

WISER: Multimodal variational inference for full-waveform inversion without dimensionality reduction

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ABSTRACT

We develop a semiamortized variational inference (VI) framework designed for computationally feasible uncertainty quantification in full-waveform inversion to explore the multimodal posterior distribution without dimensionality reduction. The framework is called full-waveform VI via subsurface extensions with refinements (WISER). WISER builds on top of a supervised generative artificial intelligence method that performs approximate amortized inference that is low-cost albeit showing an amortization gap. This gap is closed through nonamortized refinements that make frugal use of wave physics. Case studies illustrate that WISER is capable of full-resolution, computationally feasible, and reliable uncertainty estimates of velocity models and imaged reflectivities.

INTRODUCTION

Full-waveform inversion (FWI) aims to estimate unknown multidimensional velocity models \mathbf{x} from noisy seismic data \mathbf{y} by inverting the nonlinear forward operator \mathcal{F} , which relates \mathbf{x} and \mathbf{y} via $\mathbf{y} = \mathcal{F}(\mathbf{x}) + \boldsymbol{\epsilon}$ with measurement noise $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$. FWI poses significant challenges because it requires solving a high-dimensional, nonconvex, and ill-posed inverse problem, with a computationally demanding forward operator. In addition, the inherent nonuniqueness of FWI results leads to multiple possible earth models compatible with the observed data, underscoring the need for uncertainty quantification (UQ) to handle this multimodality.

The trade-off between accuracy and computational cost is always a critical consideration of UQ. To circumvent the costs associated with global optimization, several approaches have attempted localized UQ (Fang et al., 2018; Keating and Innanen, 2021; Hoffmann et al., 2024; Izzatullah et al., 2024). However, these approaches may

not capture the full complexities of multimodal parameter spaces. In contrast, a Bayesian inference approach offers a costly but comprehensive characterization of the posterior distribution $p(\mathbf{x}|\mathbf{y})$.

Bayesian inference algorithms are broadly categorized into two groups. The first category, sampling-based methods, such as Markov-chain Monte Carlo (MCMC), struggle with high-dimensional parameter spaces. To meet this challenge, they often rely on too restrictive low-dimensional parameterizations to reduce the number of sampling iterations (Fang et al., 2020; Liang et al., 2023; Wei et al., 2023, 2024a, 2024b, Dhabaria and Singh, 2024), which could bias the inference results, rendering them impractical for multidimensional UQ studies especially when solutions are nonunique.

The second category, optimization-based methods, such as variational inference (VI) (Zhang et al., 2021), seek to approximate the posterior distribution using classes of known parameterized distributions. VI can be subdivided into amortized and nonamortized methods. Amortized VI involves a computationally intensive offline training phase, leveraging advances in generative artificial intelligence (genAI), particularly with models such as conditional diffusion (Baldassari et al., 2024) and conditional normalizing flows (CNFs) (Winkler et al., 2019). After training, amortized VI provides rapid sampling during inference (Orozco et al., 2023a; Siahkoobi et al., 2023; Sun et al., 2024), exemplified by the full-waveform variational inference via subsurface extensions (WISE) framework (Yin et al., 2024b) for FWI problems. However, these methods may suffer from an *amortization gap* — implying that the amortized networks may only deliver suboptimal inference for a given observation during inference, particularly when trained with limited examples or when there exists a discrepancy between training and inference (Marino et al., 2018). Conversely, nonamortized VI dedicates all computational resources to the online inference (Zhao et al., 2022; Zhang et al., 2023; Zhang and Curtis, 2024). They result in more accurate inference, but the costly optimization has to be carried out repeatedly for new observations. In addition, incorporating realistic priors requires embedding them through density

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evaluations, such as those enabled by normalizing flows (Kruse et al., 2021; Louboutin et al., 2023; Yin et al., 2023).

This paper introduces the full-waveform VI via subsurface extensions with refinements (WISER) algorithm (shown in Algorithm 1) as a semiamortized VI framework to facilitate computationally feasible and reliable UQ for multidimensional FWI without dimensionality reduction. Building on WISE, we train CNFs for efficient, suboptimal amortized inference, but then follow up with a crucial refinement step that only makes frugal use of the forward operator and its gradient. The refinement step aligns the posterior samples with the observation during inference, effectively bridging the amortization gap and enhancing inference accuracy. The performance of WISER is demonstrated through realistic synthetic 2D case studies using the Compass model (Jones et al., 2012).

Algorithm 1. WISER: full-waveform VI via subsurface extensions with refinements.

```

1: Offline training phase
2:
3: Data set generation
4: for  $i = 1:N$  do
5:    $\mathbf{x}^{(i)} \sim p(\mathbf{x})$ 
6:    $\boldsymbol{\epsilon}^{(i)} \sim p(\boldsymbol{\epsilon})$ 
7:    $\mathbf{y}^{(i)} = \mathcal{F}(\mathbf{x}^{(i)}) + \boldsymbol{\epsilon}^{(i)}$  # forward modeling
8:    $\bar{\mathbf{y}}^{(i)} = \bar{\nabla}\mathcal{F}(\mathbf{x}_0)^\top \mathbf{y}^{(i)}$  # extended migration
9: end for
10:
11: Network training
12:  $\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N \left( \frac{1}{2} \|f_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}; \bar{\mathbf{y}}^{(i)})\|_2^2 - \log |\det \mathbf{J}_{f_{\boldsymbol{\theta}}}| \right)$ 
13:
14: Online inference phase
15:
16:  $\bar{\mathbf{y}}_{\text{obs}} = \bar{\nabla}\mathcal{F}(\mathbf{x}_0)^\top \mathbf{y}_{\text{obs}}$  # extended migration
17: for  $i = 1:M$  do
18:    $\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
19:    $\mathbf{x}_i = f_{\boldsymbol{\theta}^*}^{-1}(h_{\phi}(\mathbf{z}_i); \bar{\mathbf{y}}_{\text{obs}})$ 
20: end for
21:
22: Physics-based refinements
23: for  $ii = 1:\maxiter_1$  do
24:   for  $i = 1:M$  do # physics-based gradient update
25:      $\mathbf{g}_i = \nabla_{\mathbf{x}_i} \left[ \frac{1}{2\sigma^2} \|\mathcal{F}(\mathbf{x}_i) - \mathbf{y}_{\text{obs}}\|_2^2 + \frac{1}{2\tau^2} \|\mathbf{x}_i - f_{\boldsymbol{\theta}^*}^{-1}(h_{\phi}(\mathbf{z}_i); \bar{\mathbf{y}}_{\text{obs}})\|_2^2 \right]$ 
26:      $\mathbf{x}_i = \mathbf{x}_i - \tau \mathbf{g}_i$ 
27:   end for
28:   for  $iii = 1:\maxiter_2$  do
29:      $\mathcal{L}(\phi) = \sum_{i=1}^M \left[ \frac{1}{2\tau^2} \|\mathbf{x}_i - f_{\boldsymbol{\theta}^*}^{-1}(h_{\phi}(\mathbf{z}_i); \bar{\mathbf{y}}_{\text{obs}})\|_2^2 + \frac{1}{2} \|h_{\phi}(\mathbf{z}_i)\|_2^2 - \log |\det \mathbf{J}_{h_{\phi}}| \right]$ 
30:      $\phi \leftarrow \text{ADAM}(\mathcal{L}(\phi))$ 
31:   end for
32: end for
33:
34: Output:  $\{f_{\boldsymbol{\theta}^*}^{-1}(h_{\phi}(\mathbf{z}_i); \bar{\mathbf{y}}_{\text{obs}})\}_{i=1}^M$  as samples of  $p(\mathbf{x}|\mathbf{y}_{\text{obs}})$ 

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AMORTIZED VI WITH WISE (LINES 1–20)

WISER starts with an offline training phase that leverages conditional generative models to approximate the posterior distribution. This is achieved by WISE, which involves generating a training data set (lines 3–9 of Algorithm 1) and training the CNFs (lines 11 and 12).

Data set generation (lines 3–9)

We begin by drawing N velocity models from the prior distribution, denoted by $p(\mathbf{x})$ (line 5). For each sample $\mathbf{x}^{(i)}$, we simulate the observed data $\mathbf{y}^{(i)}$ by performing wave modeling and adding a random noise term (lines 6 and 7). Next, we compute common-image gathers (CIGs) (Hou and Symes, 2016) for each observed data with a 1D initial velocity model \mathbf{x}_0 . These CIGs, represented by $\bar{\mathbf{y}}^{(i)}$, are produced by applying the adjoint of the extended migration operator $\bar{\nabla}\mathcal{F}(\mathbf{x}_0)^\top$ to the observed data. Using CIGs as the set of physics-informed summary statistics not only preserves information from the observed seismic data (ten Kroode, 2023) but also enhances the training of CNFs in the next stage (Radev et al., 2020; Orozco et al., 2023b), as they help to decode the wave physics, translating prestack data into the image (subsurface-offset) domain.

Network training (lines 11 and 12)

CNFs are trained with pairs of velocity models and CIGs via minimization of the objective in line 12. The symbol $f_{\boldsymbol{\theta}}$ denotes the CNFs, characterized by their network weights $\boldsymbol{\theta}$ and the Jacobian $\mathbf{J}_{f_{\boldsymbol{\theta}}}$. The term “normalizing” within CNFs implies their functionality to transform the realizations of velocity models $\mathbf{x}^{(i)}$, conditioned on the summary statistics (CIGs), into Gaussian noise from a standard multivariate normal distribution (as evident by the use of the ℓ_2 norm).

Online inference (lines 14–20)

The previously mentioned data generation and CNF training procedures conclude the offline training phase. During the online inference, amortized VI is enabled by leveraging the inherent invertibility of CNFs. For a given observation \mathbf{y}_{obs} , the online cost is merely generation of a single set of CIGs (line 16). Subsequently, posterior samples are generated by applying the inverse of the CNFs to Gaussian noise realizations, conditioned on these CIGs (lines 18 and 19). Here, we use h_{ϕ} to represent the identity operator. It is a placeholder for later where h_{ϕ} will be repurposed to represent more complex operators based on physics-based corrections.

PHYSICS-BASED REFINEMENTS (LINES 22–32)

Consider a given observation \mathbf{y}_{obs} and its corresponding posterior samples $\mathbf{x}_i \sim p(\mathbf{x}; \bar{\mathbf{y}}_{\text{obs}})$. The latent space representations generated by the trained CNFs $\hat{\mathbf{z}}_i = f_{\boldsymbol{\theta}^*}(\mathbf{x}_i; \bar{\mathbf{y}}_{\text{obs}})$ may not conform exactly to the standard Gaussian distribution during inference. Thus, using $f_{\boldsymbol{\theta}^*}^{-1}(\mathbf{z}; \bar{\mathbf{y}}_{\text{obs}})$ for inference with $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ will not result in the desired posterior distribution. We refer to the distribution of $\hat{\mathbf{z}}_i$ as the shifted latent distribution, denoted by $p_{\boldsymbol{\theta}^*}(\mathbf{z}; \bar{\mathbf{y}}_{\text{obs}})$. Mathematically, the amortization gap is quantified as $\mathbb{K}\mathbb{L}(\mathcal{N}(\mathbf{0}, \mathbf{I}) \| p_{\boldsymbol{\theta}^*}(\mathbf{z}; \bar{\mathbf{y}}_{\text{obs}})) > 0$, where $\mathbb{K}\mathbb{L}$ is the Kullback-Leibler (KL) divergence. To address this issue, we follow Siahkoohi et al. (2023) to apply latent space corrections to fine tune the trained CNFs. This involves integrating a shallower, yet invertible, network, specifically trained to map

samples from the standard Gaussian distribution to the (unknown) shifted latent distribution, thereby reducing this amortization gap.

In pursuit of this goal, we adopt a transfer learning approach by freezing the weights of the trained CNFs and updating only the weights of the shallower network. The objective function reads,

$$\begin{aligned} & \underset{\phi}{\text{minimize}} \quad \mathbb{E}_{\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \mathbb{K}\mathbb{L}(p(h_{\phi}(\mathbf{z})) \| p_{\theta^*}(\mathbf{z}; \bar{\mathbf{y}}_{\text{obs}})) \\ & = \frac{1}{2\sigma^2} \|\mathcal{F} \circ f_{\theta^*}^{-1}(h_{\phi}(\mathbf{z}); \bar{\mathbf{y}}_{\text{obs}}) - \mathbf{y}_{\text{obs}}\|_2^2 \\ & + \frac{1}{2} \|h_{\phi}(\mathbf{z})\|_2^2 - \log |\det \mathbf{J}_{h_{\phi}}|. \end{aligned} \quad (1)$$

Equation 1 minimizes the reverse KL divergence between the distribution of the corrected latent variables $p(h_{\phi}(\mathbf{z}))$ and the shifted latent distribution $p_{\theta^*}(\mathbf{z}; \bar{\mathbf{y}}_{\text{obs}})$, with h_{ϕ} being the refinement network. A detailed proof can be found in [Siahkoohi et al. \(2021, 2023\)](#), along with related references. For linear inverse problems in seismic imaging, [Siahkoohi et al. \(2023\)](#) demonstrate that an elementwise scaling and shift mechanism is sufficient to close the gap. However, given the nonconvex nature of FWI, we use h_{ϕ} as a more general invertible network.

From an engineering perspective, the refinement network h_{ϕ} mitigates the amortization gap by adjusting the latent variable \mathbf{z} before feeding it to the inverse of the trained CNFs $f_{\theta^*}^{-1}$. Intuitively, minimizing the first term ties the posterior samples closer to the observed data. The second term prevents the corrected latent space from being far from the Gaussian distribution, which implicitly takes advantage of the prior information existing in the amortized training phase. The third term prevents mode collapse ([Rezende and Mohamed, 2015](#)).

Equation 1 offers a fine-tuning approach that leverages the full multidimensional wave physics to refine WISE for a given observation during inference. However, it introduces notable computational demands because it necessitates the coupling of the modeling operator and the networks. Specifically, every update to the network weights ϕ requires costly wave modeling operations. Given that network training typically involves numerous iterations, these computational demands can render it impractical for realistic FWI applications.

To relieve this computational burden, we adopt a weak deep prior strategy ([Siahkoohi et al., 2020](#)) to reformulate equation 1 into a weak form by allowing the network output to be only “weakly” enforced to be the corrected velocity models. The objective function for this weak formulation reads,

$$\begin{aligned} & \underset{\mathbf{x}_{1:M}, \phi}{\text{minimize}} \quad \frac{1}{M} \sum_{i=1}^M \left[\frac{1}{2\sigma^2} \|\mathcal{F}(\mathbf{x}_i) - \mathbf{y}_{\text{obs}}\|_2^2 + \frac{1}{2\gamma^2} \|\mathbf{x}_i \right. \\ & \left. - f_{\theta^*}^{-1}(h_{\phi}(\mathbf{z}_i); \bar{\mathbf{y}}_{\text{obs}})\|_2^2 + \frac{1}{2} \|h_{\phi}(\mathbf{z}_i)\|_2^2 - \log |\det \mathbf{J}_{h_{\phi}}| \right], \end{aligned} \quad (2)$$

where $\{\mathbf{z}_i\}_{i=1}^M$ is the M realizations of standard Gaussian noise and $\{\mathbf{x}_i\}_{i=1}^M$ is their corresponding particles (i.e., velocity models) initialized in lines 17–19 of Algorithm 1. We strategically decouple the computationally expensive forward operator \mathcal{F} from the more cheap-to-evaluate networks f_{θ^*} and h_{ϕ} . This is achieved in a penalty form with the assumption that the misfit between the network outputs and the posterior samples adheres to a Gaussian distribution $\mathcal{N}(\mathbf{0}, \gamma^2 \mathbf{I})$, where γ is a hyperparameter dictating the trade-off

between data misfit and regularization. Setting γ to 0 equates this weak formulation to the constrained formulation in equation 1. This weak formulation also supports optimization strategies for updating the velocity models with physical constraints and multiscale optimization techniques ([Esser et al., 2018](#); [Peters et al., 2019](#)).

WISE takes full computational advantage of this weak formulation by using a nested loop structure. The outer loop is dedicated for updating M velocity models \mathbf{x}_i through costly gradient descent steps (lines 24–27 of Algorithm 1), whereas the inner loop (lines 28–31) focuses on more updates (with the Adam optimizer) to network weights ϕ without computationally expensive physics modeling. To achieve a balance, we conduct $\text{maxiter}_2 = 128$ iterations in the inner loop. After refinements, WISE first evaluates the refined network on the latent variables to obtain refined latent codes. Subsequently, the amortized network uses these refined codes conditioned on the CIGs to compute the corrected posterior samples (line 34).

CASE STUDIES

Evaluation of WISE is conducted through synthetic case studies using 2D slices of the Compass model and 2D acoustic-wave physics. The parameter of interest is discretized into 512×256 grid points with a spatial resolution of 12.5 m, resulting in more than 10^5 degrees of freedom. We follow [Yin et al. \(2024b\)](#) to train the amortized CNFs.

To test the robustness and adaptability of WISE when faced with unexpected conditioning data at inference, we evaluate WISE’s performance under out-of-distribution (OOD) scenarios. We introduce alterations to an unseen velocity model drawn from the same statistical distribution on which the CNFs were trained, as depicted in Figure 1c, through an elementwise perturbation shown in Figure 1a. This manipulation modifies the velocity values across different depth levels, resulting in a significant shift in their statistical distribution, as shown in Figure 1b. We use the perturbed velocity as the unseen ground-truth velocity model in this case study, as shown in Figure 1d. To further expand the amortization gap, we modify the encoding of the forward operator by introducing a higher amplitude of bandlimited Gaussian noise (signal-to-noise ratio of 0 dB).

These complexities present substantial challenges for WISE, leading to biased inference results, as shown in Figure 1e. The yellow histograms in Figure 1b show that the velocity values of the posterior samples from WISE closely resemble those of the original velocity model, despite the different distribution of the ground-truth velocity model. This indicates that WISE tends to incorporate an inductive bias from the training samples. In WISE, we conduct $\text{maxiter}_1 = 160$ outer iterations, using $M = 16$ particles and one ocean-bottom node (OBN) per gradient. We also use the frequency-continuation method ([Bunks et al., 1995](#)) to compute the gradient in line 25 of the WISE algorithm, transitioning gradually from low- to high-frequency data. This results in a total of 40 datapasses or 5120 partial differential equation (PDE) solves (datapass means a forward and an adjoint pass for the entire OBN data set).

Observations

WISE produces more accurate posterior samples, as shown in Figure 1f. Furthermore, the statistical distribution of the velocity values in the WISE posterior samples (green histogram in Figure 1b) aligns better with the distribution of the unseen ground-truth velocity values (blue histogram in Figure 1b), demonstrating WISE’s robustness against potential distribution shifts during inference.

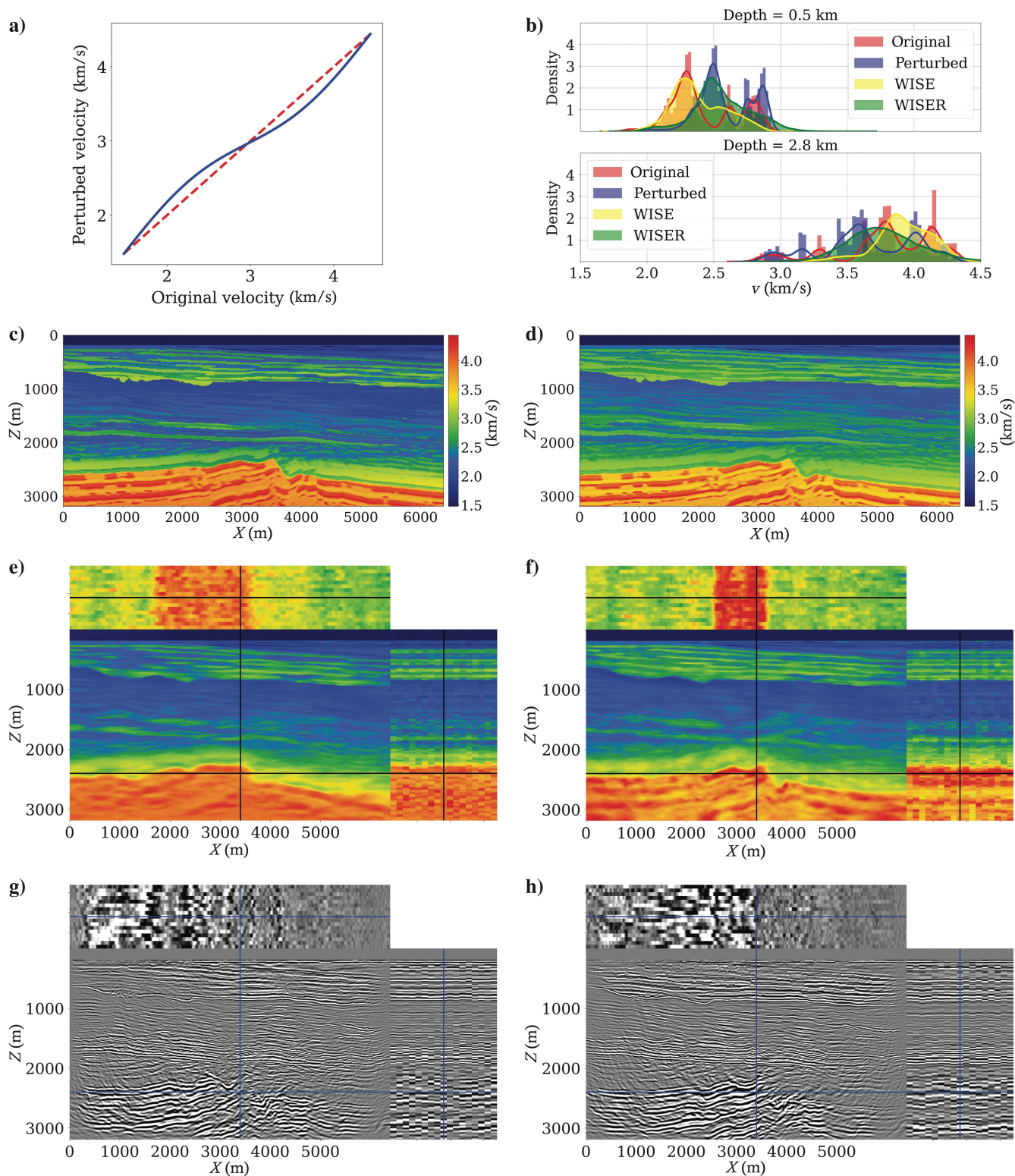


Figure 1. The OOD example. (a) Curves for velocity-value perturbations. (b) Histograms of values at the depth of 0.5 and 2.8 km in the original velocity model (c), perturbed velocity model (d), posterior samples of WISE, and WISER, shown in red, blue, yellow, and green color, respectively. (c) An unseen in-distribution velocity model. (d) Unseen ground-truth velocity model. (e) Estimated velocity models from WISE. The CM estimate is shown in the center. For posterior samples, horizontal traces at $Z = 2.7$ km and vertical traces at $X = 3.6$ km are displayed on the top and the right, respectively. (g) Imaged reflectivity samples from WISE. (f and h) The same as (e and g) but for WISER, showcasing significant improvements.

Impact on imaging

The imaging results from WISE (Figure 1g) and WISER (Figure 1h) reveal noticeable discrepancies in quality. The conditional mean (CM) migration-velocity model from WISE leads to discontinuities in the imaged reflectivities, particularly at the horizontal layer at a depth of approximately 1.8 km and more so below the unconformity. In contrast, the CM from WISER significantly improves the continuity in the imaged reflectivities across the entire seismic section. The imaged reflectivity samples from WISER also align more accurately with the estimated CM migration-velocity model, which is particularly visible in supplemental Text S1.

DISCUSSION

WISER leverages genAI and physics to achieve a semiamortized VI framework for scalable and reliable UQ for FWI even in situations where local approximations are unsuitable. At its core, WISER harnesses the strengths of amortized and nonamortized VI: the amortized posterior obtained through offline training provides a low fidelity but fast mapping, and the physics-based refinements offer reliable and accurate inference. Both approaches benefit from information preservation exhibited by CIGs, rendering our inference successful where conventional FWI fails due to cycle skipping.

Related work and computational cost analysis

Compared with MCMC methods that rely on low-dimensional parameterizations, WISER does not impose intrinsic dimensionality reductions or simplifications of the forward model. Therefore, WISER is capable of delivering full-resolution UQ for realistic multidimensional FWI problems.

UQ problems inherently involve a trade-off between offline and online computational costs. Access to a larger number of velocity models and CIGs during the offline phase enhances the accuracy of amortized inference in WISE. In addition, training samples that closely resemble actual earth models could further improve this accuracy. Preliminary studies have demonstrated that genAI workflows can create earth models from well measurements and imaged seismic data (Erdinc et al., 2024). Leveraging these automated workflows allows us to generate high-fidelity velocity models for the subsequent training of WISE, potentially reducing the online costs required in WISER. Striking the right balance between these offline and online costs remains a crucial consideration. In Table 1, we list the required number of PDE solves for several Bayesian inference methods applied to FWI.

Compared with nonamortized VI methods, WISER requires significantly fewer computational resources during the online phase. This efficiency arises because WISE, the precursor to WISER, already provides near-accurate posterior samples, making the subsequent refinement procedure computationally feasible. In addition, stochastic optimization techniques can be used in line 25 of Algorithm 1 to control online refinement costs. Therefore, we anticipate that $\text{datapass}_1 \ll \text{datapass}_2$ in Table 1 and expect that datapass_1 will not be prohibitively large. We believe this computational cost analysis would benefit from a benchmark case study in which different methods are applied and relatively compared, which we leave for future work.

Furthermore, WISER uses WISE as a *conditional* prior. During the inference phase, the approximated posterior from WISE is conditioned on the observed data, and WISER uses this approximated posterior as its prior in the objective function, effectively performing sequential Bayesian updating (Rubio et al., 2023). The conditional prior offers a more accurate approximation to the posterior compared to an unconditional prior trained solely on prior samples (Orozco et al., 2021). Arguably, this approach makes WISER more cost efficient than nonamortized inference methods that only have uninformative priors (Zhang et al., 2023) or that use a data driven but unconditional prior (Kelkar et al., 2021). Beyond reducing computational costs, WISER also ensures that the posterior samples realistically resemble earth models, thanks to the integration of conditional prior information from WISE.

In Wang et al. (2023) and Taufik et al. (2024), the authors trained a nonconditional diffusion model and conditioned it on various observations by performing gradient steps on the data likelihood, using the learned denoiser as a prior. Although diffusion models have shown promise in generating realistic-looking samples, using them for density estimation is not straightforward (Song et al., 2021), whereas it is straightforward with NFs. The WISER algorithm was built using NFs, motivated by memory efficiency, but it could be extended to use diffusion models as the backbone generative model, as demonstrated by Orozco et al. (2024a).

Correctness of posterior approximation

Because h_ϕ is trained to minimize the reverse KL divergence in equation 1, its composition with the amortized network f_θ is theoretically capable of representing the full Bayesian posterior (Winkler et al., 2019), which is likely multimodal in FWI problems. Especially, the amortized network minimizes the forward KL divergence, preventing mode collapse (Minka, 2005). In addition, WISER combines forward and reverse KL divergence minimization, guiding the sampling toward high-probability regions (Vaitl et al., 2024). This theoretical capability has been empirically validated on toy examples (Orozco et al., 2024c) and poststack seismic inversion examples (Rizzuti and Vasconcelos, 2024), where analytical posterior solutions exist.

Supplemental Text S1 shows that WISERs posterior samples respect likelihood and prior terms, indicating successful refinement of WISEs amortized posterior. However, verifying the correctness or multimodality of the approximated posterior remains challenging due to the high dimensionality and nonlinearity of FWI. A low-dimensional FWI case study could use calibration tests (Guo et al., 2017) and compare WISERs posterior samples with those from MCMC and other inference methods — an endeavor we reserve for future work.

Table 1. Number of PDE solves for several Bayesian inference methods for FWI.

| Method | Offline PDE solves $\times n_{\text{OBN}}$ | Online PDE solves $\times n_{\text{OBN}}$ |
|--------------------------|--|---|
| WISE (Yin et al., 2024b) | $3 \times N$ | 2 |
| WISER (proposed) | $3 \times N$ | $2 + 2 \times \text{datapass}_1$ |
| Nonamortized inference | 0 | $2 \times \text{datapass}_2$ |

Here, N represents the number of training pairs; n_{OBN} represents the number of OBNs in the seismic survey; and datapass_1 and datapass_2 represent the number of datapasses through the entire OBN data set using WISER and a nonamortized inference method, such as the ones presented in Zhang et al. (2023).

Scalability

Neural network implementations often face significant memory challenges in 3D problems due to the need to store intermediate activations for backpropagation. However, NFs, composed of invertible layers, mitigate this issue by recomputing intermediate activations during backpropagation instead of storing them in memory. Orozco et al. (2024d) exploit this property for memory efficiency by manually implementing gradient calculations, ensuring that memory consumption during backpropagation remains constant regardless of the number of layers (as shown in Figure 2 of Orozco et al., 2024d). Practically, this means a CNF with greatly many layers can be used for maximal expressiveness, provided that a constant factor of memory (related to the input and the condition) fits on the device. This inherent memory efficiency makes CNFs particularly suitable for 3D applications, as demonstrated by the 3D WISE case study in Orozco et al. (2024c).

Although our computational toolchain supports 3D forward and gradient calculations, deploying WISER in large-scale 3D FWI remains a valuable direction for future research. In our case study, the dimensions of network parameters θ and ϕ are $O(10^6)$ and $O(10^5)$, respectively, with the velocity model size being $O(10^5)$. Further studies should explore how the required number of training samples and network parameters for accurate WISER inference scale with the dimensionality of the parameter of interest.

Simulation gap and OOD inference

The presented case study illustrates WISER's capability when the ground-truth velocity model used during inference is geologically similar to those in the training samples. In practical terms, this suggests that WISER can be effectively applied when WISE is trained using velocity models that are drawn from the same region and share similar geologic structures, e.g., from the same area in a basin. Although these preliminary results are promising, further investigation is needed to determine the extent to which WISER can handle OOD scenarios during inference. Another way to fundamentally address the OOD issues is to diversify the training samples of WISE through a foundation model (Sheng et al., 2024).

We acknowledge that a simulation gap between synthetic and field data is inevitable. However, using CIGs, we can map information into the extended image space even when the data originate from a mis-specified forward model (e.g., elastic versus acoustic). Improving network training to better process this information remains an important avenue for future research. Although the simulation gap may persist during WISE inference, WISER is specifically designed to mitigate this issue by using a physics-based fine-tuning process that aligns the posterior samples with the observed data.

Extension to other geophysical inverse problems

Finally, the WISE(R) framework can extend to quantify uncertainty in other Bayesian inference problems, such as time-lapse monitoring (Gahlot et al., 2023, 2024b; Yin et al., 2024a). The estimated uncertainties can guide reservoir management decisions within a digital twin framework (Herrmann, 2023), including controlling injectivities (Gahlot et al., 2024a) and designing follow-up monitoring surveys and wells (Orozco et al., 2024b). In addition, mappings learned from CIGs to the velocity domain can be applied to salt segmentation problems (Muller et al., 2023, 2024).

CONCLUSION

WISER sets the stage for deploying genAI models to facilitate high-dimensional Bayesian inference with computationally intensive forward operators. Deep learning and AI have been criticized for their reliance on realistic training samples, but WISER helps to reduce this dependence and still offers computationally feasible and reliable inference through a blend of offline training and online frugal physics-based refinements, preparing our approach for large 3D deployment.

DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

During the preparation of this work, the authors used ChatGPT to improve readability and language. After using this service, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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DATA AND MATERIALS AVAILABILITY

Data associated with this research are available and can be accessed via the following URL: <https://github.com/slimgroup/WISER.jl>.

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Biographies and photographs of the authors are not available.