Traversing within the Gaussian Typical Set: Differentiable Gaussianization Layers for Inverse Problems Augmented by Normalizing Flows

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Abstract

Generative networks such as normalizing flows can serve as a learning-based prior to augment inverse problems to achieve high-quality results. However, the latent space vector may not remain a typical sample from the desired high-dimensional standard Gaussian distribution when traversing the latent space during an inversion. As a result, it can be challenging to attain a high-fidelity solution, particularly in the presence of noise and inaccurate physics-based models. To address this issue, we propose to re-parameterize and Gaussianize the latent vector using novel differentiable data-dependent layers wherein custom operators are defined by solving optimization problems. These proposed layers enforce an inversion to find a feasible solution within a Gaussian typical set of the latent space. We tested and validated our technique on an image deblurring task and eikonal tomography – a PDE-constrained inverse problem and achieved high-fidelity results.

1. Introduction

Many scientific imaging problems are essentially inverse problems, which use observed data to infer properties of a physical system. For example, astrophysicists use radio electromagnetic data to image galaxies and black holes [1, 21]. Geoscientists use seismic recordings to reveal the internal structures of Earth [51, 52, 55]. Biomedical engineers and doctors use X-ray projections, ultrasound measurements, and magnetic resonance data to reconstruct images of human tissues and organs [17, 31, 37]. However, inverse problems are typically ill-posed with incomplete information provided by data, and thus there are infinitely many compatible solutions. Worse still, the observed data are usually noisy, and the assumed physics-based model may not be accurate. All these challenges require using regularization to inject a priori knowledge into inversion processes to obtain plausible results.

Recently, deep-learning-based models have shown great promise for augmenting various inverse problems [3, 9, 20, 32, 36, 38, 42, 47, 50, 53, 54, 58, 59, 64]. In particular, deep generative models, such as VAEs [29], GANs [19], and normalizing flows [15, 16, 28, 48], which directly learn from training data distributions, are a powerful and versatile prior. Our work progresses from the prior art [3] that utilizes Glow [27] to augment inversion-based imaging problems, which demonstrates that normalizing flows are superior to other architectures such as GANs for such tasks.

Although normalizing flows are a very effective regularizer, we find that the quality of inversion results reduces significantly in the presence of noise and inaccurate physics-
based models (Figure 1). This is caused by the deviation of
the latent vector from a typical sample from a stan-
dard Gaussian distribution, on which pre-trained norma-
llizing flows are defined. The majority of probability mass of a
high-dimensional distribution lies within a so-called typical
set, which may not necessarily correspond to the region of
the highest probability density of the prior or the posterior
distributions. Typical samples from a high-dimensional
distribution rarely reside outside this typical set. This issue has
also been discussed in out-of-distribution (OOD) detection
literatures (e.g., [12, 41, 43, 44, 57]).

In this paper, we propose a set of differentiable Gaussi-
annization layers to re-parameterize and Gaussianize the
latent vectors of normalizing flows for inverse problems.
These layers mainly consist of an orthogonal transforma-
tion that increases the statistical independence among latent
vector components and nonlinear activation functions for
(marginal) 1D Gaussianization. Although our technique is
developed for normalizing flows, it can also be applied to
other deep generative models.

The remainder of this article is organized as follows. Sec-
tion 2 provides the background and mathematical state-
ment of the problem. Section 3 introduces the Gaussianiza-
tion layers, and Section 4 discusses related work. In Sec-
tion 5, we first present both quantitative and qualitative re-
results from a deblurring task on a downsampled CelebA-HQ
dataset [25]. Then, we present an additional example from
eikonal tomography. Section 6 discusses the limitations of
this work and concludes the paper.

2. Background & Problem Statement

Suppose the forward mapping can be symbolically writ-
ten as

\[ d = g(m) + \epsilon, \]

where \( g \) stands for the physics-based model that can be gov-
erned by a partial differential equation (PDE), \( \epsilon \) denotes
noise, \( d \) the observed data, and \( m \) the physical parameters
to be determined. In the augmented inversion framework, we
solve the inverse problem by finding the maximum 'a
posteriori' (MAP) estimate from

\[
p_M(m|d) \propto p(d|m)p_M(m)
\]

using gradient-based optimization methods, such as the
conjugate gradient method or quasi-Newton methods. The
probability density \( p_M \) introduces our 'a priori' knowledge
and is represented by a normalizing flow (Glow) \( f_\theta \), which
is a differentiable invertible mapping between two distribu-
tions, parameterized by neural network parameters \( \theta \):
\( m = f_\theta(z) \), where \( z \) is the latent vector. After training,
the log probability density of a given model \( m \) is

\[
\log p_M(m; \theta) = \log p_Z(f_\theta^{-1}(m)) + \log \left| \det J_{f_\theta}(m) \right|
\]

\[
= \log p_Z(z) - \log \left| \det J_{f_\theta}(z) \right|,
\]

where \( p_Z \) is the probability density function of a standard
Gaussian distribution.

In an augmented inversion, we freeze the network
weights; hence, we drop \( \theta \) in \( f_\theta \) hereafter in our notation.
Therefore, the original inverse problem can be formulated
in the following form, parameterized by a latent space rep-
resentation:

\[
\arg \min \| d - g(f(z)) \|^2_z - \beta \left( \log p_Z(z) - \log \left| \det J_f(z) \right| \right),
\]

where \( \beta \) is a weighting factor. We can retrieve an inverted \( m \)
by a forward pass of mapping from an inverted \( z \). In all our
experiments, we only use the additive coupling layer rather
than the affine coupling layer since we observe instabilities
with the latter, which is also mentioned in [5].

However, this formulation of augmented inversion leads
to unsatisfactory results, as shown in Figure 1. In addition,
if we put a large weight on the prior term, we also see strong
artifacts, as shown in Figure 5.

In high-dimensional spaces, counterintuitively, the mass
of a standard Gaussian distribution concentrates in a typi-
ical set \([6, 14]\), which we refer to as the Gaussian typical
set and give its formal definition in the supplementary
materials. A well-trained normalizing flow maps samples from
the target distribution into the Gaussian typical set with very
high probability and vice versa (supplementary materials).
Therefore, the normalizing flow may map atypical latent
vectors to unrealistic images or physical parameters out of
the target distribution.

Unfortunately, the latent vector can move outside the
Gaussian typical set during inversion with formulation 4.
For example, the MAP estimate may reside outside the typi-
cal set (e.g., a very large \( \beta \) drives the latent vector towards
the center), or in general the latent vector entries become
non-i.i.d. Noises or inaccurate physics model assumptions
would exacerbate this situation. Therefore, we need to con-
strain the latent vector within the Gaussian typical set dur-
ing inversion.

3. Method

3.1. Re-parameterization with Gaussianization

Layers

Our proposed solution is to re-parameterize the latent
space vector \( z \) by another random vector \( v \) with different-
tiable layers that “Gaussianize” the inputs, such that \( z =
patches of dimension \( n \cdot n \) tent space tensor also has the same dimension. In addition, and here \( z \) ping dom vectors. I Suppose that an inversion? The answer is to Gaussianize latent patches. Dmore tractable optimization perspective, we want to minimize \( D \) has a shape of \( m \times n \) components. The Gaussianization layers keep the optimization problem unconstrained, enabling us to use highly efficient unconstrained optimizers, such as the L-BFGS solver [45]. Remark: It is also reasonable to use a maximum-likelihood formulation instead of the maximum a posteriori formulation in Problem 5 since the Gaussianization transformation imposes a hard constraint on latent vectors. For comparison purposes, we keep using the MAP formulation in our experiments.

Now the question is: what do we mean by requiring \( z = h(v) \sim \mathcal{N}(0, I) \) since there is only one realization in an inversion? The answer is to Gaussianize latent patches. Supposing that \( m \) has a shape of \( n_c \times n_x \times n_y \), the latent space tensor also has the same dimension. In addition, the latent tensors can be partitioned into non-overlapping patches of dimension \( n_c \times w \times w \). We here make an assumption that the patch tensors are independent and identically distributed (i.i.d.), i.e., the vectorized patch tensors \( v_i \in \mathbb{R}^D (D = n_c \times w \times w, i = 1, \cdots, N) \) are i.i.d. random vectors.

The task now comes down to constructing a mapping \( z_i = h(v_i) \), such that \( z_i \sim \mathcal{N}(0, I) \). As a result, the concatenation of \( z_i, i = 1, \cdots, N \) will also be a random vector \( z \) distributed as a standard Gaussian. From a more tractable optimization perspective, we want to minimize \( D_{KL}(z_i, \mathcal{N}(0, I)) \), which can be decomposed as the sum of mutual information \( I(z_i) \) and marginal negentropy \( J_m(z_i) \) [11]:

\[
D_{KL}(p(z_i) \parallel \mathcal{N}(0, I)) = I(z_i) + J_m(z_i),
\]

where

\[
I(z_i) = D_{KL} \left( p(z_i) \parallel \prod_{j} p_j(z_i^{(j)}) \right),
\]

and

\[
J_m(z_i) = \sum_{j=1}^{D} D_{KL} \left( p_j(z_i^{(j)}) \parallel \mathcal{N}(0, 1) \right).
\]

Here \( z_i^{(j)} \) denotes the \( j \)-th component of patch vector \( z_i \), and \( p_j \) stands for the marginal PDF for that component.

Taking advantage of the fact that the KL divergence and a standard Gaussian in Equation 6 are invariant to an orthogonal transformation and that the mutual information term is invariant to a component-wise invertible transformation, we propose to conduct the Gaussianization in the following steps, similar to [11, 30]:

1. Minimize the mutual information \( I(z_i) \) – making the components statistically independent. This is done by an orthogonal transformation that keeps the KL divergence the same but increases the negentropy \( J_m(z_i) \).

2. Minimize the marginal negentropy \( J_m(z_i) \) by component-wise operations that perform 1D Gaussianization of marginal distributions \( p_{j, j=1, \cdots, D} \). The mutual information does not change under component-wise invertible operations. Therefore, the overall KL divergence between \( z_i \) and the Gaussian distribution decreases.

The orthogonal matrix and the nonlinear element-wise operations resemble neural network layers, but there are no extra parameters introduced. The nonlinear activation layers are data-dependent, and the outputs are obtained by solving optimization problems; therefore, special care should be taken to implement the gradient computation correctly and ensure that they pass the finite-difference convergence test (see the supplementary materials).

### 3.2. Reducing Mutual Information – ICA Layer

The orthogonal matrix \( W \) is constructed by the independent component analysis. As we stated previously, patch vectors \( \{v_i\}, i = 1, \cdots, N \) from \( v \) are assumed as i.i.d. random vectors; therefore, \( p_i = W v_i \) are also i.i.d. Besides, the orthogonal matrix \( W \) makes the entries of each \( p_i \) independent random variables. Therefore, the concatenated output random vector \( p = [p_1, p_2, \cdots, p_N] \) has independent components. The default patch size is \( 3 \times 8 \times 8 \).

Our proposed layer to reduce mutual information is based on the FastICA algorithm [22, 24], which employs a fixed-point algorithm to maximize a contrast function \( \Phi \) (e.g., the logcosh function).

The FastICA algorithm typically requires that the data are pre-whitened. We adopt the iterative whitening method introduced in [22] (see supplementary materials). With whitened data, we compute \( W \) using a damped fixed-point iteration scheme (\( w_i \) is the \( i \)-th column vector of \( W \)):

\[
w_i = \alpha \mathbb{E} [v \phi(w_i^\top v)] - \mathbb{E} [\phi'(w_i^\top v)] w_i,
\]

or in the matrix form:

\[
W = \frac{1}{N} \left[ \alpha V \phi'(W^\top V) - W \text{diag}(\phi'(W^\top V) \mathbf{1}) \right],
\]
where \(1\) is an all-one vector, \(\phi(\cdot) = \Phi^t(\cdot), \alpha \in (0, 1)\), and we use \(\alpha = 0.8\) throughout our experiments. To save computation time, we only perform a maximum of 10 iterations. The details of the whole algorithm can be found in the supplementary materials.

We set the initial \(W\) as an identity matrix. If the input vectors are already i.i.d. Gaussian (within the Gaussian typical set), the computed \(W\) will still be an identity matrix, which maps the input to the same output. This theoretical situation means that our ICA layer maps vectors in the supplementary materials.

In practice, the empirical situation means that our ICA layer maps vectors in the Gaussian typical set to themselves. In practice, the empirical distribution from finite samples is not a standard Gaussian typical set, the computed \(W\) vectors are already i.i.d. Gaussian (within the Gaussian typical set), the computed \(W\) vectors are already i.i.d. within the Gaussian typical set. This corresponds to the fact that ICA cannot differentiate Gaussian sources, but our inversion application works fine with this case.

### 3.3. Reducing Marginal Negentropy

For 1D Gaussianization, we choose a combination of the Yeo-Johnson transformation that reduces skewness and kurtosis to i.i.d. standard Gaussian vectors. This corresponds to the fact that ICA cannot differentiate Gaussian sources, but our inversion application works fine with this case.

#### Power Transformation Layer

We propose to use the power transformation or Yeo-Johnson transformation [60] to reduce the skewness of distributions:

\[
s(\lambda, p) = \begin{cases} 
\frac{(p + 1)^\lambda - 1}{\lambda}, & p \geq 0, \lambda \neq 0, \\
\log (p + 1), & p \geq 0, \lambda = 0, \\
\frac{(-p + 1)^{2-\lambda} - 1}{2-\lambda}, & p < 0, \lambda \neq 2, \\
\log (-p + 1), & p < 0, \lambda = 2,
\end{cases}
\]

where \(p\) is an input value, \(s\) is an output value, and \(\lambda\) is the parameter to be estimated. As shown in Figure 2(a), the form of the Yeo-Johnson activation function depends on parameter \(\lambda\). If \(\lambda = 1\), the mapping is an identity mapping. If \(\lambda \geq 1\), the activation function is convex, which compresses the left tail and extends the right tail, reducing the left-skewness. If \(\lambda \leq 1\), the activation function is concave, which oppositely reduces the right-skewness. The only parameter \(\lambda\) is determined by solving an optimization problem that minimizes the negentropy:

\[
\lambda = \arg \max_\lambda I(\lambda|p) = \arg \max_\lambda \frac{n}{2} \log(\text{Var}(s(\lambda, p_i))) + (\lambda - 1) \sum_{i=1}^{n} \text{sign}(p_i) \log(|p_i| + 1),
\]

where \(p\) is an input data vector with entries \(p_i, i=1, \ldots, n\). We refer the readers to the supplementary materials for details in implementation and algorithm summary.

#### Lambert \(W \times F_X\) Layer

Due to noise and inaccurate physics-based models, we observe that the distribution of latent vector values tends to be shaped as a heavy-tailed distribution during the inversion process. To reduce the heavy-tailedness, we adopt the Lambert \(W \times F_X\) method detailed in [18].

Let \(X\) be a random variable whose CDF is \(F_X\), with mean \(\mu_X\) and standard deviation \(\sigma_X\). The following transformation with a heavy-tail parameter \(\delta \geq 0\):

\[
S = \left( U \exp \left( \frac{\delta}{2} U^2 \right) \right) \sigma_X + \mu_X,
\]

where \(U = (X - \mu_X) / \sigma_X\), is a bijection and maps \(X\) to another random variable \(S\) with heavier tails.

We use the parameterized Lambert \(W \times F_X\) distribution family to approximate a heavy-tailed input and solve an optimization to estimate an optimal \(\delta\) (see the supplementary materials), with which the inverse transformation maps an output as Gaussian as possible.

Figure 2(b) shows that the Lambert \(W \times F_X\) layer acts as a nonlinear squashing function. As \(\delta\) increases, it compresses more the large values and reduces the heavy-tailedness. Intuitively, the Lambert \(W \times F_X\) layer can also be interpreted as an intelligent way of imposing constraints on the range of values instead of a simple box constraint. We refer the readers to the supplementary materials for more details about the optimization problem and implementation.
Standardization with Temperature. Since the output of the Lambert $W \times F_X$ Layer may not necessarily be zero mean and unit (or a prescribed) variance, we standardize the output using

$$z = (x - \bar{x})/\sqrt{\text{Var}(x)} \times \gamma, \quad (14)$$

where $\gamma$ is the temperature parameter suggested in [27].

Figure 3. The effects of Gaussianization layers. As an exaggerated example, we use a standardized (with the temperature as 0.8) image as a latent tensor. The latent tensor components are not independent, and the values of latent tensor do not follow a Gaussian distribution as indicated by the QQ-plot. Then, we apply the proposed Gaussianization layers twice, which destroy the patterns and make the values approximately distributed as a Gaussian with a temperature of 0.8. After only one pass, the image output using the normalizing flow becomes plausible. In fact, only one set of these layers are adequate for inversion. We talk about the rolling operation in the supplementary materials.

In summary, we illustrate the effects of the Gaussianization layers in Figure 3, which shows that these layers eliminate latent space patterns, i.e., making latent pixels independent, and shape their value distribution towards an isotropic Gaussian distribution (with a given temperature).

4. Related Work

Gaussianization. Chen and Gopinath [11] proposed an EM algorithm to iteratively Gaussianize high-dimensional data. The rotation-based iterative Gaussianization (RBIG) method [30] consists of iterations of a marginal Gaussianization transformation and an orthogonal transformation. These methods laid the foundation for our strategy: an orthogonal transformation to minimize mutual information and 1D Gaussianization transformations to minimize marginal negentropy. Meng et al. [40] proposed a normalizing flow named the Gaussianization flow based on the same strategy. Their 1D Gaussianization transformation resembles the one in [11], where they use kernel density estimation (KDE) with learnable parameters (i.e., 20 to 100 anchor point locations and bandwidths) to approximate the CDF and apply inverse CDF transformation to map data to a Gaussian. This approach also inspired us to experiment with the same parameterization in our optimization-based layers. However, we found it hard to obtain a non-singular Hessian for backward propagation of gradients and at the same time achieve good forward Gaussianization performance. Also, the computation cost for this approach is higher than our single-parameter optimization. We also would like to acknowledge that the “latent space normalization” trick in the super-resolution normalization flow – SRFLOW [35], a method for end-to-end super-resolution, inspired us to design Gaussianization layers to regularize inverse problems.

Implicit Layers. In contrast to traditional feed-forward neural network layers, implicit layers like OptNet [2] and the deep-equilibrium networks [4] compute the output either by solving an optimization problem or finding the solution to a nonlinear equation. Their gradient computation is similar to the adjoint-state method in computational physics, where automatic differentiation can be used to compute a vector-Jacobian product. More details and examples can be found in [39].

5. Experiments

5.1. Deconvolution with Noise and Inaccurate Kernel

We first tested our method on a deconvolution (deblurring) task. The inverse problem is to recover high-resolution images given blurred observations with possible noises, assuming we have a good knowledge of the smoothing kernel. Deconvolution has wide applications in image deblurring, astronomical imaging, and geophysical inversion. In our experiments, we use an isotropic Gaussian smoothing kernel $G$ parameterized by its standard deviation $\tau$. The math-
The mathematical formulation of the forward process is as follows

\[ d = G \ast m + \epsilon, \tag{15} \]

where \( \epsilon \) is added noise, and \( \ast \) is the convolution operator. In our experiments, we assume that \( \epsilon \sim \mathcal{N}(0, \sigma^2 I) \). This ill-posed problem is especially challenging when the noise is strong or the smoothing kernel estimate is inaccurate.

We used the CelebA-HQ dataset [25] (under the Creative Commons CC BY-NC 4.0 license) for testing and evaluation. All images were downsampled to the resolution of 128×128. We trained the Glow network with the original training-validation-testing split configuration as the CelebA dataset [34] (see the supplementary materials). For the inversion tests, we randomly selected 100 images from the test set. All inversions started with the same Gaussian random vector in the latent space.

There are two parameters for experiments: the standard deviation of the Gaussian smoothing kernel \( \tau \) and the standard deviation of the added Gaussian noise \( \sigma \). Besides, there are also two hyper-parameters for the inversion: the weighting parameter \( \beta \) from Problem 5 and the temperature \( \gamma \) of the latent space Gaussian.

We set the base case with \( \tau = 3.0, \sigma = 50.0, \beta = 10^3 \). For comparison, we also changed each of these parameters one at a time to investigate their impact on inversion results. LPIPS [62] is the primary metric in our study to measure the similarity between the deconvolved results and the ground truth because it is closer to human perception than other metrics such as PSNR and SSIM [56]. Figure 4 summarizes the quantitative evaluation results at each inversion step, where we plot the averaged LPIPS metric curve and the standard deviation in the shaded area. In addition, we report the minimum mean values on the LPIPS curves. In all cases, our Gaussianization layers, on the one hand, enable inversions to achieve a lower restoration error, and on the other hand, keep results plausible throughout the entire inversion processes.
5.2. Ablation Study

![Figure 6. Ablation study. The results indicate that the ICA layer plays the most critical role in improving inversion results. The temperature was set to 0.7 in all cases.]

We performed an ablation study to investigate the contribution from the components of the proposed Gaussianization layers. We first removed the ICA layer: we only kept the 1D Gaussianization layers (power transformation and Lambert $W \times F_X$) and the last standardization layer with a temperature of 0.7. Compared with the base case with Gaussianization layers, the minimum LPIPS increases from 0.15 to 1.61. The LPIPS curve also moves up as inversion continues, which means that the latent vectors of the deblurred images are getting out of the Gaussian typical set. Despite their inability to keep the LPIPS curve from going up, the 1D Gaussianization layers with standardization are able to reduce the minimum LPIPS compared with the base case without any part of Gaussianization layers (0.173).

We then removed all but the last standardization layer with a temperature of 0.7. The minimum LPIPS increases slightly from 1.61 to 1.62, suggesting the marginal improvement from only adding the power transformation and Lambert $W \times F_X$ layers. Considering both ablative procedures, it is clear that the ICA layer has the most significant contribution to keep results meaningful throughout inversion.

5.3. Eikonal Tomography

In this section, we perform tests on a highly ill-posed tomography problem where the physics phenomenon is described by a nonlinear PDE. The task of tomography is to use data recorded at the boundary of an object to reconstruct its internal structures. In acoustic wave imaging, the following eikonal equation approximately describes the shortest travel time $T(x; x_s)$ that the acoustic wave emerging from source location $x_s$ takes to reach location $x$ [61]:

$$ |\nabla T(x; x_s)| = \frac{1}{c(x)}, \quad x \in \mathbb{R}^2 $$

$$ T(x_s; x_s) = 0, $$

where $c(x)$ is the wave propagation speed at each location. The goal is to reconstruct $c(x)$. Figure 7(a) shows the experiment setup where we placed sources at the left boundary and receivers at the right one. We excited waves from each source and recorded travel time at the receiver array, which constituted the observed data. We solved the eikonal equation using the fast sweeping method [63] and computed the gradient using the discrete adjoint-state method [33].

We used 100 randomly selected model parameters $m(x)$ from the test set for inversion, and Figure 7(a) shows one typical example. For simplicity, the parameter values were defined between 0 and 1 and then converted to $c(x)$ by the formula: $c(x) = 100m(x) + 1500$, which was hence used in the forward physics model.

A good starting model $m_0(x)$ is necessary for this type of inversion with nonlinear physics-based models. In our synthetic tests, we obtained it by smoothing $m(x)$ by a Gaussian kernel with a standard deviation of 5. Then we found its projection in the latent space and started inversion from there. More details can be found in the supplementary materials.

We added noise to the recorded travel time using the following formula: $T_{\text{noisy}}(x_r; x_s) = T(x_r; x_s)(1 + \epsilon)$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$ and $x_r$ denotes any receiver location. In other words, a longer travel time corresponds to larger uncertainties.

![Figure 7. Comparison of results from eikonal tomography. (a) The true physical parameters and the source-receiver configuration. This represents a generic tomography setup; (b) Inversion results with traditional total variation regularization, where the result is blown up by noise; (c) Augmented inversion without Gaussianization layers, where grid-like artifacts exist; (d) Augmented inversion with Gaussianization layers, where the result has the highest quality.]
With the projected latent vectors obtained with and without Gaussianization layers, we conducted inversion by solving Problem 4 and Problem 5, respectively. As an additional comparison, we did a conventional eikonal tomography inversion without the augmentation from a normalizing flow, but with the total variation regularization and a box constraint to force values to stay in $[0, 1]$. Figure 7 shows a qualitative comparison of inversion results when $\sigma = 0.1$. In augmented inversions, we set weighting parameter $\beta = 0.001$ and temperature $\gamma = 1.0$ in both cases with and without the Gaussianization layers. Comparing Figures 7(c) and 7(d), we see that the result with the Gaussianization layers has no mesh-like artifacts and stays within a more accurate value range.

Table 1 summarizes the best average metrics (LPIPS and SSIM) from inversions with 100 examples, with different noise levels $\sigma$ and different $\beta$. This comparison favors inversions without the proposed layers since we are comparing the best results attained during the whole inversion process. Still, in almost all cases, inversion using our Gaussianization layers (the “on” cases) outperforms that without such layers (the “off” cases). Finally, we show in Figure 8 that if $\beta$ is set too large as 0.1, the inverted wave speed parameters without the Gaussianization layers diverge to unrealistic results.

| $\beta$ | $\sigma = 0.0025$ | $\sigma = 0.005$ | $\sigma = 0.01$ |
|---|---|---|---|
| $10^{-5}$ | 0.443 | 0.437 | 0.366 | 0.368 | 0.291 | 0.295 |
| $10^{-3}$ | 0.439 | 0.440 | 0.366 | 0.369 | 0.290 | 0.297 |
| $10^{-1}$ | 0.312 | 0.375 | 0.329 | 0.372 | 0.289 | 0.294 |
| SSIM↑ | | | | | | |
| $10^{-5}$ | 0.184 | 0.177 | 0.213 | 0.198 | 0.247 | 0.228 |
| $10^{-3}$ | 0.185 | 0.175 | 0.212 | 0.201 | 0.251 | 0.228 |
| $10^{-1}$ | 0.293 | 0.216 | 0.260 | 0.202 | 0.257 | 0.232 |
| LPIPS↓ | | | | | | |

6. Discussion & Conclusions

We point out some limitations of this work. First, traversing within the Gaussian typical set means that the statistics of the training dataset will dominate the results. Figure 9 shows that our method cannot restore the eyeglasses because of the strong constraint of traversing within the Gaussian typical set. The results are dominated by the bias of the training dataset.

In summary, we have proposed a set of Gaussianization layers: the ICA layer, the power transformation layer, the final standardization layer $X = 0$ and the transformation $F_X$ layer, and the final standardization layer $X = 0.30$ seconds and 18.18 seconds.

Figure 8. Comparison of eikonal tomography results with a large $\beta (0.1)$ during the inversion process. (a) SSIM; (b) LPIPS. Without the Gaussianization layers, the inverted physical parameters diverge to unrealistic results.

Figure 9. A failure example where inversion is not able to restore the eyeglasses because of the strong constraint of traversing within the Gaussian typical set. The results are dominated by the bias of the training dataset.
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A. Gaussian Typical Set

The formal definition of a typical set is as follows.

**Definition 1 (Cover & Thomas [14])** Let \( p_X(x) \) be a distribution whose support is \( \mathcal{X} \). The typical set \( A_{n}^{(n)} \) is defined as the set of sequences \( (x_1, x_2, \ldots, x_n) \in \mathcal{X}^n \), \( x_i \) i.i.d. \( p_X \) that satisfy

\[
\left| H \left[ x \right] + \frac{1}{n} \log p_X(x_1, \ldots, x_n) \right| \leq \epsilon, \tag{17}
\]

where \( H \left[ x \right] \) is the entropy of random variable \( x \).

Now a random vector \( x \in \mathbb{R}^n \sim \mathcal{N}(0, \sigma^2 I) \) can be factorized as i.i.d. random variables that are distributed as \( \mathcal{N}(0, \sigma^2) \). Therefore, we can regard \( x \) as an i.i.d. sequence and give the following definition:

**Definition 2 (Gaussian Typical Set)** A Gaussian typical set is the typical set \( A_{n}^{(n)} \) of \( x \in \mathbb{R}^n \sim \mathcal{N}(0, \sigma^2 I) \).

The following theorem guarantees that a typical sample from \( x \in \mathbb{R}^n \sim \mathcal{N}(0, \sigma^2 I) \) resides in the Gaussian typical set with very high probability.

**Theorem 1 (Cover & Thomas [14])** For every \( \epsilon > 0 \), the typical set has probability \( P \left( A_{n}^{(n)} \right) > 1 - \epsilon \) with a sufficiently large dimension \( n \).

These theoretical facts again justify our Gaussianization approach, which first makes each component as independent as possible and then shapes each component towards the same marginal 1D Gaussian distribution. As a result, the Gaussianization layers shape a latent vector towards a typical example from the desired high-dimensional isotropic Gaussian distribution.

B. More Details of the Gaussianization Layers

B.1. ICA Layer

The overall ICA layer is summarized in Algorithm 1. We set a maximum number of the fixed-point iterations to reduce computational cost and ensure accurate gradient computation that can pass the finite-difference convergence test.

**Data Iterative Whitening.** The FastICA algorithm typically requires that the data are pre-whitened. After subtracting the mean, we use the following steps to whiten the data, which are also used later in ICA iterations to decorrelate column vectors in the orthogonal matrix \([22]\):

1. Compute

\[
W = W/\sqrt{\|W^\top CW\|_2}, \tag{18}
\]

2. Repeat until convergence

\[
W = \frac{3}{2}W - \frac{1}{2}WW^\top CW, \tag{19}
\]

where \( C = E[v_i v_i^\top] + \eta I \) is the data covariance matrix, to which we add a small constant (e.g., \( \eta = 0.001 \)) on the diagonal entries to avoid ill-conditioning.

**The Modified FastICA Iterations.** As stated in [23], the objective function for one neural unit of the weight vector \( w_i \) and input \( v \) is

\[
\arg \max_{w_i} E \left[ \Phi \left( w_i^\top v \right) \right], \tag{20}
\]

\[
s.t., E \left[ (w_i^\top v)^2 \right] = 1,
\]

where \( \Phi \) is the contrast function (e.g., logcosh). The original derivations convert this constrained optimization to an unconstrained one using Lagrange multipliers. However, this procedure is unnecessary since the matrix \( W \) is orthogonalized after each iteration, and the input vectors have been pre-whitened. Therefore, we only need to solve the following equation

\[
E[v \phi'(w_i^\top v)] = 0, \tag{21}
\]

whose Jacobian is

\[
J = E[v v^\top \phi'(w_i^\top v)]
\]

\[
\approx E[v v^\top]E[\phi'(w_i^\top v)] = E[\phi'(w_i^\top v)], \tag{22}
\]

where \( \phi \) is the derivative of \( \Phi \). The Newton iteration scheme is thus

\[
w_i = w_i - E[v \phi'(w_i^\top v)]/E[\phi'(w_i^\top v)]. \tag{23}
\]

To improve the convergence, we damp the iterations by a parameter \( \alpha \in (0, 1) \). Also, using the same technique to convert the Newton iterations to fixed-point iterations in [22, 23], we arrive at the modified fixed-point iteration scheme (Equation 9):

\[
w_i = \alpha E[v \phi'(w_i^\top v)] - E[\phi'(w_i^\top v)] w_i, \tag{24}
\]

followed by the aforementioned decorrelation procedure after each step.
The convergence of the modified FastICA iterations can be proved similarly as in [46]. Without the damping factor, it is required that

$$E[b_i \phi(b_i) - \phi'(b_i)] \neq 0,$$

where $b_i, i = 1, \ldots, n$ are entries of the original random vector before mixing. If the distribution of $b_i$ is a Gaussian, this condition is violated, corresponding to the fact that ICA cannot resolve Gaussian source vectors. Our introduction of $\alpha$ avoids this problem at the theoretical level.

B.2. Power Transformation Layer

We use a custom operator based on SciPy’s implementation using Brent’s algorithm [10] to find an approximate minimum of Problem 12. Continuing from the approximate minimum, we use Brent’s root finding algorithm [10] to find the minimum where the gradient vanishes. Since the parameter $\lambda$ depends on input data, we need to back-propagate the gradient through the optimization process.

The power transformation layer is summarized in Algorithm 2.

B.3. Lambert W Layer

The transformation Equation 13 is bijective if $\delta \geq 0$, and we can use the Lambert W function to find its inverse. The Lambert W function $W$ is defined as the inverse of $q = W^{-1} (t) = t \exp (t)$, where $t$ and $q$ are scalars. Given $q$, Halley’s method can be used to find $t = W (q)$ [13]. Hence, the inverse of Equation 13 is

$$X = W_\delta \left( \frac{S - \mu_X}{\sigma_X} \right) \sigma_X + \mu_X, \quad (26)$$

where

$$W_\delta (u) = \text{sign} (u) \sqrt{\frac{W (\delta u^2)}{\delta}}. \quad (27)$$

We use the parameterized Lambert $W \times F_X$ distribution family to approximate a heavy-tailed input distribution and use Equation 26 to recover a distribution with lighter tails. In order to make the recovered distribution close to a Gaussian distribution, we compute the optimal heavy-tail parameter $\delta$ by minimizing the difference of the kurtosis of the output distribution and 3 (Kurtosis is a common surrogate measure of negentropy [24]):

$$\delta_{\text{GMM}} = \arg \min_{\delta > 0} \left| \text{Kurt} \left(W_\delta \left( \frac{s - \mu_X}{\sigma_X} \right) \right) - 3 \right|^2, \quad (28)$$

where $s$ is the data vector, and Kurt is the kurtosis. We constrain $\delta > 0$, and solve Equation 28 using the L-BFGS-B optimizer.

In addition, we estimate the mean $\mu_X$ and standard deviation $\sigma_X$ along with $\delta$ using the Iterative Generalized Method of Moments (IGMM) [18], which embeds an optimization problem for $\delta$ in an outer loop of iterations to estimate $\sigma_X$ and $\mu_X$ (see Algorithm 3). If the kurtosis of input data vector is not greater than 3, we skip the whole Lambert $W \times F_X$ layer by directly outputting the data vector.
C. Details of Training

For the deconvolution experiments, we split the 30000 images from CelebA-HQ into the subsets of training (24183 images), validation (2993 images), and testing (2824 images) following the original splits from CelebA [34]. These images were also downsampled to the resolution of 128×128.

To construct the dataset of layer models, we created layer geometries by intersecting sine functions of randomly generated wavelengths, initial phases, and dip angles. Then, we generated an array of 20 numbers equally spaced between 0.1 and 0.9. Each layer picked one number a from the array with equal probability and sampled a value from the distribution $N(a, 0.01^2)$ as the value of the layer. There are 16000, 4000, and 2000 examples in the training, validation, and testing sets. We used 100 randomly selected examples from the test set for inversion. We show 32 training and 32 generated examples in Figure 10.

For the hyper-parameters of the Glow networks, we used 4 multi-scale levels and 32 flow-steps for both CelebA-HQ and the layer models. As mentioned in the main text, we only used additive coupling layers. Figure 11 reports the training process. For each epoch, we computed the training negative log-likelihood (NLL) averaged throughout the epoch, and the validation NLL at the end of the epoch. For both CelebA-HQ and layer models, the validation curves suggest that it is better to use 4 multi-scale levels. We chose the network weights from the epoch before the validation NLL stopped to decrease: 850 for the CelebA-HQ dataset and 460 for the layer models. All training was conducted using $8 \times 32$ GB Nvidia V100 GPUs with a batch size of 64. We used the Adam optimizer [26] with a learning rate of 1e-4, as well as $\beta_1 = 0.9$ and $\beta_2 = 0.99$.

D. Gradient Computation of the Optimization-based Differentiable Layers

In the power transformation and Lambert $W \times F_X$ layers, there are operators whose outputs are obtained by solving optimization problems formally described as

$$y = \arg \min_y l(x, y),$$

where $l$ denotes the objective function that defines the operator, symbol $y$ stands for the output, a scalar in our cases but can also be a vector in general situations. The optimal condition is

$$l_y(x, y) := L(x, y) = 0,$$

where the subscript denotes partial differentiation.
Figure 11. The negative log-likelihood or NLL (reported in bits per dimension) on the training and validation splits with different numbers of multi-scale levels. (a) CelebA-HQ; (b) Layer models.

The optimal condition implicitly defines a forward operator of the following form:

$$y = \mathsf{op}_{\text{forward}}(x).$$

(31)

The backward operator is

$$\frac{\partial \chi}{\partial x} = \mathsf{op}_{\text{backward}}\left(\frac{\partial \chi}{\partial y}, x\right),$$

(32)

where $\chi$ is the objective function of an inverse problem.

Differentiating Equation 30 with respect to $x$, we have

$$L_x + L_y y_x = 0 \implies y_x = -L_y^{-1} L_x,$$

(33)

using the implicit function theorem. Then, to backpropagate the gradient from $\frac{\partial \chi}{\partial y}$ to $\frac{\partial \chi}{\partial x}$, we use

$$\frac{\partial \chi}{\partial x} = \frac{\partial \chi}{\partial y} y_x = -\frac{\partial \chi}{\partial y} L_y^{-1} L_x = -\frac{\partial \chi}{\partial y} H_y^{-1} L_x,$$

(34)

where $H_y$ is the Hessian matrix of $\chi$ with respect to $y$.

In our problems, the output $y$ is a scalar, so it is easy to use automatic differentiation to compute $L_y$ directly and hence $L_y^{-1}$. Otherwise, if $y$ has many parameters, we can first solve the following linear system with an auxiliary vector $\lambda$:

$$\lambda H_y = -\frac{\partial \chi}{\partial y},$$

(35)

and then compute the gradient using

$$\frac{\partial \chi}{\partial x} = \lambda L_x,$$

(36)

a technique also known as the adjoint-state method. Note that there is no need to compute the Hessian explicitly, but one can use automatic differentiation to compute the vector-Hessian product $\lambda H_y$ and utilize iterative linear solvers like GMRES [49] to solve the linear system.

As a final note, we check the accuracy of our gradient computation using the finite-difference convergence test based on Taylor expansion:

$$f(x + \epsilon \delta x) = f(x) + \epsilon \nabla f(x)^\top \delta x + O(\epsilon^2),$$

(37)

where $\delta x$ is a random vector with a unit $\ell_2$ norm, and $\nabla f(x)$ is computed using our custom gradient. We here define $f$ as a composite function that maps the (vector) output of an forward operator to a scalar, e.g., $f(x) = \|\mathsf{op}_{\text{forward}}(x)\|_2^2$. Once we decrease $\epsilon$, we should see that the error term $f(x + \epsilon \delta x) - f(x) - \epsilon \nabla f(x)^\top \delta x$ decreases at a speed of second order. All our layers passed this test, as the example shown in Figure 12. This test should be conducted in double precision.

E. Miscellaneous Topics

E.1. Gaussian Annulus Theorem.

Theorem 2 ([7]) For a $n$-dimensional standard Gaussian, for any $\beta \leq \sqrt{n}$, all but at most $3e^{-c\beta^2}$ of the probability mass lies within the annulus $\sqrt{n} - \beta \leq |x| \leq \sqrt{n} + \beta$, where $c$ is a fixed positive constant.
Bojanowski et al. [8] recognized this issue in their generative latent optimization processes and projected the latent vector onto a sphere. In addition to constraining the norm of latent vectors only, our approach Gaussianizes the latent vectors. In fact, a latent vector staying within the Gaussian annulus geometrically does not necessarily map to a plausible image. For example, all latent vectors in Figure 3 have almost the same $\ell_2$ norm, but the uppermost one does not correspond to a meaningful normalizing flow output.

E.2. Duality of KL Divergence

As also shown in [48], the KL-divergence between two distributions does not change under a differentiable invertible transformation, so

$$D_{KL}[p^*_M(m)||p_M(m; \theta)] = D_{KL}[p^*_Z(z; \theta)||p_Z(z)],$$

(38)

where $p^*_M$ is the target distribution in the physical parameter space, and $p^*_Z$ is the corresponding latent-space distribution under the normalizing flow. This means that minimizing the forward KL divergence in the $M$ domain or physical parameter space is equivalent to minimizing the reverse KL-divergence in the $Z$ domain or the latent space.

This fact and Theorem 1 imply that a well-trained normalizing flow maps samples from the target distribution into the Gaussian typical set with very high probability and vice versa.

E.3. The Rolling Operation

After applying one set of the Gaussianization layers to the latent tensor, it might be desirable to apply the layers to a different set of non-overlapping patches from the latent tensor at a second time. The rolling operation shifts the latent tensor in the horizontal and vertical directions by half of the patch size $w$ before patch extractions. The values at the boundaries are wrapped around to the opposite sides. One can, for example, use the `torch.roll` command to implement this functionality.

E.4. Initial Model Projection for Eikonal Tomography

The first step of inversion is to find the latent vector that has a minimum $\ell_2$ distance to that of an initial model in the physical parameter domain, given the prior from the network. To this end, we solve the following optimization problems for a maximum of 100 iterations:

$$\arg\min_{z} \| m_0 - f(z) \|^2_2 - \beta \left( \log p_Z (z) - \log |\det J_f (z)| \right),$$

(39)

and

$$\arg\min_{v} \| m_0 - f \circ h(v) \|^2_2 - \beta \left( \log p_Z (h(v)) - \log |\det J_f (h(v))| \right),$$

(40)

where $m_0$ is the vector representation of the initial physical property field $m_0(x)$. Note that this step is necessary since we find that an inversion usually gets stuck at the beginning if we directly start from the inverse of the initial model under the normalizing flow: $z_0 = f^{-1}(m_0)$ without the Gaussianization layers.