DeepGEM: Generalized Expectation-Maximization for Blind Inversion

Angela F. Gao\(^1\)  Jorge C. Castellanos\(^2\)

Yisong Yue\(^1\)  Zachary E. Ross\(^2\)  Katherine L. Bouman\(^1\)

\(^1\)Computing and Mathematical Sciences, California Institute of Technology
\(^2\)Caltech Seismological Laboratory, California Institute of Technology

\{afgao, jcastellanos, yyue, zross, klbouman\} \(\circ\) caltech.edu

Abstract

Typically, inversion algorithms assume that a forward model, which relates a source to its resulting measurements, is known and fixed. Using collected indirect measurements and the forward model, the goal becomes to recover the source. When the forward model is unknown, or imperfect, artifacts due to model mismatch occur in the recovery of the source. In this paper, we study the problem of blind inversion: solving an inverse problem with unknown or imperfect knowledge of the forward model parameters. We propose DeepGEM, a variational Expectation-Maximization (EM) framework that can be used to solve for the unknown parameters of the forward model in an unsupervised manner. DeepGEM makes use of a normalizing flow generative network to efficiently capture complex posterior distributions, which leads to more accurate evaluation of the source’s posterior distribution used in EM. We showcase the effectiveness of our DeepGEM approach by achieving strong performance on the challenging problem of blind seismic tomography, where we significantly outperform the standard method used in seismology. We also demonstrate the generality of DeepGEM by applying it to a simple case of blind deconvolution.

1 Introduction

Physics-based inversion methods typically recover an unknown source from indirect measurements by assuming that the source and measurements are related via a known forward model \([15, 7, 30]\). For example, non-blind deconvolution algorithms often assume that a measured blurry image is related to its true sharp image via a known spatially-invariant blur kernel \([9]\); and traditional seismic inversion methods assume that the spatially-varying velocity of the Earth’s interior is known \(a\ priori\) when solving for an earthquake’s hypocenter \([30]\). However, these “known” forward models are generally idealized and ignore intricacies of the systems that are either hard to capture or simply unknown. Inversion algorithms with forward \textit{model mismatch} result in biased reconstructions. For instance, bias is regularly seen in non-blind deconvolution results, where reconstruction artifacts are often present due to the use of an incorrect blur kernel \([9]\).

In order to reduce the effects of model mismatch, in this paper we tackle the problem of \textit{blind inversion}: solving an inverse problem without knowledge of the underlying forward model parameters. When considering how learning can help, a natural first idea might be to learn a direct map from measurements to the desired source via supervised learning. However, such a “model-free” approach is generally not practical, due to the lack of available ground truth training data. For example, the blur kernel caused by handheld camera shake cannot be reproduced to get a training set of...
sharp-blurry pairs to train a deconvolution approach. In seismic tomography, synthetic earthquakes cannot be placed densely throughout the interior of the Earth to measure the ground response as a function of hypocenter location. An alternative approach, which we adopt, is to develop unsupervised methods that treat the true forward model as something that is unobserved and must be inferred. An additional consideration is that we must solve for the true forward model from a single dataset, without knowledge of the true source that produces the measurements.

In this paper, we propose Deep Generalized Expectation-Maximization (DeepGEM) for solving blind inverse problems. Using the indirect measurements as input, DeepGEM jointly estimates the source and forward model that together produce the observed measurements. DeepGEM is a variational inference based framework that makes use of deep learning machinery to easily capture and optimize complex probabilistic distributions that cannot be easily integrated in analytic Expectation-Maximization (EM) solutions. Our proposed framework is generic and can be applied to blind inversion problems described by differentiable forward models. In Section 4 we showcase the effectiveness of our DeepGEM approach on the challenging problem of blind seismic tomography, where we significantly outperform methods used in seismology. We also demonstrate the generality of DeepGEM by applying it to blind deconvolution in Section 5.

Figure 1: DeepGEM applied to blind seismic tomography. (a) A simulated cross section of the Earth's interior (velocity structure), along with the locations of receivers on the surface (red triangles) that collect measurements. (b) The time it takes for a wave traveling from a source below the surface to reach the specified receiver is visualized for each location in the region of interest. The overlaid dots represent the true locations of simulated earthquakes and indicate the measured travel times that constrain optimization. (c) The subsurface velocity reconstruction obtained using a baseline approach optimized with the help of a seismologist. Note that the bright anomaly is missing from this reconstruction. Overlaid dots represent the inferred earthquake locations. (d) DeepGEM reconstructed subsurface velocity and inferred earthquake locations. Note that DeepGEM is able to accurately recover the gradient of the velocity field as well as partially recover the central anomaly.

2 Background and related work

The joint optimization of a forward model with source recovery is a very challenging ill-posed problem, leading to many possible solutions that are hard to disambiguate. For example, in blind deconvolution the blurry image observed can be equivalently explained by a sharp source image convolved with an extended kernel or a blurry source image convolved with an impulse kernel; to prefer one solution over another, additional information, such as image priors, must be considered. Previous work on inversion in poorly characterized systems focused on limited contexts, such as spatially-invariant blind deconvolution [21, 22, 14, 10] and CT with a simple rotational error [35]. These methods tend to be highly specialized to each application domain, and cannot be easily generalized. In contrast, we propose a flexible model-based Bayesian framework that can be applied across multiple differentiable blind inversion problems.

2.1 Model-based Bayesian inversion

In model-based inversion, unobserved sources \( x \) and observed measurements \( y \) are related through a forward model: \( y = f(x) \). When the parameters of the underlying model are unknown, one can parameterize the forward model as \( f_\theta(x) \) and then solve for the true model parameters \( \theta^* \). A common approach is to solve a maximum a posteriori (MAP) objective: either MAP\( _{\theta,x} \) or MAP\( _{\theta} \).
MAP_{θ,x} solves for the optimal point estimate of the pair \{\hat{θ}, \hat{x}\} that maximizes a joint objective:

\[
\{\hat{θ}, \hat{x}\} = \arg \max_{θ, x} \left[ \log p(θ, x | y) \right] = \arg \max_{θ, x} \left[ \log p(y | θ, x) + \log p(θ) + \log p(x) \right]. \tag{1}
\]

In practice, formal probabilistic definitions of \(p(θ)\) and \(p(x)\) are often unknown and replaced with regularization terms (e.g., total variation, sparsity) \([22, 21]\). Although MAP_{θ,x} provides a straightforward approach to solve for \(θ\), the energy landscape of Eq. (1) is typically poorly behaved due to the ill-posed nature of the problem \([22]\). As a result, optimization is likely to get stuck in a (bad) local minimum.

MAP_{θ} attempts to smooth the energy landscape by reducing the number of parameters that must be optimized. This is done by solving for parameters of the forward model, \(θ\), that perform best under the full volume of possible \(x\) interpretations:

\[
\hat{θ} = \arg \max_{θ} \left[ \log p(θ | y) \right] = \arg \max_{θ} \left[ \log \left( \int_x p(y | θ, x) p(x) dx \right) + \log p(θ) \right]. \tag{2}
\]

Since this marginalization integral is often intractable, Expectation-Maximization (EM) algorithms have long been used for solving MAP_{θ} efficiently \([11]\). EM is an iterative algorithm that alternates between: “E”-Step (calculating the posterior of \(x\) conditioned on the current estimated forward model parameters \(θ^{(t-1)}\); and M-Step) updating \(θ\) to maximize the expected value of the log likelihood:

\[
θ^{(t)} = \arg \max_{θ} \left[ \mathbb{E}_{x \sim p(x | y, θ^{(t-1)})} \left[ \log p(y | θ, x) \right] + \log p(θ) \right]. \tag{3}
\]

The advantage of MAP_{θ} over MAP_{θ,x} optimization for the blind deconvolution problem was described in \([22]\) and its success demonstrated via EM optimization in \([21]\). However, it is important to note that evaluating the expectation in of Eq. (3) over complex distributions is often intractable. For instance, the authors of \([21]\) were forced to restrict the posterior distribution to a Gaussian distribution. Alternatively, stochastic EM methods \([5, 8]\) bypasses the need to evaluate the expectation directly, approximating it by sampling the distribution. In this paper, we solve MAP_{θ} using complex distributions parameterized by deep neural networks.

Forward model parameterization Model-based inversion requires that the parametric form of \(f_θ(x)\) is well matched with the true forward model, which is not always known. Alternatively, neural networks can be used to approximate the forward model, where \(θ\) represents the network weights. This setup is flexible, in that it can be used to approximate arbitrarily complex forward models, with the downside that it is often not interpretable when the parameters have no physical meaning. In this work, we develop and make use of interpretable, physically-motivated deep neural networks to parameterize \(f_θ(·)\) for the problems of blind seismic tomography and blind deconvolution.

2.2 Deep variational distributions

We are interested in solving blind inverse problems using the EM algorithm to optimize the MAP_{θ} objective. Optimizing in this fashion requires the use of the posterior distribution \(p(x | y, θ^{(t-1)})\) in evaluating Eq. (3). As inverse problems are often ill-posed, we expect that the posterior distribution of source \(x\) conditioned on the forward model parameters \(θ\) is likely to be complex and perhaps even multi-modal. Therefore, it is important to be able to parameterize a flexible family of distributions to best estimate this conditional posterior.

Deep Probabilistic Imaging (DPI) \([32]\) uses a normalizing flow-based generative model, \(G_φ(·)\), to solve for the uncertainty of an unknown source \(x\) given a fixed forward model \(f(·)\) and measurements \(y\). DPI solves the variational objective:

\[
\hat{φ} = \arg \min_φ \text{KL}(q_φ(x) || p(x | y)) = \arg \min_φ E_{x \sim q_φ(x)} \left[ -\log p(y | x) - \log p(x) + \log q_φ(x) \right], \tag{4}
\]

where \(q_φ(x)\) is the implicit distribution defined by \(G_φ(·)\) for \(z \in \mathcal{R}^{|x|} \sim \mathcal{N}(0, 1)\) and \(\log p(y | x) \propto \|y - f(x)\|_2 + c\) when there exists i.i.d. Gaussian noise on the measurements, \(y\). After inference, \(q_φ(x)\) can be efficiently sampled by evaluating \(G_φ(z)\) for a Gaussian sample \(z\).

The DPI variational objective is equivalent to the Variational Autoencoder \([17, 28]\) objective, except with a fixed decoder, \(f(·)\). In practice, vanilla VAEs constrain the posterior to be a Gaussian

\[|x| \] is the dimension of \(x\)
distribution, relying on the reparameterization trick for tractable optimization. Alternatively, DPI uses flow-based networks to efficiently sample and directly compute \( q_{\phi}(x) \) [12][13][18]. DPI’s use of a flow-based network allows for complicated and multi-modal posterior distributions constrained only by the space of possible invertible network architectures. Our proposed DeepGEM approach utilizes similar tools to model flexible distributions over \( x \), while simultaneously learning the forward model parameters \( \theta \).

3 Methods

We propose a deep variational EM approach (DeepGEM) that optimizes the MAP\(_{\theta} \) objective in Eq. [2] to recover the parameters of a forward model \( f_\theta(x) \) using only a single static set of measurements \( y \). Once learned, the updated forward model can then be used to estimate the posterior distribution of the unknown source, \( x \). DeepGEM iterates between two stages that are inspired by the standard EM algorithm: (1) an “E”-step that learns a variational distribution, \( q_{\phi(t)}(x) \), to approximate the posterior distribution of \( x \) given the current forward model parameters \( \theta^{(t-1)} \), and (2) an M-step (refer to Eq. [3]) that solves for \( \theta^{(t)} \) that maximizes the expected value of the log likelihood function of \( \theta \), with respect to the posterior distribution \( q_{\phi(t)}(x) \) estimated in the prior “E”-step. Each step is alternated and solved to convergence. Since this is an EM algorithm (up to the variational approximation), our method inherits properties of EM, including convergence to a local minimum of Eq. [2].

3.1 “Expectation” step (“E”-step)

The goal of DeepGEM’s “E”-step is to solve for the posterior distribution \( p(x|y, \theta^{(t-1)}) \) that facilitates optimizing Eq. [3]. Because this posterior distribution can be very complex, and even multi-modal, we propose to use a flexible variational approach to learn the parameters \( \phi \) of an approximate posterior distribution \( q_{\phi}(x) \). The variational distribution \( q_{\phi}(x) \) can then be used to evaluate Eq. [3] via efficient sampling.

Using DPI we solve for a flexible variational distribution, \( q_{\phi}(x) \) that well approximates the posterior distribution \( p(x|y, \theta^{(t-1)}) \). DPI uses a normalizing flow network, \( G_{\phi}(z) \), with input \( z \in \mathbb{R}^{[d]} \), where \( x = G_{\phi}(z) \sim q_{\phi}(x) \) when \( z \sim \mathcal{N}(0, 1) \). Normalizing flow networks allow for exact computation of the log-likelihood \( \log q_{\phi}(x) \) needed to solve

\[
\phi^{(t)} = \arg \min_{\phi} \text{KL}(q_{\phi}(x) || p(x|y, \theta^{(t-1)}))
\]

\[
\approx \arg \min_{\phi} \frac{1}{N} \sum_{n=1}^{N} \left[ -\log p(y|\theta^{(t-1)}, x_n) - \log p(x_n) + \log q_{\phi}(x_n) \right]
\]

for \( x_n = G_{\phi}(z_n), \ z_n \sim \mathcal{N}(0, 1) \),

(5)

(as derived from Eq. [4]) for a batch size of \( N \) where \( \log p(x) \) is a prior on the source and \( \log p(y|x, \theta^{(t)}) \) is the data likelihood. When assuming the measurements \( y \) experience i.i.d additive Gaussian noise with standard deviation \( \sigma_y \), \( \log p(y|\theta^{(t)}, x_n) = \frac{1}{2\sigma_y^2} \| y - f_{\theta^{(t)}}(x_n) \|^2 + c \).

3.2 Maximization step (M-step)

The goal of DeepGEM’s M-step is to use the parameterized approximate posterior distribution, \( q_{\phi(t)}(x) \), from the prior “E”-step to update \( \theta \), the parameters of the unknown forward model \( f_\theta(\cdot) \). This is achieved by sampling from the learned normalizing flow network, \( G_{\phi(t)}(\cdot) \), to stochastically solve Eq. [5]:

\[
\theta^{(t)} \approx \arg \max_{\theta} \left[ \frac{1}{N} \sum_{n=1}^{N} \log p(y|\theta, x_n) + \log p(\theta) \right] \quad \text{for} \quad x_n = G_{\phi(t)}(z_n), \ z_n \sim \mathcal{N}(0, 1),
\]

(6)

where \( p(\theta) \) is a prior on the forward model. This prior can be used to encourage the forward model parameters to remain close to an initial model \( \hat{\theta} \) by defining \( \log p(\theta) \propto ||\theta - \hat{\theta}||_2 + c \).
4 Case study: blind seismic tomography

Two fundamental seismic inverse problems are spatially localizing an earthquake’s hypocenter (also referred to as source localization) and tomographic reconstruction of the Earth’s subsurface [30]. These problems are interconnected: source localization relies on knowing how fast waves propagate through different regions of the Earth’s interior, referred to as the Earth’s velocity structure. However, in standard seismological practice, due to difficulties in solving these problems jointly, they are generally treated separately: source localization is performed initially using oversimplified velocity models [30], and then the tomography problem is performed by taking those best-fitting hypocenters as ground truth [26]. This approach typically results in the need to over-regularize the inverse problem by smoothing out high-frequency information [2], and can only be improved by carefully incorporating other forms of information such as waveform-derived quantities [16, 23, 4, 24] or by performing costly experiments such as controlled explosions. In contrast, we demonstrate our DeepGEM approach on blind seismic tomography, solving for the subsurface velocity (parameterized by $\theta$) when the source hypocenters, $x$, are unknown. Measurements, $y$, used to constrain the inverse problem are the time it takes for the first wave to propagate from its source to a receiver on the Earth’s surface, referred to as a travel time measurement (refer to Fig. [1]).

4.1 Seismic tomography background

Physics of earthquake source localization: The earthquake source location, also called the hypocenter, is the location where the earthquake nucleates [30]. The source location can be triangulated using travel times from multiple receivers. However, when there are very few receivers ($< 3$ in 3D, $< 2$ in 2D), the source localization is ill-posed and there exists multiple equally optimal solutions.

Physics of travel time tomography: Travel time tomography is a method for reconstructing the velocity structure using the absolute arrival times of earthquake waves from the earthquake to the receiver [30]. Given perfect knowledge of the earthquake locations $x$ and receivers $r$ at every position in the ground, the exact velocity can be computed by solving the Eikonal equation $V(r) = \|\nabla T(x, r)\|^{-1}_2$, where $T(x, r)$ is the travel time from an earthquake to a receiver. There exists an analytical solution to the Eikonal equation; however, seismologists often use simplifications, such as straight ray tomography, for efficiency [2].

Deep Learning for travel time tomography: EikoNet [31] implicitly solves the Eikonal equation [33] by learning a mapping from a source-receiver pair $(x, r)$ to its associated travel time, learning $\theta$ such that $f_\theta(x, r) \approx T(x, r)$ where $T(x, r)$ is the true travel time. The velocity structure can then be extracted from the learned EikoNet by solving the Eikonal equation through automatic differentiation. In particular, the computed velocity $V(s)$ at location $s$ is $\|\nabla_s f_\theta(x, s)\|^{-1}_2$. Note that this computed velocity depends on the source location $x$. Ideally, the velocity should be invariant to the source location; however, in practice, this is only true when EikoNet is trained with densely-sampled $(x, r)$ pairs. Additionally, the travel time from a source to a receiver, $T(x, r)$, should be identical to the travel time from a receiver to a source, $T(r, x)$, but remains unconstrained by EikoNet.

![Figure 2: (Left) A visualization of the homogeneous, gradient, and layer models used in $p(\theta)$’s $\mathcal{L}_\theta$ term. (Right) Visualizations used to describe source configurations and earthquake source posteriors. (a) Visualizations of the true and initialized source locations are plotted as stars (true) connected to circles, which indicate the expected source locations according to $p(x)$. Note that the expected source locations deviate significantly from the true locations. (b) Visualizations of the learned posterior distribution, $q_\theta(x|y, \theta)$, for each source are plotted as colored histograms and overlaid with stars (of the same color) indicating the true source location.](image)


We construct a prior over the forward model, $p(\theta)$ within the region of interest. Before DeepGEM optimization, we first initialize with respect to the source location, and (2) travel time symmetry between sources and receivers. We augment the prior

$$p(\theta) = \lambda_\theta \sum_{s \in S} ||\tilde{V}_s - V_s||_2 + \lambda_V \sum_{s_i, s_j \in S} ||V_{s_i}(s) - V_{s_j}(s)||_2 + \lambda_T \sum_{s \in S} ||T(s, r) - T(r, s)||_2.$$  

The velocity constraint is represented through $L_V$ and travel time constraint through $L_T$, with corresponding hyperparameters $\lambda_V$ and $\lambda_T$. $S$ is a set of points sampled uniformly from the region of interest, $R$ is the set of all receiver locations, and $V_s = ||\nabla_s f_0(r, s)||_2^{-1}$.

**Implementation details:** In our experiments we define a realistic prior over unknown source locations as $p(x) = \mathcal{N}(\bar{x}, \sigma_x)$, where $\bar{x} \sim \mathcal{N}(x, \sigma_x)$ and $\sigma_x = 2$ km. We assume the measurements $y$ are sampled from a Gaussian distribution with mean $\bar{y} - \text{true travel times computed using the package eikonal1fm}$ and a realistic standard deviation of $\sigma_y = 0.2$ seconds. To simulate real world passive tomography, we assume receivers are located only along the surface (the top edge of the 2D image) of the region of interest, which is 20 km $\times$ 20 km, and sources can be anywhere within the region of interest. Before DeepGEM optimization, we first initialize $\theta$ using maximum likelihood estimation assuming $\bar{x}$ is the true source location.
Figure 4: **DeepGEM consistently recovers prominent features across various earthquake source configurations.** Row 2 shows DeepGEM results obtained using different random source configurations, where the true Earth velocity is shown in Fig. 1(a). As a reference, row 1 shows the velocity reconstruction obtained using DeepGEM under fixed, perfectly known source locations. As can be seen by the table, both velocity and localization error decrease with an increasing number of sources in the region of interest. Each mean and standard deviation is computed using 5 random realizations of true source configurations.

The posterior distribution of the source locations, \( x \), is estimated using a Real-NVP network \( G_\theta(\cdot) \) with 16 affine coupling layers. An updated EikoNet (described in the supplemental material) has been modified to parameterize \( f_\theta(x) \). This EikoNet is pretrained with samples from the prior \( p(x) \) as input and the simulated travel time measurements as output. We use Adam as the optimizer [36] with a batch size of 32 and an E-step learning rate of 1e-3 and M-step learning rate of 5e-5. Hyperparameters \((\lambda_T, \lambda_V, \lambda_\theta)\) were empirically chosen by inspecting the loss on a grid search over hyperparameters. Results presented have been run with 10 EM iterations, each with 800 “E”-step epochs and 2000 M-step epochs. Each DeepGEM model takes \( \sim6 \) hours on a NVIDIA Quatro RTX 5000.

### 4.3 Results

**Comparison to Baseline Approaches:** We compare results from DeepGEM to results obtained using a baseline run by a seismologist. This iterative baseline alternates between source inversion and straight ray tomography, and is the standard approach used for blind tomography. Further detail on this baseline is provided in the supplemental material. The gradient model shown in Fig. 2 is used to perform the initial source inversion for this baseline; nonetheless, we find that the solution quickly diverges. Therefore, we rely on the expertise of the domain expert to decide when to terminate the optimization. As seen in Fig. 3, DeepGEM consistently outperforms this human-in-the-loop baseline across all source configurations. In Fig. 3 we also compare with a MAP\(_\theta,x\) solution. MAP\(_\theta,x\) is consistently outperformed by the DeepGEM MAP\(_\theta\) approach across all source configurations. Additional results highlighting the sensitivity of MAP\(_\theta,x\) to hyperparameters and initialization are shown in the supplemental material.

**Sensitivity to \( L_\theta \) Prior Choice:** We evaluate DeepGEM’s recovery of the true velocity structure shown in Fig. 1 using one of three different \( L_\theta \) priors shown in Fig. 2: homogeneous, gradient, and layer, as well as \( L_\theta = 0 \). The homogeneous model takes on value of 6.419 km/s, the average velocity value of the true velocity structure. The gradient captures the increasing velocity as depth increases, and the layer model represents the true model without the added anomaly. As shown in Fig. 3 the mean squared error tends to decrease with the gradient and layer \( L_\theta \) prior models, which are closer to the true velocity structure.

**Sensitivity to Source Configuration:** We evaluate results with sources that are both uniformly and randomly spaced throughout the region of interest. Improved performance is expected when the number of sources is increased and/or when sources are well distributed. To better understand DeepGEM’s performance we introduce an ablation, where the velocity structure is learned by training \( f_\theta(\cdot) \) with access to perfect source locations \( x \) (i.e., \( p(x) \) is a delta function). As is shown in Fig. 5 even when training with true source locations, the anomaly is not well resolved until \( \sim49 \) sources.

<table>
<thead>
<tr>
<th>Source Count</th>
<th>Velocity Error (km/s)</th>
<th>Source Loc. Error (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>0.52 ± 0.063</td>
<td>62.88 ± 21.77</td>
</tr>
<tr>
<td>25</td>
<td>0.42 ± 0.043</td>
<td>36.62 ± 4.93</td>
</tr>
<tr>
<td>49</td>
<td>0.44 ± 0.181</td>
<td>33.78 ± 4.56</td>
</tr>
<tr>
<td>100</td>
<td>0.27 ± 0.021</td>
<td>30.38 ± 1.43</td>
</tr>
</tbody>
</table>

Table 1: Velocity and source localization error on random source configurations.
Figure 5: DeepGEM recovery with a single receiver. Velocity reconstructions shown in columns 3 and 5 demonstrate that DeepGEM is able to learn some of the true velocity features (see Fig. 1(a)), even when limited to measurements from a single receiver. However, these reconstructions show clear signs of overfitting to the measurement data. This is demonstrated by observing that the DeepGEM reconstruction with perfectly known source locations is significantly better with a single receiver when no measurement error is included on the measurements (comparing columns 1 and 2). Note that the learned posterior in column 4 appears to be non-Gaussian, but not multimodal.

Figure 6: Performance of DeepGEM recovery on random velocity fields. Ten random velocity fields were drawn from a GRF-based distribution and used to simulate travel time measurements with 20 receivers and 100 randomly placed sources. (left) Reconstructions obtained for 3 of these configurations are shown. (right) A table lists the mean and standard deviation of velocity and source error obtained across the ten models, each recovered using different $\mathcal{L}_\theta$ priors.

Table 2: Velocity and source localization error on random velocity fields

<table>
<thead>
<tr>
<th>Model</th>
<th>True &amp; Prior Source Locs</th>
<th>No $\mathcal{L}_\theta$</th>
<th>Gradient $\mathcal{L}_\theta$</th>
<th>$\mathcal{L}_\theta$</th>
<th>Velocity Error (km/s)</th>
<th>Source Loc. Error (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>None (&amp; Known Source Locs.)</td>
<td>0.57 ± 0.25 NA</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>None</td>
<td>0.51 ± 0.30 24.40 ± 7.18</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Homogenous</td>
<td>0.94 ± 0.45 21.37 ± 5.34</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gradient</td>
<td>1.07 ± 0.53 26.20 ± 6.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Sensitivity to Number of Receivers: In the case of a single receiver, there exists an entire ring of source locations that result in the same travel time measurement. Fig. 5 contains results from this challenging one-receiver setting using DeepGEM with/without measurement noise and with/without known source locations. Since there is only one receiver, the velocity model is able to easily overfit. However, perhaps surprisingly, artifacts are more severe when source locations are perfectly constrained. These artifacts are caused by the velocity model overfitting to noise in the travel time measurements, and are substantially reduced when noise-free travel time measurements are used. Note that the recovered source location posterior $q(x)$ obtained by the “E”-step is non-Gaussian.

Sensitivity to Velocity Structure: In Fig. 6, DeepGEM is tested on randomly generated velocity fields, each generated from a Gaussian random field (GRF) described in the supplemental material.
These results show that DeepGEM works well at recovering the primary features across a variety of different velocity structures. As compared to when $L_\theta = 0$, the $L_\theta$ gradient prior biases the reconstruction towards smoother velocity structures. The accompanying table contains error statistics for ten different randomly generated velocity fields.

5 Case study: blind deconvolution

We apply DeepGEM to the problem of blind deconvolution to further demonstrate the generality of our approach. Blind deconvolution is a classic ill-posed imaging problem that aims to reconstruct a sharp image from a blurry image with an unknown PSF [19, 14, 25, 21, 22, 20, 6, 1, 27]. Blurry images, caused by handheld camera shake, can be modeled using a single spatially-invariant blur kernel:

$$y = x * k_\theta + \varepsilon \quad \text{for} \quad \varepsilon \sim \mathcal{N}(0, \sigma),$$  \hfill (8)

where $y$ is the blurry image, $*$ represents a 2D convolution, $x$ is the true sharp image, $k_\theta$ is the spatially invariant blur kernel, and $\varepsilon$ is additive Gaussian noise.

5.1 DeepGEM setup for blind deconvolution

For blind deconvolution, we parameterize the forward model $f_\theta(\cdot)$ using a deep network consisting of multiple convolution layers without non-linear activation, as proposed in [3]. Multiple convolutional layers without activation simply overparameterizes a linear blur kernel, which has been empirically shown to produce multiple good minima that are easier to converge to. To ensure the blur kernel is non-negative and volume preserving, we use a Softmax layer and normalize the kernel. For an $n$ layer network with weights $\theta_i$ for $i = 1, ..., n$, the resulting parameterized forward model is:

$$f_\theta(x) = x * \hat{k}_\theta = x * \left[ \frac{\text{Softmax}(\theta_1 * \theta_2 * \theta_n)}{\|\text{Softmax}(\theta_1 * \theta_2 * \theta_n)\|_1} \right]$$ \hfill (9)

![Figure 7: DeepGEM results are comparable to inversion with known blur kernels for simple Fashion MNIST images. Blurry measured images (column 1) are generated using the true sharp image and blur kernel (shown in column 2). The deconvolved images obtained using the true blur kernel are shown in column 3. Reconstructed deconvolved images and corresponding inferred blur kernel from DeepGEM are shown in column 4.

Implementation details: We demonstrate DeepGEM using simple Total Variation (TV) regularization in place of $\log p(x)$. We assume a Gaussian prior on the noise on the blurry measurements where $\varepsilon \sim \mathcal{N}(0, 0.01)$ as well as a sparsity prior on the reconstructed kernel through an $\ell_{0.8}$ soft constraint.
The posterior distribution of the sharp image, $x$, is estimated using a Real-NVP network $G_\phi(\cdot)$ with 16 affine coupling layers. We use 5 convolution layers to parameterize $k_\theta$. We use Adam as the optimizer \[36\] with a batch size of 64 and an E-step learning rate of 5e-4 and M-step learning rate of 1e-4. Hyperparameters, weights used for sparsity and TV priors, were empirically chosen by a grid search over hyperparameters. Results presented have been run with 10 EM iterations, each with 400 “E”-step epochs and 400 M-step epochs, which takes \(~1\) hour on a NVIDIA Tesla V100.

5.2 Results

In Fig. 7 we show results from DeepGEM on three different Fashion-MNIST \[34\] images. The Fashion MNIST images are $64 \times 64$ pixels in size and each blur kernel is contained within $15 \times 15$ pixels. We choose to use images from Fashion-MNIST because they are compatible with the TV prior used in place of $\log p(x)$. In contrast, other natural images such as images from \[22\] (which were originally curated for deconvolution) are not compatible with this handcrafted prior. While this highlights that handcrafted priors such as TV are often insufficient, we choose to leave this to future work. Please refer to the supplemental material for more details about the performance of a TV prior on different types of images.

The blurry images in the first column of Fig. 7 exhibit artifacts from the blur kernel in the form of repeated features, caused by the bi-modal blur kernel. The images recovered via DeepGEM are much sharper and are comparable to the images reconstructed with the known blur kernel. Additionally, DeepGEM reconstructs blur kernels (i.e., $k_\theta$) that are similar to the true kernel shape, with two lobes along the same diagonal. Note that even when there is perfect knowledge about the shape of the blur kernel, detailed structures on the images are not recovered due to the TV prior.

6 Conclusions

In this paper we present DeepGEM, a deep probabilistic framework for tackling blind inverse problems through estimation of the forward model. DeepGEM achieves strong performance in the task of joint seismic tomography and earthquake source localization, substantially outperforming standard approaches currently being used in seismology on synthetic data. The proposed framework is flexible and can be applied to different applications that require estimation or fine tuning of forward model parameters. We demonstrate this flexibility by also applying the approach to a simple, but challenging, blind deconvolution problem. Future work includes applying this method to real seismic data, extending to other applications, and incorporating data-driven priors. Our results highlight the benefit of blending physically sound model-based techniques with learning machinery for blind inverse problems.

Broader Impact

DeepGEM can be used to solve for a system’s model mismatch, which can then help improve our understanding of complex physical systems. However, this tool is not trustworthy enough for safety-critical systems. Nonetheless, this approach can benefit society through a better understanding of fundamental science and advanced earthquake prediction models via seismic imaging.

Acknowledgments and Disclosure of Funding

This work was sponsored by Beyond Limits, Jet Propulsion Laboratory Award 1669417, NSF Award 2048237, and generous gifts from Luke Wang and Yi Li. Additionally, we would like to thank He Sun for many helpful discussions. We declare no competing interests.

References


DeepGEM: Generalized Expectation-Maximization for Blind Inversion

Angela F. Gao1  Jorge C. Castellanos2
Yisong Yue1  Zachary E. Ross2  Katherine L. Bouman1

1Computing and Mathematical Sciences, California Institute of Technology
2Caltech Seismological Laboratory, California Institute of Technology
{afgao, jcastellanos, yyue, zross, klbouman} @ caltech.edu

Contents

1 Related works for blind inversion

2 Blind seismic tomography

2.1 EM derivations
2.1.1 “E”-Step derivation
2.1.2 M-Step derivation

2.2 Baselines
2.2.1 Iterative straight ray baseline
2.2.2 MAP_{\theta,x}

2.3 Gaussian random field

2.4 Forward model parameterization

2.5 Additional results
2.5.1 Posterior visualizations
2.5.2 M-Step only reconstructions with known sources
2.5.3 Full GRF results
2.5.4 Regularization
2.5.5 Loss curves

3 Blind deconvolution

3.1 Total Variation Prior

3.2 Additional results

1 Related works for blind inversion

Similar works that use expectation maximization (EM) based deep learning approaches are usually specific to a single task, often times image classification. These similar works typically assume that
Figure 1: **Velocity reconstructions from MAP\(_{\theta,x}\) with varying \(\lambda_\theta\) and \(\lambda_V\) prior weights.** Each column corresponds to the reconstructions obtained from a single noisy observation of travel times using MAP\(_{\theta,x}\), where the true Earth velocity is shown in Fig. 1(a) from the main paper. Each row’s reconstruction corresponds to different \(\lambda_\theta\) and \(\lambda_V\) values corresponding to varying strengths of the gradient \(L_\theta\) and \(L_V\) priors. Results shown are simulated using 20 surface receivers and a varying number of sources (9, 25, and 49) in a uniform grid. Note that as the prior \(\lambda_\theta L_\theta\) increases, the closer the velocity reconstruction becomes to the gradient prior model shown in Fig. 2 from the main paper. The velocity reconstruction MSE is included in the top right of each reconstruction. The model with the highest data likelihood is highlighted in orange.

Using alternative loss functions instead of the standard \(\ell_2\) is another way to accommodate model mismatch into inversion. For example, Wasserstein distance is a loss function that has been used in many applications related to optimal transport, from seismology \([12]\) to image reconstruction \([11]\). Since the dual of the Wasserstein distance \([11]\) is differentiable, we may also be able to use it to better approximate \(p(y|x)\) in the future.
Figure 2: **Posterior visualization with varying number of random sources.** Results shown are simulated using 20 surface receivers and a varying number of sources (9, 25, 49, and 100) that are randomly sampled, with the legend shown in Fig. 2 of the main paper. Note that as the depth increases, the inferred posterior distribution has more uncertainty.

Figure 3: **Velocity reconstructions corresponding to the sources reconstructed in Fig. 2.** Results shown are simulated using 20 surface receivers and a varying number of sources (9, 25, 49, and 100) that are randomly sampled. The velocity reconstruction MSE is included in the top right of each reconstruction, where the true Earth velocity is shown in Fig. 1(a) of the main paper. Note that as the number of sources increase, the MSE tends to improve. Additionally, even with 9 sources, the anomaly is able to be reconstructed.
2 Blind seismic tomography

2.1 EM derivations

2.1.1 “E”-Step derivation

We include expanded derivations of Section 3.1 Eq. 5 from the main paper. Here $q_\phi(x)$ represents a flexible variational distribution that well approximates the posterior distribution $p(x|y, \theta^{(t-1)})$. A normalizing flow network, $G_\phi(z)$, has input $z \in \mathbb{R}^{|x|}$, where $x = G_\phi(z) \sim q_\phi(x)$ when $z \sim \mathcal{N}(0, 1)$ and $|x|$ is the dimension of $x$. Normalizing flow networks allow for exact computation of the log-likelihood $\log q_\phi(x)$, which is needed to solve Eq. 5. Eq. 5 can be derived using the variational objective to get

$$
\phi^{(t)} = \arg \min_\phi KL(q_\phi(x)||p(x|y, \theta^{(t-1)}))
$$

$$
= \arg \min_\phi \mathbb{E}_{x \sim q_\phi(x)} \left[ \log q_\phi(x) - \log p(x|y, \theta^{(t-1)}) \right]
$$

$$
= \arg \min_\phi \mathbb{E}_{x \sim q_\phi(x)} \left[ -\log p(y|\theta^{(t-1)}, x) - \log p(x) + \log q_\phi(x) \right]
$$

$$
\approx \arg \min_\phi \frac{1}{N} \sum_{n=1}^{N} \left[ -\log p(y|\theta^{(t-1)}, x_n) - \log p(x_n) + \log q_\phi(x_n) \right]
$$

for $x_n = G_\phi(z_n), z_n \sim \mathcal{N}(0, 1), (1)$

for a batch size of $N$ where $\log p(x)$ is a prior on the source and $\log p(y|x, \theta^{(t)})$ is the data likelihood. When assuming the measurements $y$ experience i.i.d additive Gaussian noise with standard deviation $\sigma_y$, $\log p(y|\theta^{(t)}, x_n) = \frac{1}{2\sigma_y^2} \|y - f_{\theta^{(t)}}(x_n)\|^2 + c$.

![M-step with Known Source Locs.](image)

Figure 4: **M-step solutions (with known source locations) improve with more sources and better $\mathcal{L}_\theta$ prior models.** Each row corresponds to the reconstructions obtained from a single noisy observation of travel times, where the true Earth velocity is shown in Fig. 1(a) in the main paper. Results shown are simulated using 20 surface receivers and a varying number of sources (9, 25, and 49) in a uniform grid. Columns 2-5 show M-step results with known source locations obtained using different $\mathcal{L}_\theta$ priors. Note that results tend improve as the $\mathcal{L}_\theta$ prior becomes closer to the true velocity structure and as the number of sources increases. Note that these reconstructions tends to be blurrier than those shown in Fig. 5 due to the presence of Gaussian noise in the receiver measurements.
Figure 5: **M-step solutions (with known source locations) from noise-free measurements improve with more sources and better $\mathcal{L}_\theta$ prior models.** Each row corresponds to the reconstructions obtained from a single observation of noise-free travel times, where the true Earth velocity is shown in Fig. 1(a) in the main paper. Results shown are simulated using 20 surface receivers and a varying number of sources (9, 25, and 49) in a uniform grid. Columns 2-5 show M-step results with known source locations obtained using different $\mathcal{L}_\theta$ priors. Note that results tend improve as the $\mathcal{L}_\theta$ prior becomes closer to the true velocity structure and as the number of sources increases.

### 2.1.2 M-Step derivation

We include expanded derivations of Section 3.2 Eq. 6 from the main paper. The parameterized approximate posterior distribution, $q_{\phi(t)}(x)$, is used from the “E”-step to update $\theta$, the parameters of the unknown forward model $f_{\theta}(\cdot)$. This is achieved by sampling from the learned normalizing flow network, $G_{\phi(t)}(\cdot)$, to stochastically solve:

\[
\theta^{(t)} = \arg \max_{\theta} \{ \log p(\theta | y) \}
\]

\[
= \arg \max_{\theta} [\log p(y | \theta) + \log p(\theta)]
\]

\[
= \arg \max_{\theta} \left( \log \left( \int_x p(y | \theta, x)p(x)dx \right) + \log p(\theta) \right)
\]

\[
= \arg \max_{\theta} \left[ \mathbb{E}_{x \sim p(x | y, \theta^{(t-1)})} \{ \log p(y | \theta, x) \} + \log p(\theta) \right]
\]

\[
\approx \arg \max_{\theta} \left[ \frac{1}{N} \sum_{n=1}^{N} \{ \log p(y | \theta, x_n) \} + \log p(\theta) \right] \text{ for } x_n = G_{\phi(t)}(z_n), \ z_n \sim \mathcal{N}(0, 1),
\]

where $p(\theta)$ is a prior on the forward model. This prior can be used to encourage the forward model parameters to remain close to an initial model $\theta$ by defining $\log p(\theta) \propto ||\theta - \theta||_2 + c$.

### 2.2 Baselines

#### 2.2.1 Iterative straight ray baseline

The tomography baseline that we use is a straight ray tomography method based on [2]. The source localization baseline is the maximum a posteriori (MAP) solution given by

\[
\hat{x} = \arg \min_{x} \sum_{r} \frac{1}{2\sigma_y^2} ||T(x^*, r) - \hat{T}(x, r)||^2 - \log p(x)
\]
Figure 6: **Results from ten different GRF velocity models.** Ten random velocity fields were drawn from a GRF-based distribution and used to simulate travel time measurements with 20 receivers and 100 randomly placed sources. Reconstructions obtained for all of these configurations are shown. Velocity structure recovered using different $L_0$ priors. The straight ray baseline is included.
Higher $\lambda$ $
abla$ $
abla$

Higher $\lambda$ $\theta$

Lower $\lambda$ $\theta$

Figure 7: Velocity reconstruction with varying prior parameters $\lambda_\theta$ and $\lambda_V$. Each reconstruction is obtained from a single noisy observation of travel times, where the true Earth velocity is shown in Fig. 1(a) from the main paper. Each row corresponds to different $\lambda_\theta$ values corresponding to varying strengths of the layers $L_\theta$ prior. Each column corresponds to different $\lambda_V$ values corresponding to varying strengths of the velocity invariance prior. $\lambda_\theta$ with values $1e^{-5}$, $1e^{-6}$, $1e^{-7}$ and $\lambda_V$ with values $1e^{-4}$, $1e^{-5}$, $1e^{-6}$ are used. The optimal parameters ($\lambda_\theta = 1e^{-6}$ and $\lambda_V = 1e^{-5}$) are used for all results shown in the paper. Results shown are simulated using 20 surface receivers and 100 sources in a uniform grid. The velocity reconstruction MSE is included in the top right of each reconstruction.

where $\sigma_y$ is the standard deviation of the measurement error, $T(x^*, r)$ is the true travel time measurement generated from the true source $x^*$ and receiver $r$, $\hat{T}(x, r)$ is the travel time measurement from an assumed velocity model and test source $x$, and $\log p(x)$ is the prior on the source location. We assume a Gaussian prior on the source where $x^* \sim N(\bar{x}, \sigma_x)$. We discretize the possible source positions $x$ for efficiency.

The baseline solution results from alternating between the source localization and tomography to perform joint source and velocity inversion. The source baseline is initialized using a 1D gradient velocity model shown in Fig. 1(a) from the main paper. The iterative method usually converges when there is low uncertainty of the source location even with high uncertainty in the velocity model. However, when the 1D gradient velocity model poorly approximates the true velocity model, the iterative solution diverges. This is the case for the 1D gradient initialization. Thus, we chose to show only one iteration for our baseline results, a choice made by an expert seismologist with experience using the technique.

2.2.2 MAP $\theta, x$

We show MAP $\theta, x$’s sensitivity to $L_\theta$ and $L_V$ in Fig. 11. Note that with a stronger prior where $\lambda_\theta = 1e2$ and $\lambda_V = 1e2$, the reconstruction converges to the gradient prior model. With a weaker prior where $\lambda_\theta = 0$ and $\lambda_V = 1e-2$, the reconstruction is far from the true underlying velocity, and is very sensitive to initialization choices. The model with the highest data likelihood is highlighted in orange. Note that this model does not have the lowest velocity reconstruction MSE.

2.3 Gaussian random field

The Gaussian Random Field (GRF) based velocity models were sampled such that:

$$V = 1.3(G + 0.5) * R + 2$$ (7)
Figure 8: **Example loss curve from M-step only with known sources.** Noisy measurements are generated from 961 sources and 20 receivers. Total loss is plotted in purple.

Figure 9: **Example loss curves for both “E” and M steps for DeepGEM reconstruction with 961 sources and 20 receivers.** Top plot shows the loss curves from the “E”-steps with the full loss plotted in blue. Bottom plot shows the loss curves from the M-steps with the full loss plotted in purple. Note that initially the $-\log q_\phi(x)$ term is increasing due to the data likelihood term taking over in optimization at early iterations.

where $G$ is a sample from a zero-mean Gaussian random field (with a von Karman covariance function that has parameters for correlation length, standard deviation, and the Hurst exponent), $*$ is element-wise multiplication, and $R$ is a 1D velocity model with layers.
2.4 Forward model parameterization

The EikoNet [9] is used to parameterize $f_{\theta}(x)$ in the blind seismic tomography problem. The EikoNet architecture used has been modified to have four residual blocks with sine activation [8]. Instead of training EikoNet using velocity, as in [9], our results are trained using simulated travel time measurements.

2.5 Additional results

2.5.1 Posterior visualizations

We show the visualized posterior along with true source locations for 9, 25, 49, and 100 random source locations and 20 fixed receivers in Fig. 2. As depth increases, the estimated posterior increases in size as is expected. The corresponding velocity reconstructions are shown in Fig. 3. The overall mean squared error (MSE) of the velocity reconstruction tends to increase as the number of sources increases, but this is source-receiver configuration dependent.

2.5.2 M-Step only reconstructions with known sources

In Fig. 4 and Fig. 5, we show more M-step only reconstruction (with known source locations) as comparisons to Fig. 3 in the main paper, where the true Earth velocity is shown in Fig. 1(a) from the main paper. Fig. 4 shows velocity reconstructions from a set of noisy measurements for 9, 25, and 49 sources with different priors on the velocity structure. In most cases, the M-step results in Fig. 4 have a lower MSE than the EM results in Fig. 3 from the main paper. Fig. 5 shows M-step velocity reconstructions from noise-free measurements for 9, 25, and 49 sources with different priors on the velocity structure. The reconstructions in Fig. 5 are better than Fig. 3 in the main paper when comparing MSE, which is due to the absence of measurement noise.

2.5.3 Full GRF results

Results from ten different GRF velocity models are shown in Fig. 6 each with a different random source configuration. DeepGEM reconstructions without $L_\theta$ prior and gradient $L_\theta$ prior both outperform the straight ray baseline for all velocity models. The GRF anomaly is reconstructed in all reconstructions without $L_\theta$ prior except for model 3, which does not have enough sources within the anomaly. DeepGEM reconstructions are able identify the anomaly much more consistently than the straight ray baseline.

2.5.4 Regularization

In Fig. 7 velocity reconstructions with 100 sources and varying the hyperparameters are shown, where the true Earth velocity is shown in Fig. 1(a) from the main paper. $\lambda_\theta$ with values 1e-5, 1e-6, 1e-7 and $\lambda_V$ with values 1e-4, 1e-5, 1e-6 are used. The optimal parameters ($\lambda_\theta = 1e-5$ and $\lambda_V = 1e-4$) are used for all results shown in the paper.

2.5.5 Loss curves

We show that our method converges for the M-step optimization with known sources, shown in Fig. 8 and the joint DeepGEM optimization for blind inversion, shown in Fig. 9. Note that these curves are plotted in log$_{10}$ scale.

3 Blind deconvolution

3.1 Total Variation Prior

Traditional approaches to blind deconvolution often solve for a sharp target image while simultaneously solving for the kernel $k$, which represents the camera’s point spread function (PSF) [3,5,6]. These techniques make use of regularizers, such as total variation (TV) regularization on the sharp image and $\ell_1$ sparsity on the kernel, to constrain the ill-posed inverse problem [4].

TV assumes that the image gradients follow a Laplacian distribution. While TV is commonly used for many different image processing problems [4,5,7], it is (perhaps surprisingly) not a good model
Figure 10: **Total variation (TV) values for the different true sharp images and blurry images used.** TV values for the true images (row 1) and blurry images (row 2). Note that the TV value is being used as $-\log p(x)$. Therefore a higher TV value indicates that an image is less likely.

Figure 11: Blurry measured images (columns 1 and 4) generated using the true sharp image and blur kernel (shown in columns 2 and 5). Reconstructed sharp image and the corresponding inferred blur kernel from DeepGEM (columns 3 and 6).

There are two ways to avoid preference towards the blurry image delta PSF solution: (1) better image priors and (2) over-estimating the uncertainty in the posterior conditional distribution during EM optimization. Both solutions can be easily incorporated in DeepGEM. Data-driven priors can easily be incorporated since our method only requires evaluation of the prior. We choose to leave this to later work.

### 3.2 Additional results

Here our goal is to highlight that a TV prior leads to poor deconvolution results for many natural images, unlike the results shown in Fig. 7 in the main paper. In Fig. 11 we show additional results for images from [5], which are of size $255 \times 255$. As described in the previous section, for these images the TV prior prefers the blurry image with an impulse kernel over the true sharp images.

The blurry images in Fig. 11 exhibit artifacts due to the shape of the blur kernel. In Fig. 11(a), the text in the deconvolved image is more legible, but there are still some ringing artifacts due to model mismatch. The reconstructed kernels roughly match the true kernels’ shape with two lobes along the same diagonal. In Fig. 11(b), the edges in the blurry image are sharper in the reconstructed image. Although the reconstructed kernel is not located spatially at the same location as the true kernel, this does not significantly harm reconstruction; since the kernels are shift-invariant, the reconstructed image and learned kernel can both be shifted such that they reconstruct the same blurry image.

Note we suspect that the reason we converge to a sharper image than the initial blurry image is due to the fact that we initialize the blur kernel to a Gaussian kernel. The solution converges to a local minimum rather than the blurry image with impulse kernel explanation.
References


