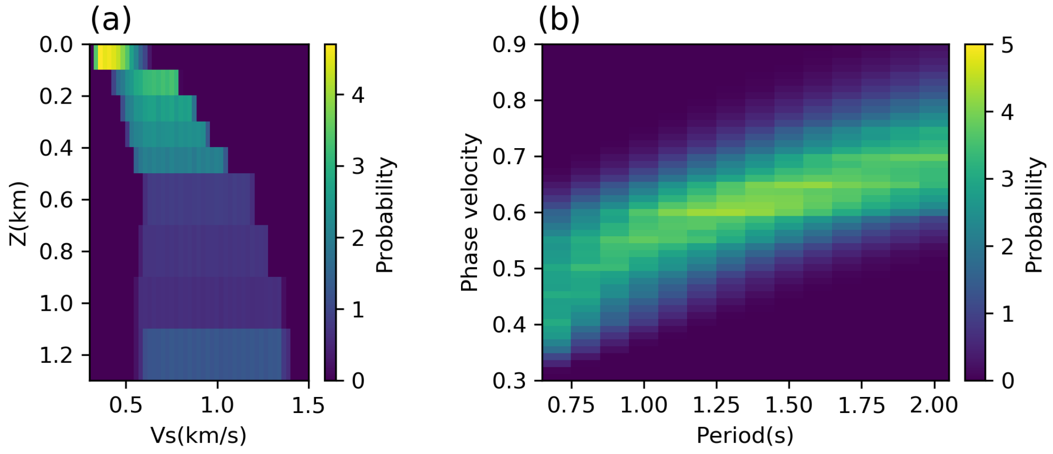

Figure 3. **(a)** Marginal prior distributions of shear velocities, and **(b)** the prior distribution of dispersion curves used to train neural networks.

pdf and calculate Rayleigh wave dispersion curves corresponding to each model using a modal approximation method (Herrmann 2013) over the period range 0.7 s to 2.0 s with 0.1 s spacing (Figure 5b). We added Gaussian noise with a standard deviation of 5 m/s to those calculated dispersion curves, which is a typical noise level in near surface ambient noise studies (Zhang et al. 2020a). Note that to ensure the computed dispersion curves are fundamental mode Rayleigh waves, within the prior pdf we ensured that the top layer has smallest shear velocity – - otherwise the wave recorded on the Earth's surface would be a higher mode Rayleigh wave (Zhang et al. 2020a). We use 90 percent of those model and dispersion curve pairs as training data, and the remaining 10 percent as test data used for independent evaluation of network performance.

The INN was designed using four reversible blocks, each of which contains fully connected subnetworks (see details in Appendix A1), and was trained using the ADAM optimizer (Kingma & Ba 2014). We assume the neural network has converged when both the training loss and test loss become stationary or when the test loss starts increasing. The trained neural network is then used to predict posterior pdfs by running the network backwards using many random values of $\mathbf{d}'$ in equation 4 for each fixed data vector $\mathbf{d}_{obs}$, and we histogram the resulting set of samples of $\mathbf{m}$ to approximate the posterior marginal distribution over each shear velocity. We show two examples of the set of predicted marginal posterior pdfs in Figure 4a and 4d. To better understand the results, we compared them with those obtained using McMC and MDNs. For McMC we use an adaptive Metropolis-Hastings algorithm (Haario et al. 2001; Salvatier et al. 2016) with 3 chains,

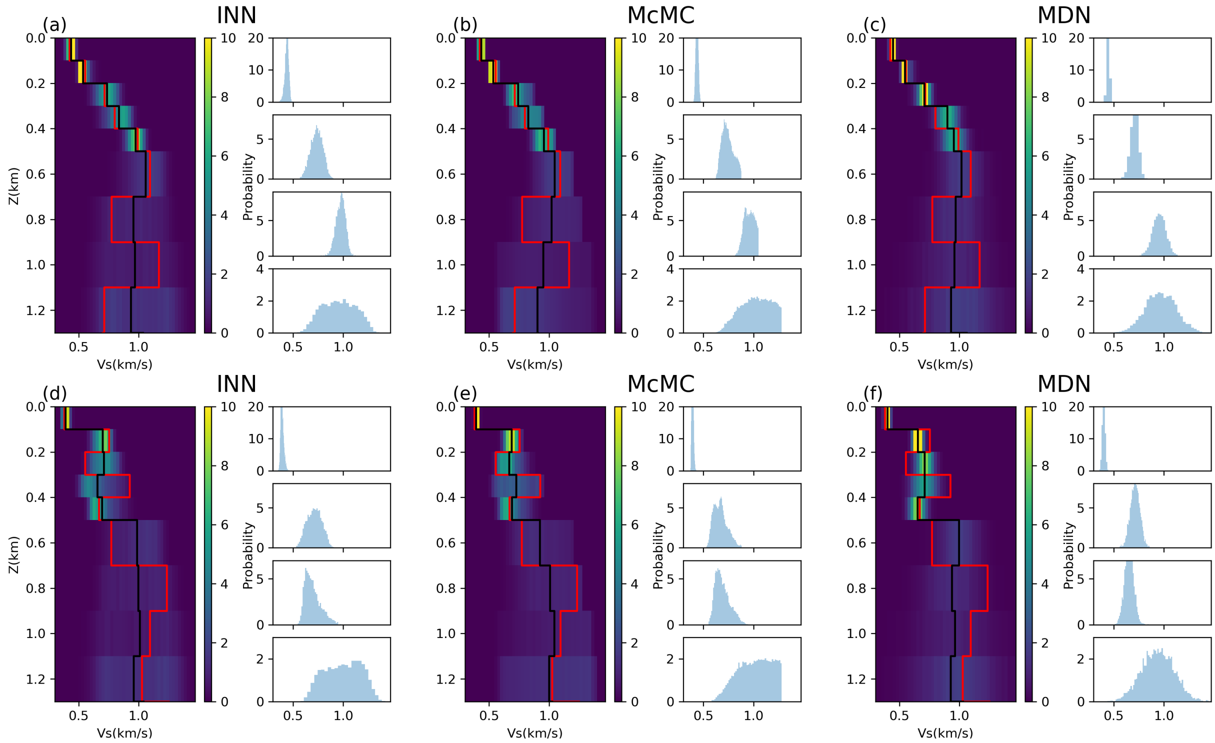

Figure 4. The marginal posterior distributions obtained using (**a** and **d**) an INN, (**b** and **e**) McMC and (**c** and **f**) MDNs for two different shear velocity structures. Red lines show the true shear velocity and black lines show the mean velocity. At the right side of each panel we plot marginal distributions for four layers: 0 - 0.1 km, 0.2 - 0.3 km, 0.5 - 0.7 km and 0.9 - 1.1 km depth.

each of which contains 250,000 samples including a burn-in period of 50,000 samples; the burn-in samples were ignored, and every 20th of the remaining 200,000 samples was included in the final set of McMC samples used for calculating statistics and marginal distributions. The results are shown in Figure 4b and 4e. For the MDN we use 20 mixture Gaussian kernels and use a network design from Earp & Curtis (2020). The network is then trained 20 times with random initialization and the network with best performance on the test data is used to produce final results. The results are shown in Figure 4c and 4f. Overall the three methods produce similar results for both examples. For example, in the top row the results show lower uncertainties at shallower depths ($< 0.8km$) due to the fact that surface waves are more sensitive to shallower structure. In the bottom row the results of all three methods exhibit higher uncertainties in the third and forth layers and the mean velocities deviate from the true velocity. This is because surface waves are not sensitive to complex structures with thin low velocity zones (Jan van Heijst et al. 1994). However, marginal distributions from the MDNs show clear Gaussian shapes, whereas the results from INNs and McMC have non-Gaussian shapes. This suggests that MDNs are not accurately approximating non-Gaussian pdfs, and in comparison the INNs have produced more accurate results. Note that this limitation of MDNs cannot be resolved by increasing the number of kernels as in these results only a few kernels contribute to the final pdfs (all others are assigned near-zero weights), a property found also in previous studies (Hjorth & Nabney 1999; Rupprecht et al. 2017; Curro & Raquet 2018; Cui et al. 2019; Makansi et al. 2019; Earp & Curtis 2020).

Figure 5 shows the correlation coefficients between parameters estimated using the three methods. The results from INNs and McMC show clear correlations between different parameters (Figure 5a,d and 5b,e), whereas the results from MDNs only show correlations for velocities of shallow layers in the top row. While this result probably occurs because we used a standard MDN which only contains kernels with diagonal covariance matrix, given the number of kernels (20) it is certainly theoretically possible that the MDN could have represented the true correlations, at least approximately (in Figure 5c, the signs of correlations between the first, second and third layers are correct). Again, this relatively poor result is explained by the fact that MDNs tend to use only a few kernels to represent the solution (Hjorth & Nabney 1999; Rupprecht et al. 2017; Curro & Raquet 2018; Cui et al. 2019; Makansi et al. 2019; Earp & Curtis 2020). Although a MDN with full covariance matrix might produce better results, the problem becomes far more complex which can cause numerical instability and computationally expense due to the approximately squared number of network outputs (Williams 1996).

In comparison INNs naturally estimate full correlation information. For example in our tests INNs provide the right correlation information for the first and second off-diagonal elements in the correlation matrix, that is, the correlation information between neighbouring and every second neighbouring layers (although the magnitudes are slightly lower than those from McMC). Even for more distant correlations, INNs still provide a reasonable approximation. For example, the results from INNs show correlations between the first and forth layer that are similar to results from McMC.

Overall INNs provide more accurate approximations to the results obtained using McMC compared to those obtained using MDNs. After training, both INNs and MDNs provide very efficient calculations of posterior distributions. For example, the above tests took about 2 seconds to pre-

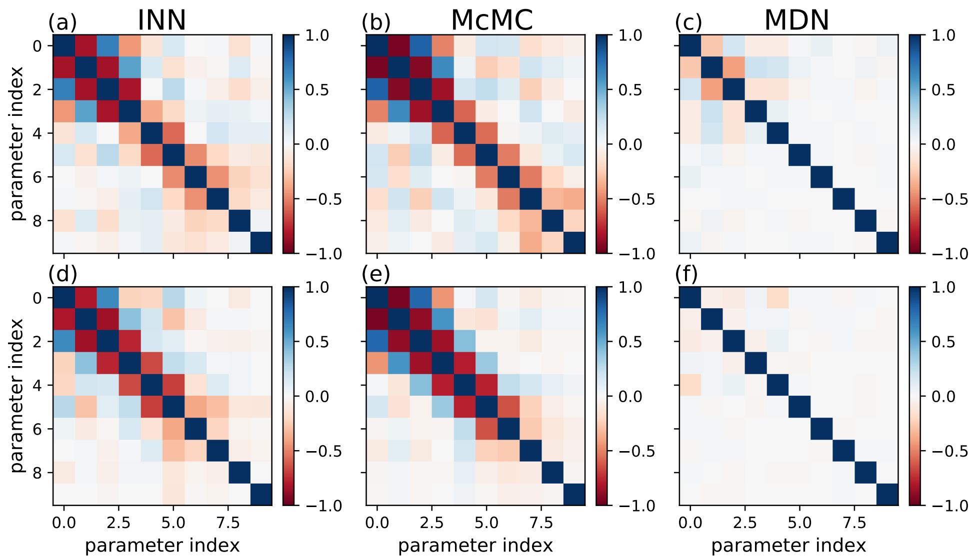

Figure 5. Correlation coefficients between shear velocities of different layers obtained using (**a** and **d**) an INN, (**b** and **e**) McMC and (**c** and **f**) MDNs for the two different velocity profiles in Figure 4.

dict posterior distributions using a trained INN or MDN on a typical desktop, whereas McMC took about 3 hours on the same machine. Thus trained INNs can be applied in scenarios where many repeated inversions are necessary to provide accurate shear velocity posterior distributions of the changing subsurface over time (Cao et al. 2020). We discuss the compute power required for training the INN in the Discussion section below.

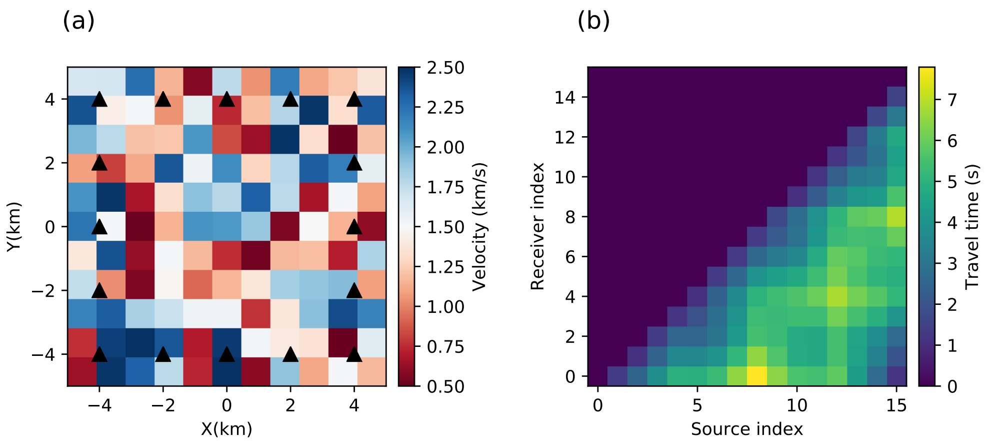

Figure 6. Experimental design for 2D travel time tomography. **(a)** Receiver locations (black triangles) and an example of a random velocity model. Each receiver also acts as a virtual source to mimic an ambient noise tomography experiment. **(b)** An example travel time field.

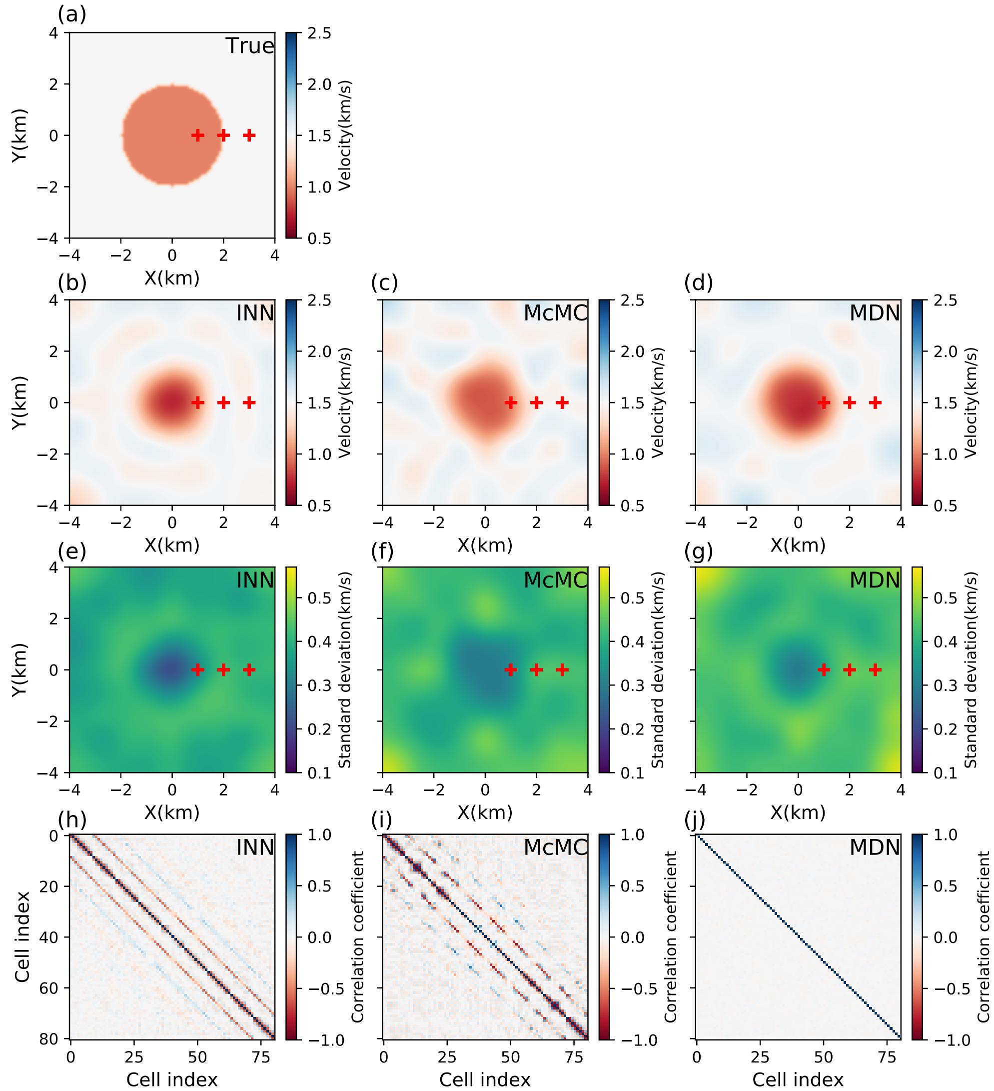

Figure 7. **(a)** The true velocity model. **(b)**, **(c)** and **(d)** show the mean velocity models obtained using INN, McMC and MDN respectively. **(e)**, **(f)** and **(g)** show the standard deviation at each point obtained using the three methods respectively.**(h)**, **(i)** and **(j)** show the correlation coefficient matrices obtained using the three methods respectively. Red pluses show locations referred to in the text, at which marginal probability distributions are shown in Figure 8.

3.2 Travel time tomography

We next examine performance of the methods on a 2D travel time tomographic problem similar to those which appear in ambient noise tomography (Shapiro et al. 2005). We solve a problem similar to that described in Earp & Curtis (2020) so that the results can be compared with theirs obtained using MDNs. A total of 16 receivers are used in our study, each of which also acts as a virtual source (Figure 6a). The velocity model is parametrized using a 9×9 regular grid (Figure 6a); for ease of visual interpretation we interpolate between the cell centres to construct smooth

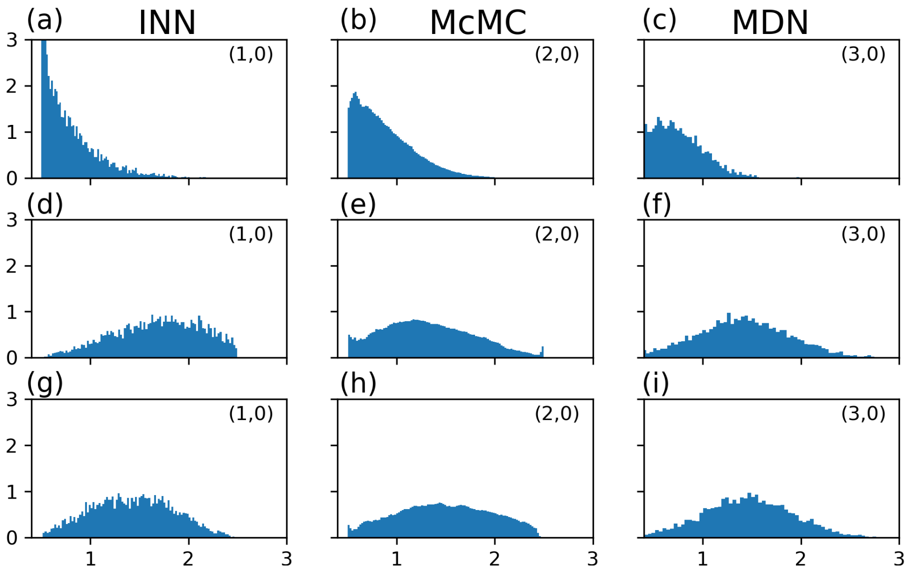

Figure 8. The marginal distributions at three points (red pluses in Figure 7) derived using different methods. **(a)**, **(b)** and **(c)** show the marginal distributions at point (1,0) obtained using INN, McMC and MDN respectively. **(d)**, **(e)** and **(f)** show similar marginal distributions at point (2,0), and **(g)**, **(h)** and **(i)** show results for point (3,0).

tomographic maps (e.g., Figure 7). At each grid point the prior distribution of velocity is set to be a Uniform distribution in the range 0.5 km/s to 2.5 km/s. We generate 200,000 velocity models from the prior distribution, for each of which the inter-receiver travel time data (Figure 6b) are calculated using a fast marching method (Rawlinson & Sambridge 2004) with 0.05 s standard deviation Gaussian noise added. Note that we added a halo of cells with random velocities around the receiver array; these will not be be imaged but which allow waves to travel both outside and inside of the array during inter-receiver propagation. Again we use 90 percent of those data as training data and the remaining 10 percent as test data.

For the INN we use a network that contains eight reversible blocks (details in Appendix A2) trained using the ADAM optimizer (Kingma & Ba 2014). To better understand the method, we compared the results with those obtained using MDNs and McMC. We train MDNs of the same network design as described in Earp & Curtis (2020) with 100 Gaussian kernels. Again the network is trained 20 times with random initialization, and the network with best performance on test data is used to produce final results. For McMC we use a standard adaptive Metropolis-Hastings algorithm with a total of 6 chains, each of which contains 1,600,000 samples including a burn-in period of 600,000. Again the burn-in samples were ignored, and every 20th of the remaining

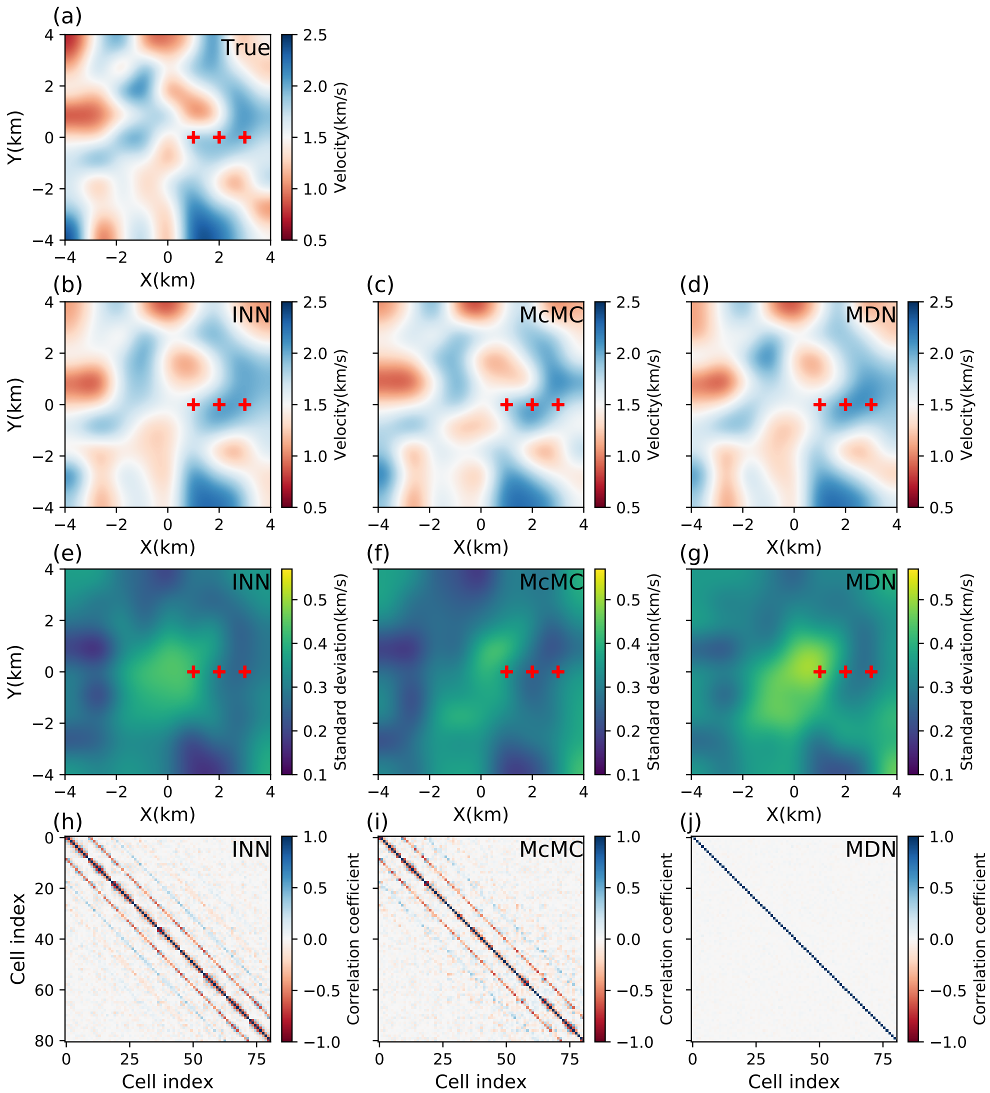

Figure 9. A random velocity example. Key as in Figure 7

1,000,000 samples was included in the final set of McMC samples used for calculating statistics and marginal distributions.

As a first example we show results for data generated using a smooth velocity model which contains a low velocity anomaly in the centre within a homogeneous background (Figure 7a), similar to the test model in Galetti et al. (2015); Zhang et al. (2018); Earp & Curtis (2020); Zhang & Curtis (2020a). While simple (which permits some degree of intuition about tomographic solution), the tomography problem is nevertheless substantially nonlinear (Galetti et al. 2015). The model also consists of both perfectly smooth regions and a sharp, spatially coherent boundary, whereas smooth regions are not represented by any randomly-selected training example (they are

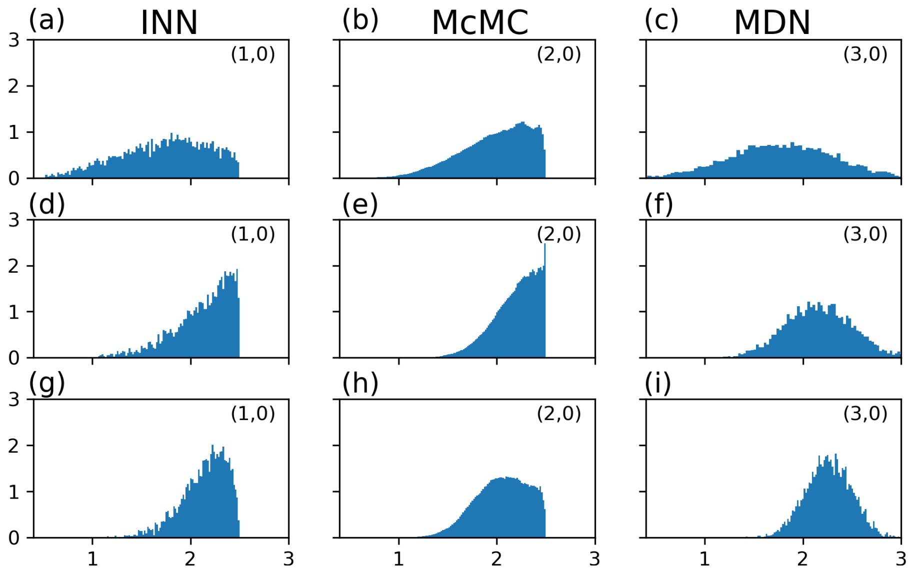

Figure 10. The marginal distributions at three points (red pluses in Figure 9) derived using different methods. Key as in Figure 8

all of similar roughness to that in Figure 6a). The example also presents the complication that the true model is defined on a relatively high resolution grid so that the circular boundary is not representable in the lower resolution parameterizations used for tomography (and for the set of training examples above). Zhang & Curtis (2020a) showed that the Bayesian solution to this problem varies significantly depending on the parameterization adopted, so in this example we use identical parameterizations for each of the three methods.

The data are then fed into the trained INNs and MDNs to predict posterior pdfs, and are also inverted using McMC to generate posterior samples. Overall the three methods produce similar mean (Figure 7b, c and d) and standard deviation models (Figure 7e, f and j). For example, all mean models show the middle low velocity anomaly, and small velocity variations around the anomaly which might be caused by lower resolution in those areas or by the random noise added to the data. Note also that we do not expect the mean model to match the true model. The mean is a statistic of the family of all models that might be true given the data; together with the standard deviation, it helps us to describe that family (the goal of uncertainty analysis). Hence the mean is not an estimator of the true model, and particularly in nonlinear problems it is expected to deviate from the true model. All standard deviation models show low uncertainties across the central anomaly and higher uncertainties around the anomaly and in the four corners of the grid.

Note that some detailed structure present in the results of McMC cannot be clearly observed in the results of INNs and MDNs. For example, there are four higher standard deviation anomalies above, below, left and right of the central anomaly, which are not clearly visible in the results of INNs and MDNs. This is probably because of cost function residuals remaining after training the INNs and MDNs.

Note that this is a high (81) dimensional problem, and there is minimal information in the uniformly-distributed prior pdf. The curse of dimensionality therefore implies that a huge number of samples would be needed to sample the parameter space adequately to explore all significant areas of the tomographic solution (Curtis & Lomax 2001). Even sampling at only 2 samples per dimension would require $2^{81} = 2.4 \times 10^{24}$ samples. Therefore the training sets used are extremely small (far closer to 1 than to 2 samples per dimension), and even after 1.6 million samples the McMC method may not have converged to a statistically stable solution as it is difficult to assess convergence of McMC (Brooks et al. 2011). Therefore in this problem we do not know the exact Bayesian solution, nor which of the three solutions in Figure 7 is the most accurate. Nevertheless, the broad character of all three sets of means and standard deviations matches those found previously (papers cited above) so we have reasonable confidence in these statistics.

The correlation coefficient matrices obtained using INNs and McMC show similar results (Figure 7h and i). For example, there are negative correlations between neighbouring cells and positive correlations between every second neighbouring cells. In comparison the results obtained using MDNs do not show any correlation information. This is probably because MDNs become numerically instable in high dimensionality and again use only a few kernels to represent the solution (Hjorth & Nabney 1999; Rupprecht et al. 2017; Curro & Raquet 2018; Cui et al. 2019; Makansi et al. 2019; Earp & Curtis 2020).

To further analyse the results, Figure 8 shows marginal pdfs obtained by histogramming samples from the solutions of each of the three methods at three locations: (1,0), (2,0) and (3,0). Overall the results show similar marginal distributions, which suggests that both INNs and MDNs can produce reasonable estimates of marginal distributions. However, the distributions obtained from different methods still show slightly different shapes which is probably caused by training residuals in INNs and MDNs.

To explore generalization properties of the trained neural networks we show another example using data generated from a random velocity model in Figure 9a. Similarly to the first example, the three methods produce similar mean and standard deviation models. The mean velocity models are largely the same as the true model. The standard deviation models show low uncertainties at the location of the high velocity anomaly at the east side of the area and at the location of the low velocity anomaly at the west side between Y=0 km and Y=2 km, and high uncertainties in the centre. Due to training residuals and possible lack of convergence of McMC the standard deviation models show other details that differ between methods. For example, the central high uncertainly anomaly adopts different shapes in the three results. Nevertheless, overall the results are fairly consistent.

The correlation coefficient matrices show similar results to the first example: the results from INNs and McMC show negative correlations between neighbouring cells and positive correlations between every second neighbouring cell, whereas the results from MDNs shows no correlation information. In Figure 10 we show marginal distributions at the same locations as for the first example. The results from MDNs are clearly approximately Gaussian, whereas the results from INNs show non-Gaussian shapes which provide more accurate approximations to results of McMC.

Again the trained INNs and MDNs provide very efficient estimates of the posterior pdfs. For example, in a typical desktop the above trained MDN and INN takes about 3 seconds to produce a prediction of posterior pdfs – slightly longer than that required for 1D surface wave dispersion inversion because of the larger networks used here. In comparison McMC takes about 3 days on the same machine to generate the above results.

4 DISCUSSION

Although trained neural networks provide efficient estimates of posterior pdfs, the methods require large numbers of training datasets to be created in advance, and training itself can still be computationally expensive. For example, on our desktop (32 Intel Xeon CPUs) it takes about 0.3

hours to generate 100,000 surface wave dispersion curves using one CPU core and 1.1 hours to generate 200,000 travel time data using 6 CPU cores. However the training data only need to be calculated once; even if additional prior information becomes available we can update the prior using the prior replacement method (Walker & Curtis 2014) or the resampling method (Sambridge 1999) rather than generating entirely new training samples.

Neural networks can take between hours and days to train. For example, the above MDNs take 15 minutes to train for 1D surface wave dispersion inversion and 3 hours to train for 2D travel time tomography using one NVIDIA Tesla K80 GPU. In comparison, the above INNs take 6 hours to train for 1D surface wave dispersion inversion and 19 hours to train for 2D travel time tomography using the same GPU. So although INNs improve the prediction accuracy of the posterior pdfs, they take longer to train. This is because INNs are trained in both directions which generally requires larger networks to represent the forward and inverse process at the same time, and bidirectional training also intrinsically requires more computation and hence training time. However, training only needs to be done once: after training both types of neural networks can predict posterior pdfs in seconds. Computational efficiency is therefore gained when trained neural networks are applied many times, e.g., in real-time monitoring scenarios (Cao et al. 2020) or in highly parallelised (task-farmed) inference problems.

Even if the networks will only be applied once, it may be that they provide a more efficient solution than standard McMC, because of the generalisation property of neural networks. Essentially training networks is equivalent to performing a regression of the functional form of each network to the training data. Once that regression has been accomplished, the functional form approximately interpolates between examples in the training set, providing estimates of forward evaluations of infinitely many other model samples. This property implies that in some problems it may not be necessary to evaluate as many samples to train a neural network as would be required to characterise the solution using Monte Carlo or other purely sampling-based methods.

For example, in the above travel time tomography problems, the 1.6 milllion McMC samples required 3 days to evaluate, while the total times required to calculate training examples and train the MDN and INN were 4.3 hours and 20.1 hours, respectively. Hence in this example both the

MDN and the INN were more efficient than McMC even for one single inversion. Of course, the computational time strongly depends on hardware used in each case. In the above study different hardware is used for neural network training and McMC because McMC is difficult to parallelize, and hence it is difficult to take advantage of GPUs. It may also be the case that if we had used more efficient McMC methods such as Hamiltonian Monte Carlo (Neal et al. 2011; Fichtner et al. 2018) or Langevin Monte Carlo (Grenander & Miller 1994) we could have improved the McMC performance to outstrip the two neural network methods. Nevertheless, this work demonstrates at least that neural network inversion can be competitive with Monte Carlo methods even for a single inversion, but additionally they allow all subsequent inversions using similar prior information to be carried out almost for free.

Since INNs are trained bidirectionally, they also provide approximate forward functions. In Appendix B we show data distributions predicted by trained INNs for both surface wave dispersion curves and travel times in the above two experiments, and compared with solutions obtained by standard numerical modelling methods. The results show that trained INNs can also provide good approximations to the standard modelling methods. In this case since the standard forward modelling methods can calculate dispersion curves and travel time data in seconds, INNs do not provide any benefits. However, for problems whose forward modelling is computationally expensive (e.g. 3D applications or full waveform modelling), INNs might provide a faster approximate forward function.

In this study we used a Uniform prior distribution which can become ineffective for large inverse problems (Curtis & Lomax 2001; Earp & Curtis 2020). If appropriate, the space of models that remain possible in the Bayesian solution can be reduced by using a smooth prior (Earp & Curtis 2020), or other more advanced priors can be used to improve computationally efficiency (Walker & Curtis 2014; Zunino et al. 2015; Ray & Myer 2019; Caers 2018; Mosser et al. 2020). We also used a fixed regular grid of cells to parametrize the subsurface, but to increase flexibility other parametrizations, such as Delauney triangulation (Curtis & Snieder 1997), Voronoi diagrams (Sambridge et al. 1995; Bodin & Sambridge 2009), wavelet representations (Fang et al. 2015; Zhang & Zhang 2015) or other advanced parametrizations (Hawkins et al. 2019) can be used. The parametrization itself might also be predicted by neural networks along with the parameter values as in reversible-jump McMC (Green 1995; Bodin & Sambridge 2009), although to our knowledge this has never been implemented.

INNs provide full posterior pdfs which might be impossible for very high dimensional problems because this may require a network that is too large to fit in memory. In this case one can train INNs to predict marginal distributions of only a few parameters, as was performed in Earp & Curtis (2020) in cases where dominant correlations were expected between parameters in some neighbourhood of each other.

In this study we used coupling layers to implement invertible neural networks which might affect the expressiveness of the network. Other designs of invertible networks may be used as alternatives, for example, invertible residual networks (Behrmann et al. 2019) or Hamiltonian neural networks (Greydanus et al. 2019). Future research that makes a fair comparison between different architectures would be a useful contribution.

5 CONCLUSION

In this study we introduced invertible neural networks (INNs) to solve geophysical Bayesian inference problems. INNs are a class of neural networks that provide bijective mappings between inputs and outputs and can be trained to produce estimates of posterior probability density functions efficiently by introducing additional latent variables on the output (data) side. We applied the method to two types of problems: 1D surface wave dispersion inversion and 2D travel time tomography, and compared the results with those obtained using Markov chain Monte Carlo (McMC) and Mixture density networks (MDNs). The results show that INNs can provide accurate approximations of posterior pdfs obtained by McMC, including correlation information between parameters which is difficult to obtain using standard MDNs. The marginal distributions from INNs can also provide clearly non-Gaussian forms which are more similar to those obtained by McMC compared to the results obtained by MDNs. After training INNs can predict posterior pdfs in seconds, and therefore can be used to provide accurate estimates of posterior pdfs in rapid, real-time monitoring scenarios. Even accounting for training time, neural networks can be more efficient than Monte

Carlo methods in applications to single inverse problems. It remains to be seen how far this latter result can be generalised to problems other than those tested here.

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Table A1. Training data and model and data dimensionalities used in different experiments

Experiment	training data	dim(inputs)	dim($\mathbf{d}$)	dim($\mathbf{d}'$)
Surface wave inversion	100,000	24	14	22
Travel time tomography	200,000	241	120	181

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APPENDIX A: NETWORK CONFIGURATION

Table 1 summarizes the training datasets and model and data dimensionalities used in 1D surface wave dispersion inversion and 2D travel time tomography. Note that in practice zeros are padded to the inputs to ensure the same dimensionality.

A1 Network configuration for surface wave dispersion inversion

INN: 4 reversible blocks, each of which contains two coupling layers as described in equation 2. Each affine function (i.e. s_i and t_i) is implemented using a neural network with 3 fully connected layers each of which contains 512 hidden units with RELU activation functions. The ADAM optimizer is used with a batch size of 1000.

MDN: 20 mixture Gaussian kernels, 4 fully connected layers with RELU activation functions. The sizes of layers are 200, 300, 200 and 200 respectively. The ADAM optimizer is used with a batch size of 1000.

A2 Network configuration for travel time tomography

INN: 8 reversible blocks as described in equation 2. Each affine function (i.e. s_i and t_i) is implemented using one convolutional layer with 32 channels for the first four blocks, and one fully connected layer containing 1024 hidden units for the remaining blocks. The ADAM optimizer is used with a batch size of 1000.

MDN: 100 mixture Gaussian kernels, 7 layers in total containing 3 convolutional layers and 4 fully connected layers. The number of channels of the 3 convolutional layers are 128, 128 and 64

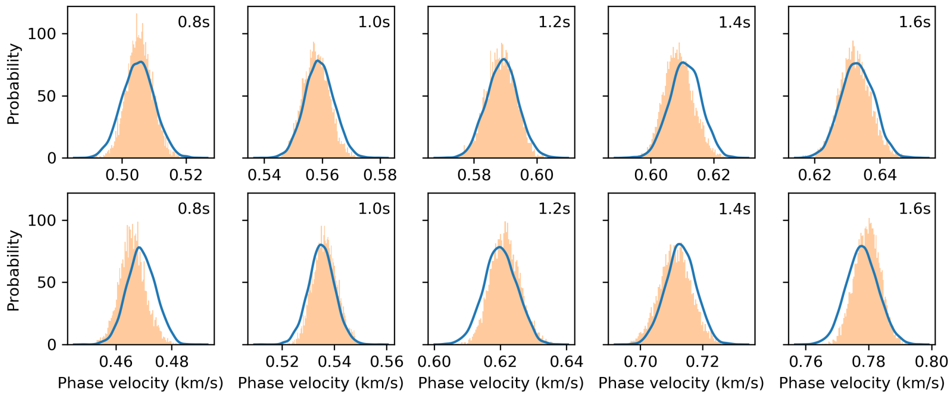

Figure A1. Distributions of phase velocities with random noise predicted by INNs (orange histograms) for a specific shear velocity model at periods 0.8 s, 1.0 s, 1.2 s, 1.4s and 1.6 s. The distributions in upper and lower rows correspond to the upper and lower models respectively, shown by red lines in Figure 4. Blue lines show true distributions obtained using the standard forward modelling method with random noise added to the synthetic data.

respectively. The size of the 4 fully connected layers are 800, 150, 600 and 1500 respectively. The ADAM optimizer is used with a batch size of 1000.

APPENDIX B: APPROXIMATE FORWARD MODELLING FUNCTION USING INNS

Since INNs are trained bidirectionally, they also provide approximate forward functions. For example, one can obtain the distribution of data with noise for a fixed model $\mathbf{m}$ by running the network forward with noise parameter ϵ (Figure 1) distributed according to its assumed distribution. Figure A1 shows phase velocity distributions obtained from INNs for those shear velocity models used in the surface wave dispersion inversion experiment at 5 different periods, and compares the results with those obtained using standard forward modelling methods using equation 10, which we refer to as true distributions. The noise of each phase velocity is assumed to follow a Gaussian distribution with a standard deviation of 5 m/s. The results show that the distributions predicted by INNs from the training samples alone, can provide good approximations to those obtained by the forward models themselves. Note that because of training residuals the distributions obtained from INNs are slightly different from the true distributions.

Similarly the upper and lower rows in Figure A2 show distributions of travel times for 5 randomly selected (virtual) source-receiver pairs predicted by INNs for the two velocity models in Figure 7 and Figure 9 respectively. The noise of each travel time is assumed to follow a Gaussian

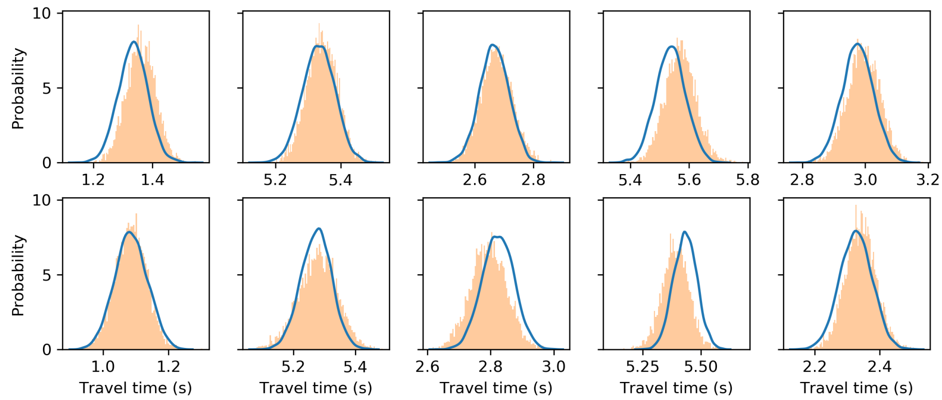

Figure A2. Travel time distributions for 5 randomly selected (virtual) source-receiver pairs predicted by INNs (orange histograms) for (**upper row**) the smooth velocity model in Figure 7a and (**lower row**) the random velocity model in Figure 9a. Blue lines show true distributions obtained using the standard forward modelling method with random noise added to the synthetic data.

distribution with a standard deviation of 0.05 s. The results show that distributions obtained from INNs are largely similar to the true distributions (those obtained using standard forward modelling method). However, there are still differences between the two distributions caused by training residuals of INNs.