Geophysical inversion versus machine learning in inverse problems

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Abstract

Geophysical inversion and machine learning both provide solutions for inverse problems in which we estimate model parameters from observations. Geophysical inversions such as impedance inversion, amplitude-variation-with-offset inversion, and traveltime tomography are commonly used in the industry to yield physical properties from measured seismic data. Machine learning, a data-driven approach, has become popular during the past decades and is useful for solving such inverse problems. An advantage of machine learning methods is that they can be implemented without knowledge of physical equations or theories. The challenges of machine learning lie in acquiring enough training data and selecting relevant parameters, which are essential in obtaining a good quality model. In this study, we compare geophysical inversion and machine learning approaches in solving inverse problems and show similarities and differences of these approaches in a mathematical form and numerical tests. Both methods aid in solving ill-posed and nonlinear problems and use similar optimization techniques. We take reflectivity inversion as an example of the inverse problem. We apply geophysical inversion based on the least-squares method and artificial neural networks as a machine learning approach to solve reflectivity inversion using 2D synthetic data sets and 3D field data sets. A neural network with multiple hidden layers successfully generates the nonlinear mapping function to predict reflectivity. For this inverse problem, we test different L1 regularizers for both approaches. L1 regularization alleviates effects of noise in seismic traces and enhances sparsity, especially in the least-squares method. The 2D synthetic wedge model and field data examples show that neural networks yield high spatial resolution.

Introduction

An inverse problem is the process of predicting the causal factor from the outcome of measurements, given a partial description of a physical system. The inverse problem is a reverse process that predicts an observation out of a model of the system (Tarantola, 2005). Application of inverse theory is applied widely in science and engineering — for example, in geophysics, signal processing, medical imaging, optics, and computer vison. In the field of geophysics, inverse problems aim to retrieve subsurface physical properties from measured geophysical data such as exploration seismic data, magnetotelluric data, and controlled-source electromagnetic (CSEM) data. Full-waveform inversion, simultaneous inversion, and amplitude-variation-with-offset (AVO) inversion are common inversion methods used to recover physical properties such as P- and S-wave velocities or impedance using prestack seismic data.

Geophysical inverse problems are often ill-posed, nonunique, and nonlinear problems. A deterministic approach to solve inverse problems is minimizing an objective function. Iterative algorithms such as Newton algorithm, steepest descent, or conjugate gradients have been used widely for linearized inversion. Geophysical inversion usually is based on the physics of the recorded data such as wave equations, scattering theory, or sampling theory. Machine learning is a data-driven, statistical approach to solving ill-posed inverse problems. Machine learning has matured during the past decade in computer science and many other industries, including geophysics, as big-data analysis has become common and computational power has improved. Machine learning solves the problem of optimizing a performance criterion based on statistical analyses using example data or past experience (Alpaydin, 2009). Machine learning uses two major approaches to solve problems — supervised and unsupervised approaches, which we will discuss later. Artificial neural networks, naïve Bayes, and support vector machines are popular supervised learning methods for classification and regression. Previous studies show that machine learning and conventional geophysical inversion can be combined to solve inverse problems. Ray et al. (2014) introduce joint inversion of marine CSEM data using Bayesian methods. The Bayesian posterior seafloor resistivity model is constrained by CSEM inversion data. The joint inversion could avoid subjective regularization in deterministic inversion and reduce computation for Bayesian methods. Reading et al. (2015) apply a random forest classifier with remote-sensed geophysical data to constrain and supplement a geophysical inversion method. Kuzma and Rector (2004) implement nonlinear AVO inversion aided by a support vector machine to yield the nonlinear inverse operator. Reflectivity inversion, or impedance inversion, has also been implemented using machine learning methods such as neural networks (Röth and Tarantola, 1994; Calderon-Macias et al., 2000; Baddari et al., 2010), support vector machines (Rojo-Álvarez et al., 2008), and Bayesian learning (Ji et al., 2008; Yuan and Wang, 2013). The machine learning methods are proven to be effective when non-linearity or noise exist in the data.

Geophysical inversion and machine learning methods both are useful for solving inverse problems. In this study, we compare geophysical inversion based on a least-squares method and a neural network as a supervised machine learning method with examples of reflectivity inversion and make clear the similarities and differences between them. Least-squares minimizes the sum of the squared error difference between the desired and the actual signal. The least-squares framework is the most popular method not only to retrieve reflectivity but also to recover geophysical properties using other inversion. A neural network, which is used extensively

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in machine learning, can model nonlinear and complex relationships between input and output (Kappler et al., 2005). We first evaluate the resolution of these methods on thin beds using a 2D wedge reflectivity model. Regularization is a key factor to aid gradient descent to converge in an ill-posed problem. We present how a regularization term operates in two algorithms, especially in the presence of Gaussian noise. We also test sensitivity with regard to noise in the data. Finally, we apply these algorithms to field data sets and discuss the results.

Similarities and differences between geophysical inversion and machine learning approaches

Both geophysical inversion and machine learning involve a process that converts input data from the data space to the model space (Constable et al., 2015). An inverse problem can be formulated as

$$y = Hx + w, \tag{1}$$

where H is a forward operator, y is observed data, and w is the noise component of the data. The objective of the inverse problem is to obtain an unknown model x. Typically in contexts of geophysical inversion, H and y are presumably known, and w and x are unknown to investigators. The objective function (also known as cost function) of the inverse problem in least-squares manner is

$$L = \left\| y - H\hat{x} \right\|_2^2, \tag{2}$$

where $\hat{x}$ is an estimate of model x.

Machine learning techniques are frequently classified depending on whether the technique is unsupervised or supervised. Unsupervised learning analyzes input data based on the distribution or underlying structure of the input data. The training data set in the supervised algorithm, on the other hand, includes input data and labels that are response values of input. In the machine learning approach, the forward operator H can be unknown. Instead, some portion of input data set x_n and output data set y_n are provided in the supervised learning case as a training data set. Machine learning approaches to inverse problems can be denoted as

$$L_{learn} = \left\| x_n - H_\Theta^\dagger y_n \right\|_2^2, \tag{3}$$

where Θ is a parameter set optimized during the learning process, and $H_\Theta^\dagger$ is a pseudoinverse operator or mapping function that is given by Θ (Adler and Öktem, 2017). For instance, neural networks approximate the inverse mapping from the data space into the model space using a nonlinear basis function with weights and biases. In this case, weights and biases that are determined during the learning process are equivalent to parameter set, Θ. The set of weights and biases in neuron layers defines the pseudoinverse operator.

Similarities

Ill-posed and nonunique problem. Inverse problems in geophysics are likely under- or overdetermined, which means fewer or more equations exist than unknowns in a system. For instance, reflectivity inversion is an underdetermined problem because convolving reflectivity with the seismic wavelet has the effect of applying a low-pass filter. Applying a low-pass filter then causes the seismic traces to miss high-frequency content. The underdetermined problem can have an infinite number of solutions if constraints are not provided. Because inverse problems can be illposed and/or nonunique, a regularization method or a priori information is adopted to reconstruct a feasible model and prevent amplifying noise. In both geophysical inversion and machine learning, overfitting is also avoided by adding regularization terms such as L1 or L2 regularizers.

Nonlinearity. Many geophysics inverse problems are nonlinear. Linear problems have a single minimum when solved with a misfit function. Nonlinear inverse problems, on the other hand, have multiple local minima (Snieder, 1998). It is challenging to search for a global minimum in large-scale nonlinear inverse problems. A deep neural network (DNN) in machine learning is an artificial neural network with multiple hidden layers between the input and output layers. A DNN can build a nonlinear mapping function with such hidden layers and nonlinear activation function (e.g., sigmoid function).

Optimization techniques. Machine learning approaches such as neural networks are similar to geophysical inversion that has a general framework of iterative error minimization using Newton method, conjugate gradient, or steepest descent. Both geophysical inversion and the training process in machine learning methods (e.g., full-waveform inversion and neural network) use forward propagation and back propagation to minimize error in gradient descent. Back propagation can be computed from a partial derivative of objective function. The goal of optimization is to reach the global minimum, the smallest value over the entire range of error functions. However, most inverse or machine learning problems are nonconvex, and thus gradient descent likely converges at local minima (Van der Baan and Jutten, 2000). Both the step size in gradient descent and learning rate in the neural network affect the speed of convergence. An adaptive step size or learning rate can converge the inversion efficiently.

Differences

To implement geophysical inversion, a forward operator should be given to investigators based on parametric equations such as Zoeppritz equations (AVO inversion) or wave equations (full-waveform inversion) describing a specific physical relation of data and model space. Machine learning uses statistical techniques and makes decision boundaries for classification based on data distribution and density for unsupervised learning or human intervention and/or a priori information for supervised learning. Because machine learning methods are data-driven approaches, the feasibility of the method depends on training data sets and hyperparameters that are selected before the learning process.

Regarding reflectivity inversion as an example, when geophysical inversion is applied, a wavelet matrix is assumed to be known as a forward operator. However, machine learning does not use the forward operator or wavelet matrix explicitly. Only sets of seismic traces and reflectivity are used as training data. A machine learning model, which acts as a pseudoinverse operator, can be

generated in an infinite number of different cases depending on an investigator's choice of hyperparameters.

Comparison of two methods applied to reflectivity inversion

Methodology. The seismic trace s(t) can be considered as a convolution of the seismic wavelet and earth's reflectivity, which is denoted by

$$s(t) = h(t) * r(t) + w(t), \qquad (4)$$

where $h(t)$ is seismic wavelet, $r(t)$ is reflectivity, and $w(t)$ is seismic noise.

We implement supervised learning to recover true reflectivity r(t) using a DNN and compare it with conventional least-squares inversion (explained later). The advantage of using multiple layers in a neural network is to generate nonlinear mapping functions with high complexity. For the neural network problem, first we need to optimize parameter set Θ and build a pseudoinverse operator $H^\dagger_\Theta$ from training data sets. The objective function for this operator building is

$$L_{learn} = \frac{1}{2}\left\| r_n(t) - H^\dagger_\Theta s_n(t) \right\|_2^2 + \lambda \|\theta\|, \qquad (5)$$

where $r_n(t)$ is modeled reflectivity as training output data, and $s_n(t)$ is measured seismic traces as training input data. The L1 weight penalty or regularization term $\lambda\|\theta\|$ is applied to lead sparsity of reflectivity and to prevent overfitting, where θ is a parameter set to be optimized, which is equivalent to a set of weight and bias values in the neural network. λ is a nonnegative regularization parameter.

The learning process of the DNN generates a nonlinear mapping function $H^\dagger_\Theta$, which is equivalent to the pseudoinverse of the forward operator. One can use any existing or synthetic data sets as the training data sets for the DNN if they represent the observed data well. We synthetically generate the training data sets from convolving a 25 Hz Ricker wavelet and reflectivity. The total number of training samples is equivalent to the multiplication of the number of reflectivity models and the number of observations in a reflectivity model (266,200 × 30 observations). Seismic traces

are modeled from each reflectivity model and include 30 time samples with 2 ms intervals. A value of feature corresponds to a seismic sample with a time window that ranges from −40 to 40 ms at the current observation (Figure 1), thus the number of features is 41. The training output is the reflectivity value that corresponds to the seismic traces. In each reflectivity model, three reflectors vary in location and magnitude. Location changes with 2 ms increments, and magnitude ranges from −1.0 to 1.0 with 0.2 increments for synthetic data sets. For field data sets, reflectivity magnitudes range from −1.0 to 1.0 with 0.1 increments. When the source wavelet is not close to 25 Hz, we can squeeze or stretch the signals and still use the mapping function for different data sets.

We construct our DNN model with an input layer, three hidden layers, and output layers. The three hidden layers have 200, 100, and 50 neuron units, respectively. In a neural network, an activation function decides whether to convert an input signal of a node to an output signal or not. A rectified linear unit (ReLU) is efficient for DNN training with large data sets (Schmidhuber, 2015). Here, we use ReLU as an activation function. To minimize the objective function (equation 5), adaptive moment estimation is adopted as a gradient-descent optimization algorithm. During the training process, 10% of neuron units are dropped to prevent overfitting of the DNN model.

After pseudoinverse operator $H^\dagger_\Theta$ is generated during the training process, we can estimate reflectivity for actual data s(t) using

$$\widehat{r(t)} = H^\dagger_\Theta s(t) , \qquad (6)$$

where $\widehat{r(t)}$ is estimated reflectivity.

The inversion scheme we compare with the machine learning method is least squares with an L1 regularizer denoted as

$$L = \frac{1}{2}\left\| s(t) - h(t) * \widehat{r(t)} \right\|_2^2 + \lambda \left\| \widehat{r(t)} \right\|, \qquad (7)$$

where λ is a nonnegative regularization parameter. We invert $\widehat{r(t)}$ by minimizing the objective function (equation 7). The convolved wavelet is the same as what we use for the neural network method. The L1-norm regularizer recovers a sparse solution and is called basis pursuit (Chen et al., 2001; Wipf and Rao, 2004; Zhang and Castagna, 2011) in signal processing and least absolute shrinkage and selection operator in statistics.

Results and discussion

Synthetic models. The wedge model was tested to evaluate the predictability on thin beds for each approach. Figure 2 shows inverted reflectivity using neural network and least-squares methods. The dominant frequency of the source wavelet is 25 Hz, and hence the tuning thickness is 20 ms (Chung and Lawton, 1995). Reflected waves of two reflectors in Figure 2c constructively interfere and produce a single event when wedge
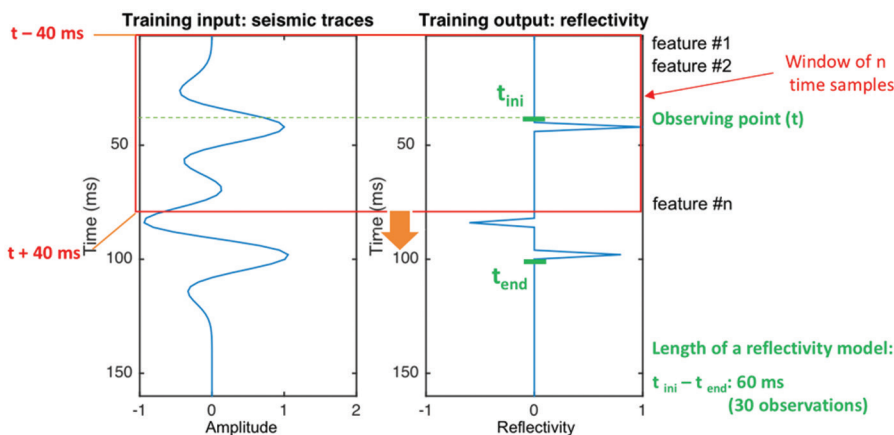

Figure 1. Description of training input and output data for reflectivity inversion using neural network methods.

thickness is less than 20 ms. The neural network approach distinguishes two separate events narrower than the tuning thickness (Figure 2e), which shows better resolution than that of the least-squares model (Figure 2g). In this example, the resolvable thickness of the neural network and least-squares methods are 4.2 and 5.4 ms, respectively. They are below the tuning thickness. (The peak frequency of the data is 25 Hz, yielding a one-quarter wavelength resolution of about 20 ms.) The neural network model classifies reflectivity based on features that are equivalent to the amplitude of seismic traces in each time sample of training data. The amplitude of two reflectors in Figure 3b can be differentiated from the amplitude of a single reflector, which is resolvable with the neural network method. Seismic traces of different polarities (Figure 2d) destructively interfere when reflectors are closely spaced. Figure 2f shows the neural network result, which resolves two reflectors even when the reflectors are closer than the tuning thickness. In the least-squares result, two reflectors are separated as two events at tuning thickness, but the locations of these events are wrong (Figure 2h).

In the case that the forward operator, which is equivalent to the wave matrix, is convolved with the reflectivity series, the problem becomes underdetermined and ill posed. Underdetermined problems can give rise to a nonunique solution. For instance, two closely spaced reflectors and one single reflector can lead to the same solution in this inversion. The neural network approach, on the other hand, has a sufficient number of dimensions or features to build the inverse operator that can resolve thin beds (Figures 2e and 2f). A potential limitation of the machine learning method arises when training data do not represent the problem because the data set is not sufficient for solving the problem and/or because input and output are not related. Also, an appropriate hyperparameter should be selected for good quality of model building. The machine learning method also suffers from the overfitting problem, which occurs when a function is closely fit to a limited set of data.

We examine the sensitivity of two methods for noisy data (Figures 4 and 5). We add white Gaussian noise to seismic traces with signal-to-noise (S/N) ratio of 0, 2, and 4 dB. Here we measure the S/N as a ratio of signal power of the true reflectivity model compared to noise power. To test the sensitivity of the noise
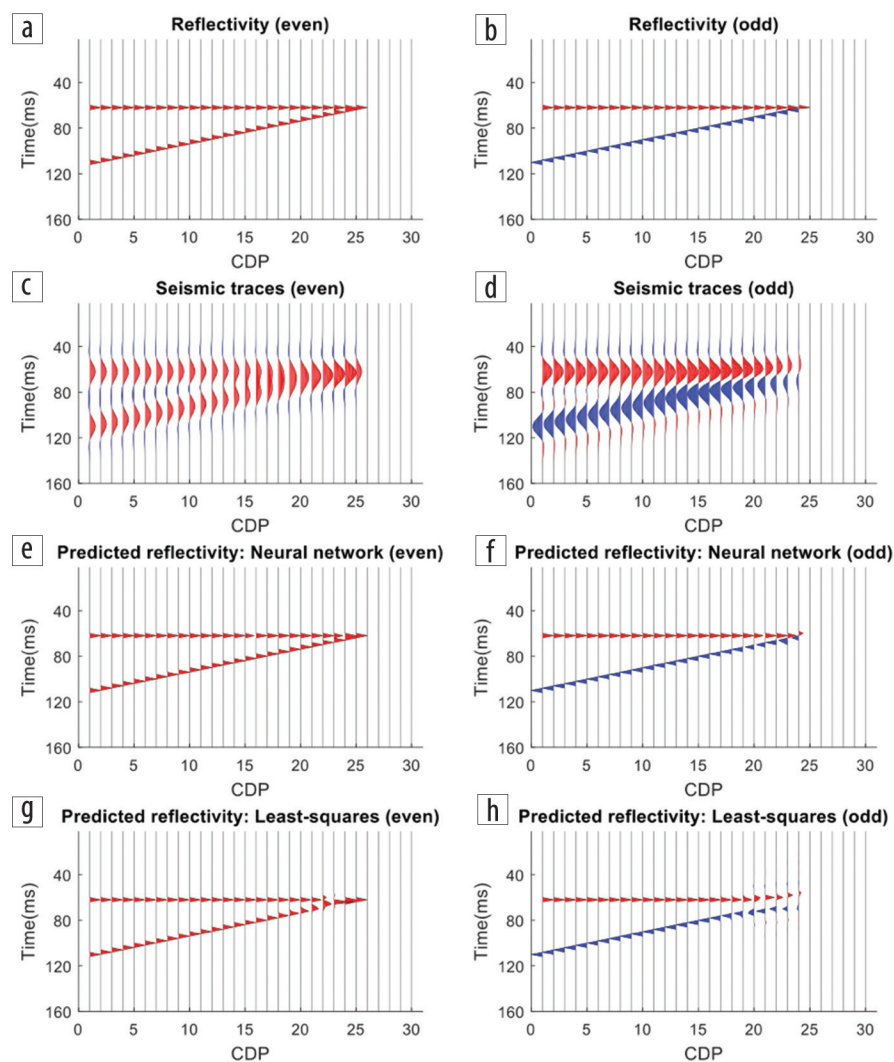

Figure 2. 2D wedge true reflectivity model with (a) two reflectors with positive impedance (even reflectivity pairs; red) and (b) two reflectors with positive impedance and negative impedance (odd reflectivity pairs; red and blue, respectively). (c) and (d) Seismic traces modeled by convolving a source wavelet (25 Hz Ricker wavelet) and reflectivity shown in panels (a) and (b), respectively. (e) and (f) Predicted reflectivity using the neural network method from the data in panels (c) and (d), respectively. (g) and (h) Same as panels (e) and (f) but using the least-squares method.
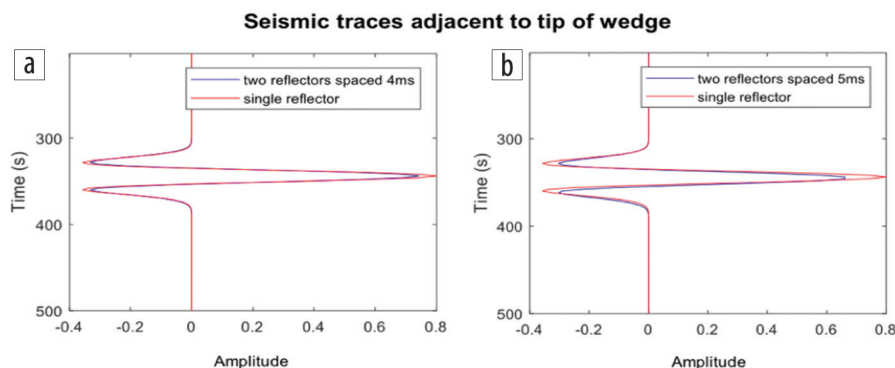

Figure 3. Seismic traces adjacent to tip of wedge. Amplitude of two reflectors spaced (a) 4 ms and (b) 5 ms.
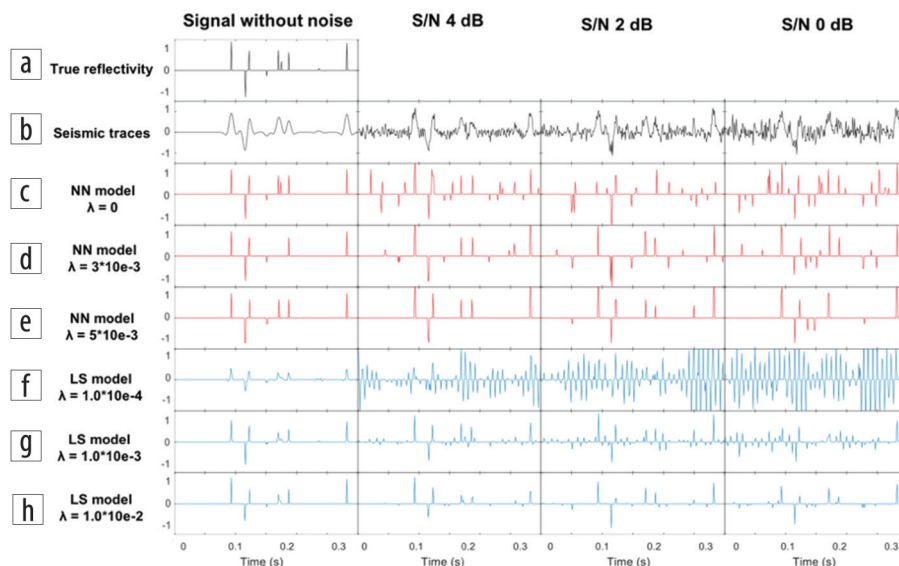
Figure 4. (a) True reflectivity. (b) Seismic traces modeled from the true reflectivity. White Gaussian noise is added with different S/N levels: noise free, 4, 2, and 0 dB. (c) through (e) Recovered reflectivity using neural network method with the L1 regularization parameter (equation 5); (c) $\lambda = 0$, (d) $\lambda = 3 \cdot 10e{-3}$, (e) $\lambda = 5 \cdot 10e{-3}$. (f) through (h) Recovered reflectivity using the least-squares method with the L1 regularization parameter (equation 7): (f) $\lambda = 10e{-4}$, (g) $\lambda = 10e{-3}$, (h) $\lambda = 10e{-2}$.
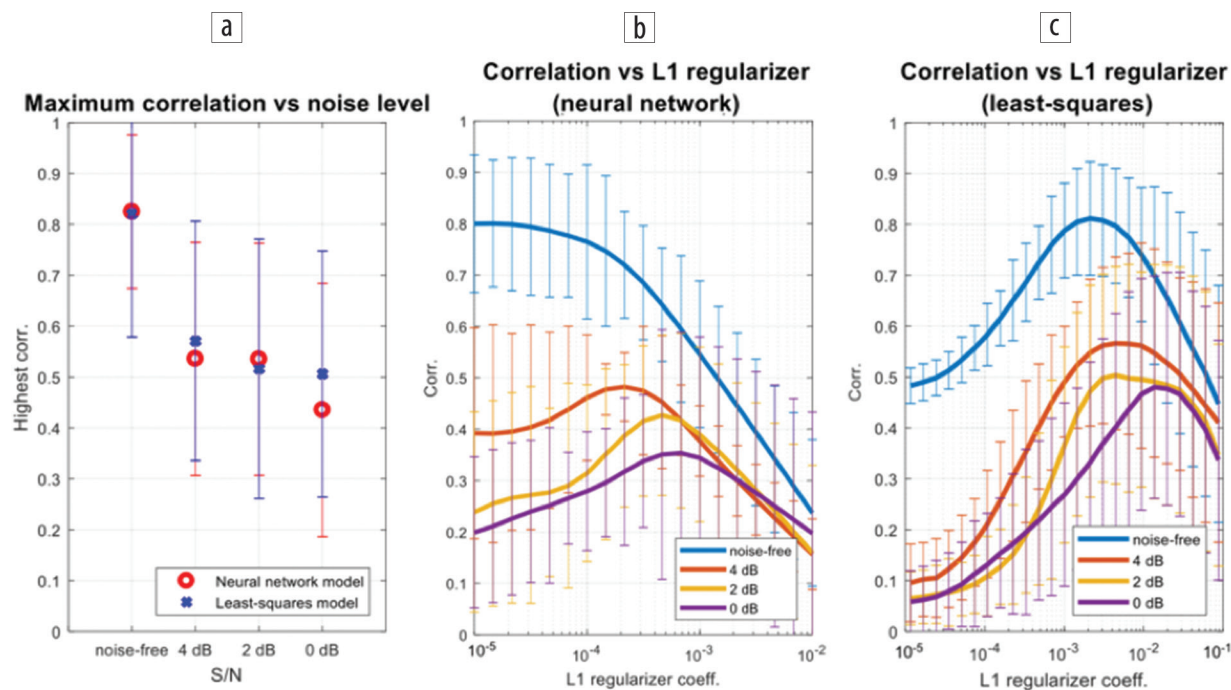

Figure 5. Sensitivity of two algorithms with regard to the noise component of data. (a) Correlation coefficients between true reflectivity model and inverted model at different noise levels. White Gaussian noise is added with S/N level: noise free, 4, 2, and 0 dB. (b) and (c) Correlation coefficients for different L1 regularization coefficients at each noise level using (b) neural network and (c) least-squares methods. We test 10 different models to compute the correlation coefficients, and the errorbars represent the standard deviation of different models.

Table 1. Computation time of reflectivity inversion neural network and least-squares methods.

Inversion methods		Number of processes	Elapsed time (in seconds)
Neural network	**Training**	1	837 s
	Inversion	1	0.344 s/trace × (367 × 271) traces = 34,213 s
Least squares		1	1.89 s/trace × (367 × 271) traces − 187,973 s

for two methods and evaluate an effect of L1 regularization with respect to the noise, we calculate the correlation coefficient between true reflectivity and inverted reflectivity for different regularization coefficients λ (Figure 5). We use 10 different models (one example is shown in Figure 4a) for estimating reliable correlation coefficients. For noise-free data, the neural network model yields high accuracy when the regularization term is not added (Figures 4c and 5a). This is because the regularization term induces underfitting, which reduces the accuracy for the data set. In the presence of noise, however, the proper value of the regularization term enhances the accuracy and suppresses noise (Figures 4d and 4e and 5a and 5b). The underfitted model means that the mapping function is smoother, and thus the model can recover the right solution in the wide range in noisy data sets. In the least-squares model, adding an L1-regularization term gives better results regardless of the existence of noise. Particularly for the least-squares model, because the inverse operator has the same effect as a bandwidth-broadening filter, the noise is amplified during the inversion process. The regularization term filters out these undesired components when their Eigen values are small.

We also add the different level of noise to training data and apply inversion to a noisy test set to test the effect of noise in neural network training. Noise in training data can alleviate the effect of noise in test data and enhance prediction accuracy (Figure 6) since it prevents overfitting in the training process. It is known that training with noise is equivalent to adding a regularization factor (Bishop, 1995). In the case of noise-free test data, however, noisy training data reduce the accuracy of the inversion, which behaves similar to a regularizer.

Field data example. We apply two algorithms to the 2D volume extracted from 3D field poststack seismic data and evaluate resolution of the inverted reflectivity. The seismic volume includes 367 × 271 traces (Figure 7a). Traces are sampled up to 2.5 s with a sample interval of 2 ms. We estimate the source wavelet using a statistical method (Figure 7b). We use the source wavelet to generate a training data set for the neural network. The forward operator in the least-squares method is also computed using the wavelet. The L1 regularization parameter λ for neural network and least-squares methods are 0 and 1.5E-5, respectively, which provides the minimum error between measured seismic traces and seismic traces modeled from the inverted reflectivity for each method. The total computation times of the two methods are compared in Table 1. Even if the neural network method requires computing time for training, the time elapsed for the inversion process in the neural network method is comparatively shorter than that of the least-squares method. The inversion result using a neural network shows higher resolution compared to measured seismic traces (Figure 8). The least-squares method also resolves thin beds; however, the reflectivity is less definite than one inverted using the neural network method. Also, the
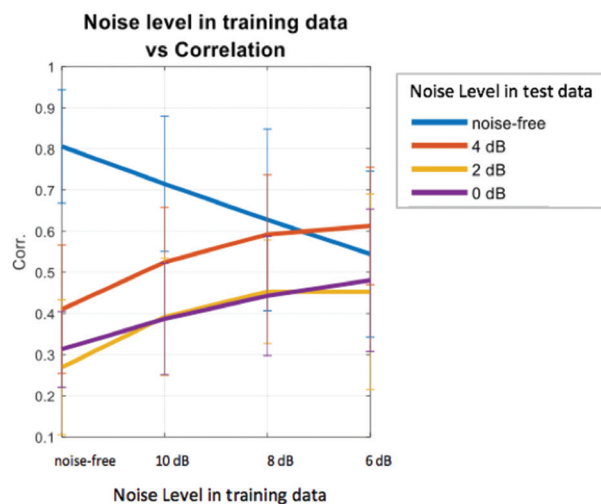

Figure 6. Correlation coefficients for different levels of noise in training data used in the neural network method. Noise in training data can alleviate the effect of noise in test data. In a case of noise-free test data, however, noisy training data reduce the accuracy of the inversion.
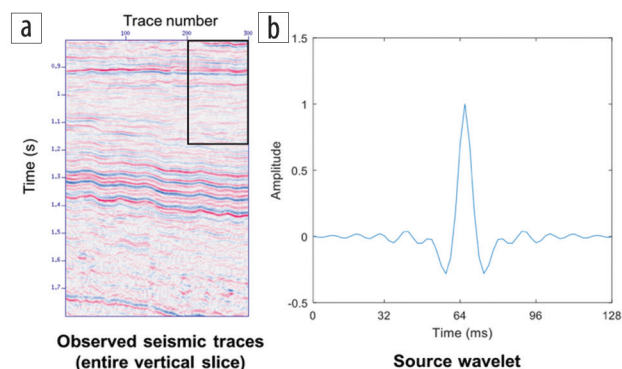

Figure 7. (a) A representative vertical slice of 3D field poststack seismic data tested for reflectivity inversion. An enlarged image of seismic traces in a black box is in Figure 8a. (b) Seismic source wavelet used for reflectivity inversion. The wavelet is extracted using a statistical method.
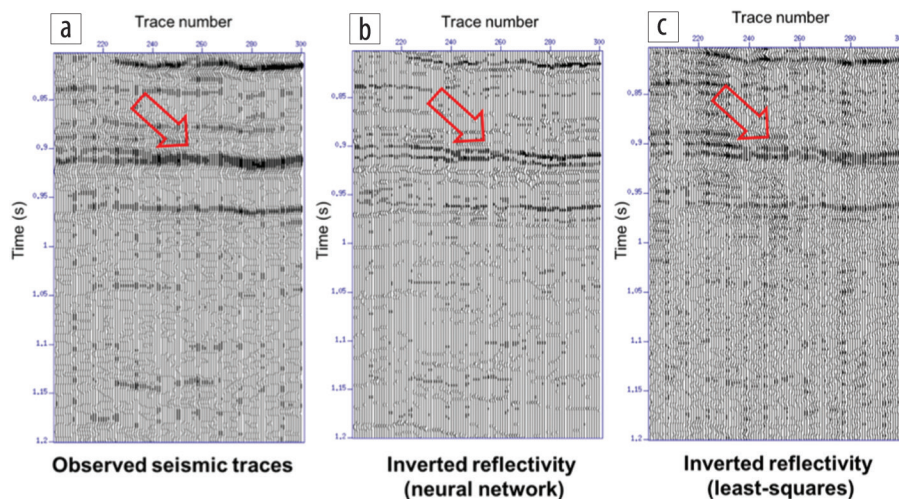

Figure 8. (a) Observed seismic traces (input data), (b) inverted reflectivity model estimated by neural network method and (c) inverted reflectivity model computed by the least-squares method. Inverted reflectivity in panels (b) and (c) show higher resolution than that of seismic traces in (a). Especially the neural network method (b) better recovers sparse reflectivity of stratigraphic boundaries, which is indicated by red arrows.
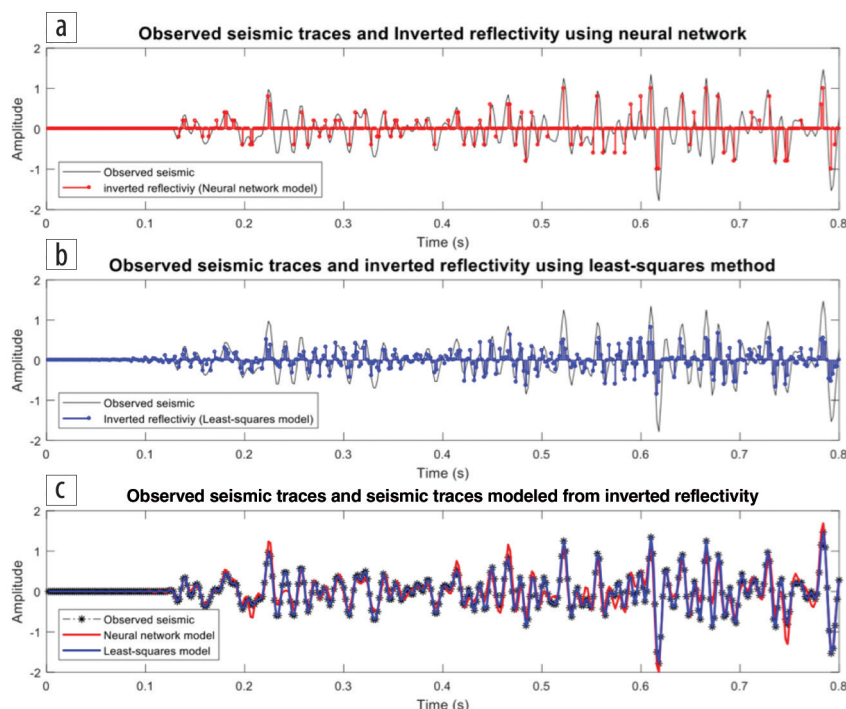
Figure 9. Comparison of observed seismic traces and inverted reflectivity using (a) neural network, (b) least-squares method, and (c) comparison of observed seismic traces and seismic traces modeled from inverted reflectivity using two methods.

least-squares method shows a ringing effect or noise, especially around traces 220–240. Comparing inverted reflectivity of a trace in a vertical slice, the neural network model recovers sparsity of reflectivity series better than the least-squares method (Figure 9). The limitation of the neural network is that the seismic traces modeled from inverted reflectivity show minor error in amplitude.

Conclusions

We examine conventional geophysical inversion and machine learning as a methodology to solve an inverse problem. We show the similarities and differences of such methods based on mathematical expression and take reflectivity inversion as an example of an inverse problem. Convolving reflectivity with seismic wavelet works as a low-pass filter, which results in reflectivity inversion as an underdetermined ill-posed problem. The least-squares methods fit the data points using a concept of normal equation. The least-squares fitting provides a compromised solution that minimizes perpendicular offset between data points and model. In the machine learning method, especially neural network in this case, a set of weight values is multiplied to each feature.

During the learning process, weights are optimized to be able to classify reflectivity even when small differences are observed between different input data samples. This explains why the neural network displays higher resolution in the thin beds example. However, enlarging the difference and yielding high accuracy in the neural network method does not necessarily guarantee that the quality of the estimated model will be good. The pseudoinverse operator generated in machine learning methods relies on training sets and hyperparameters. If training data do not represent the distribution of data sets in real-world problems, the problem of so-called overfitting occurs.

Algorithms combining two methods can be suggested for general inverse problem or reflectivity inversion. If physical equations or forward operators are known, the machine learning method can supplement geophysical inversion. For example, higher resolution in reflectivity inversion can be yielded using machine learning methods. **TLE**

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