
Score-Based Likelihood Characterization for Inverse Problems in the Presence of Non-Gaussian Noise

Ronan Legin^{1,2,3} Alexandre Adam^{1,2,3}
Yashar Hezaveh^{1,2,3,4,5,6} Laurence Perreault-Levasseur^{1,2,3,4,5,6}
¹Université de Montréal ²Ciela Institute ³Mila
⁴CCA, Flatiron Institute ⁵Trottier Space Institute ⁶Perimeter Institute
{ronan.legin, alexandre.adam, yashar.hezaveh,
laurence.perreault.levasseur}@umontreal.ca

Abstract

Likelihood analysis is typically limited to normally distributed noise due to the difficulty of determining the probability density function of complex, high-dimensional, non-Gaussian, and anisotropic noise. This work presents Score-based Likelihood Characterization (SLIC), a framework that resolves this issue by building a data-driven noise model using a set of noise realizations from observations. We show that the approach produces unbiased and precise likelihoods even in the presence of highly non-Gaussian correlated and spatially varying noise. We use diffusion generative models to estimate the gradient of the probability density of noise with respect to data elements. In combination with the Jacobian of the physical model of the signal, we use Langevin sampling to produce independent samples from the unbiased likelihood. We demonstrate the effectiveness of the method using real data from the Hubble Space Telescope and James Webb Space Telescope.

1 Introduction

The presence of measurement errors, or noise, in data leads to uncertainty in the inference of variables of interest. Modeling this uncertainty requires the likelihood function, which depends on the statistics of the measurement errors [1]. These errors can be caused by various physical processes, resulting in different forms of noise [e.g., 2–8].

Although the assumption of Gaussian noise models for the likelihood is prevalent in many fields [e.g., 9–11], in practice, however, the statistics of noise often deviate significantly from a simple normal distribution and could be highly correlated, anisotropic, and non-Gaussian [e.g., 12–19]. Traditionally, the approach to deal with these scenarios has been to adopt an approximate normal noise model for the likelihood (and accept the potential biases that result), model and remove specific forms of noise (e.g., cosmic rays removal from CCD images [20–22]), masking a subset of data with significant non-Gaussian noise, or avoiding using likelihood analysis altogether. These sub-optimal approaches are driven by the fact that the probability density of complex, high-dimensional, non-Gaussian noise is not known and is intractable with closed-form expressions.

In this work, we build a noise model using a set of observed noise realizations in high dimensions (e.g., pixel space) and show that this can produce unbiased likelihoods even for noise with highly non-Gaussian statistics. We focus on the ubiquitous case of additive noise and assume that the noise realizations used for learning the noise model are either simulated or real data in the absence of the signal of interest (e.g., regions in a CCD image that do not contain the signal of interest).

Our framework, Score-based Likelihood Characterization (SLIC), employs score-based diffusion generative models [23–25] to estimate the gradient of the probability density of noise relative to

image pixels. We demonstrate that, when combined with the Jacobian of the forward model of the signal, this approach enables unbiased inference of model parameters for inverse problems where the data contains non-Gaussian noise.

2 Methods

2.1 Learning the noise model

We assume that we have a dataset of n images of noise, where each image has m elements (i.e. the number of pixels), $D_{\text{Training}} = \{x_1; x_2; \dots; x_n\}$. We construct this training set with i.i.d. realizations of noise from an underlying true noise probability density distribution, $Q_{\text{True}}(\mathbf{x})$. Here, \mathbf{x} refers to any m -dimensional point (i.e. an image) in the data space. When evaluated on a particular data, e.g., x_0 , this function informs us of how likely it is that x_0 is a realization of noise.

In the context of score-based models, instead of learning Q directly, we learn the gradient of the logarithm of Q with respect to its variable \mathbf{x} , written as $\mathbf{s}(\mathbf{x}_0) = \nabla_{\mathbf{x}} \log Q(\mathbf{x}_0)$. We refer the reader to [25] for a comprehensive description of how to learn $\mathbf{s}(\mathbf{x})$. In summary, the method involves training a neural network model (e.g., a UNet [26]) using the score matching technique [27–29] to estimate the score of a distribution.

2.2 Sampling the parameters of the forward model

Our goal is to generate samples of the parameters of the forward model, $\boldsymbol{\eta} \in \mathbb{R}^l$, based on the likelihood function. The data-generating process can be written as

$$\mathbf{x} = \mathbf{M}(\boldsymbol{\eta}) + \mathbf{N}; \quad (1)$$

where $\mathbf{M}(\boldsymbol{\eta})$ encodes the signal (the forward model) as a function of the parameters of interest $\boldsymbol{\eta}$ and \mathbf{N} is a vector of additive noise. A particular observation could be written as $x_0 = \mathbf{M}(\boldsymbol{\eta}_{\text{True}}) + \mathbf{N}_0$, where \mathbf{N}_0 is the true (but unknown) realization of noise.

Since here we are only considering non-stochastic forward models, the likelihood $P(x_0|\boldsymbol{\eta})$ can be written as

$$P(x_0|\boldsymbol{\eta}) = Q(x_0 - \mathbf{M}(\boldsymbol{\eta})); \quad (2)$$

where Q is the probability density of noise.

If we can compute the score of the likelihood with respect to the model parameters $\nabla_{\boldsymbol{\eta}} \log Q$, we can sample from the underlying likelihood function, $Q(x_0 - \mathbf{M}(\boldsymbol{\eta}))$, using gradient-based sampling methods [23, 25, 30, 31]. To get the score of the likelihood in the parameters of the model, we use the chain rule to write:

$$\nabla_{\boldsymbol{\eta}} \log Q = \nabla_{\mathbf{x}} \log Q \nabla_{\boldsymbol{\eta}} \mathbf{x}; \quad (3)$$

Here, $\nabla_{\mathbf{x}} \log Q$ is the score of the noise model with respect to the pixel values, which is the variable learned by the neural network score function and $\nabla_{\boldsymbol{\eta}} \mathbf{x}$ is the gradient of the pixel values with respect to the variables of interest $\boldsymbol{\eta}$. Since the pixel values only change when the model $\mathbf{M}(\boldsymbol{\eta})$ changes, this is equivalent to $\nabla \mathbf{M} = \nabla_{\boldsymbol{\eta}}$, which is the Jacobian of the forward model.

Afterwards, we can generate samples from the likelihood function using a chosen sampling method. In this work, we use the unadjusted Langevin sampling algorithm

$$\boldsymbol{\eta}_{t+1} = \boldsymbol{\eta}_t + \nabla_{\boldsymbol{\eta}} \log Q(x_0 - \mathbf{M}(\boldsymbol{\eta})) + \frac{\rho}{2} \boldsymbol{\xi}_t; \quad (4)$$

where ρ is the step size and $\boldsymbol{\xi}_t \sim N(0; \mathbf{1})$ is a random variable drawn from an l -dimensional multivariate normal distribution.

To summarize, the procedure to perform inference with SLIC involves:

1. Learning a score model for the distribution of noise in the data space, $\mathbf{s}(\mathbf{x}) = \nabla_{\mathbf{x}} \log Q(\mathbf{x})$.
2. Calculating the Jacobian of the forward model, $\nabla \mathbf{M} = \nabla_{\boldsymbol{\eta}}$.
3. Use a gradient-based sampling algorithm, such as the unadjusted langevin sampling algorithm, to perform inference using equation 3 to construct the likelihood function.

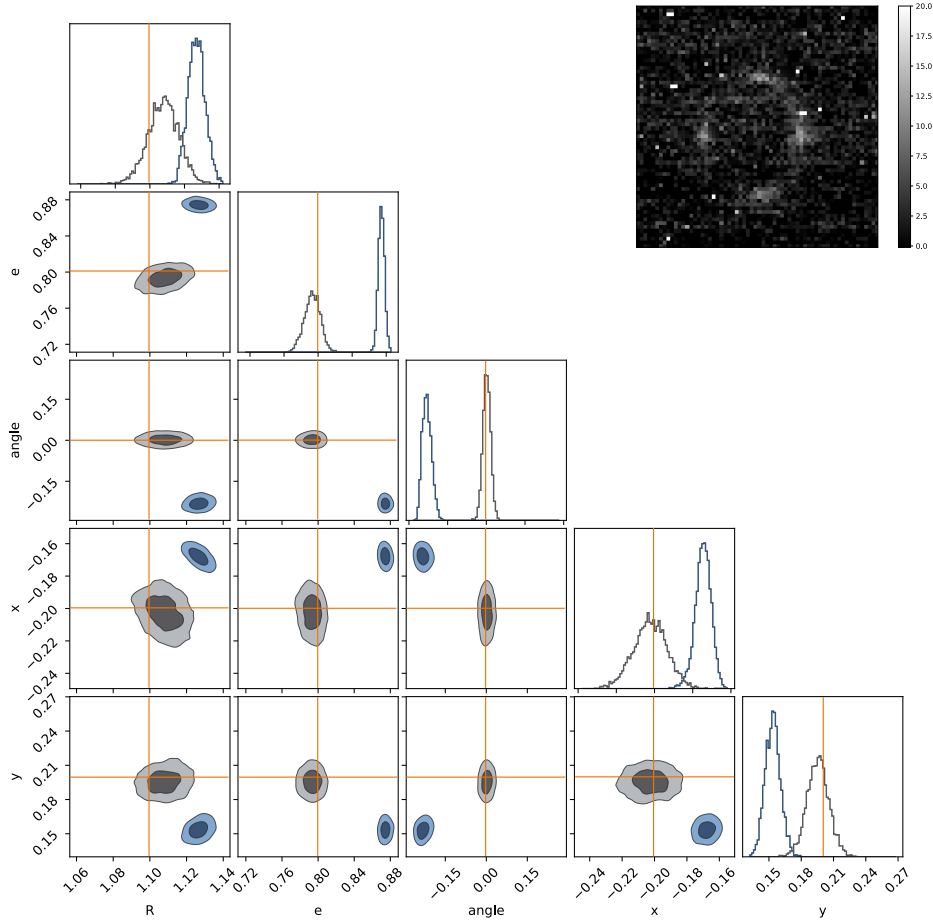


Figure 1: The analysis of a gravitational lensing signal with noise taken from *JWST* data. The data is shown on the top panel (in linear intensity units). The gray contours show samples generated with SLIC and the dark blue contours show biased results when a Gaussian likelihood is sampled.

3 Experiments and results

In this section, we present the results of our experiments to model and sample likelihood functions in the presence of non-Gaussian noise using SLIC. We use *Hubble Space Telescope (HST)* and *James Webb Space Telescope (JWST)* imaging data, publicly available at <https://archive.stsci.edu/> and <https://hla.stsci.edu/>, to test the proposed framework. We also compare the samples from our likelihood to those generated from a Gaussian likelihood with an MCMC sampler.

For *JWST*, we use five 2048 \times 2048 stage-2 calibrated exposure-based images to produce empty noise cutouts. In total, we produce a set of approximately 800 128×128 *JWST* images to train the score model. For *HST*, we use around 50 different snapshots mainly consisting of background noise and cosmic rays, and produce a second training set of approximately 150000 64×64 *HST* cutouts.

To produce simulated observations with real non-Gaussian *HST* and *JWST* noise, we inject the signal of a strongly lensed galaxy into real noise samples. The signal is produced by distorting the image of a Sérsic background source by the gravity of a Singular Isothermal Ellipsoid (SIE) foreground structure. Our gravitational lensing model is implemented in JAX and is fully differentiable, allowing us to easily calculate the Jacobian of the model. Our goal is to infer the parameters of the foreground model (mass, ellipticity, orientation angle, position x and y).

We use Langevin dynamics to produce 2000 samples from the SLIC likelihood functions using equation 4, with a step size of $\epsilon = 10^{-5}$, and compare our results for both the *HST* and *JWST* examples using a Gaussian likelihood in Figure 1 and 4.

In Figure 2, we show results of a coverage probability test calculated using 200 different realizations of *HST* noise. In every experiment, we use the same ground truth parameters but add different realizations of noise to the signal and obtain the corresponding SLIC likelihood. The coverage probabilities are calculated using the method proposed by Lemos et al. [32].

We also visually assess the quality of the score models performance by generating new realizations of noise using the method described in Song et al. [25]. Figure 3 of section A shows examples of real *HST* and *JWST* noise along with noise realizations generated from the score model.

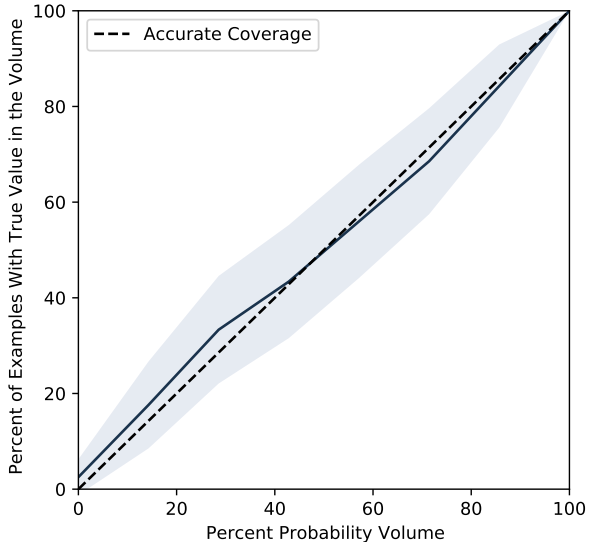


Figure 2: The coverage probability calculated by estimating the SLIC likelihoods for 200 different realizations of *HST* noise for a signal similar to that of figure 4 from section A. The 3σ error region (shaded) is calculated using jackknifing. The trend of following the dashed diagonal line shows that the likelihood is accurate (unbiased).

4 Discussion and conclusion

Our experiments show that by modeling the empirical distribution of noise and having access to differentiable forward models, it is possible to build accurate likelihood models for highly non-Gaussian noise, resulting in accurate inference without the need for major approximations.

As shown in Figure 1 and 4, the procedure provides likelihoods with high accuracy while maintaining the precision and the information content of the data. Note that the framework is not only limited to instrumental noise and can also be used to treat any other sources of additive errors. Additionally, while we demonstrated the method using gravitational lensing as an example, the framework is general and can be used for inference with any differentiable forward model.

The proposed framework also offers the advantage of utilizing the learned noise models for generating new noise realizations, as shown in Figure 3. These simulations can be used to train other inference models (e.g., in the context of simulation-based inference).

While in this work we used an unadjusted Langevin method to produce samples from the score of the likelihood, it is also possible to use Hamiltonian MCMC to sample the non-Gaussian likelihoods using only the score of the distribution [e.g., see 31].

We conclude by summarizing that given a set of possibly highly non-Gaussian noise realizations, SLIC provides a framework to use a score-based generative model to characterize the likelihood, allowing accurate analysis of highly non-Gaussian likelihoods without approximations that result in biases or loss of precision.

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A Supplementary Material

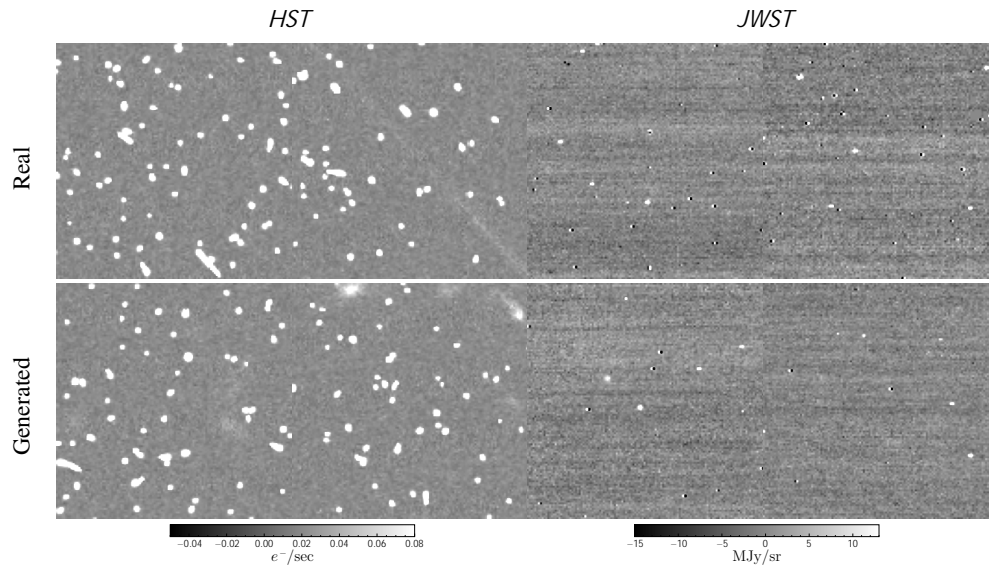


Figure 3: *Top row*: Examples of noise patches from the datasets. *Bottom row*: Examples of noise patches generated using the score models used in this work. These examples are generated by solving a reverse-time variance-exploding stochastic differential (VESDE, [25]) equation with 1000 steps of the discretized Euler-Maruyama solver.

