Application Log 1

Hanzhang Yin

September 4, 2024

[1] chung2024diffusionposteriorsamplinggeneral.

Background Summary

Note that Diffusion models have recently emerged as effective generative solvers for inverse problems, used in high-quality image reconstruction (i.e. image super-resolution tasks). This work extends diffusion models to solve general noisy (non)linear inverse problems by approximating posterior sampling. This results in a more effective generative path integrating noise statistics like Gaussian and Poisson. The approach efficiently handles complex issues, such as Fourier phase retrieval and non-uniform deblurring, surpassing previous methods in noisy settings.

Mathematical Content

MACHINE LEARNING MODEL (SCORE-BASED DIFFUSION MODELS): Diffusion models define the generative process as the reverse of the noising process. It Contains the forward and reverse (backward) diffusion process (NOTE: diffusion model aims to solve an ill-posed Inverse Problems):

• In the forward diffusion process, a data glitch is gradually perturbed by adding Gaussian noise over a sequence of time slices. This process transforms the original data distribution to a Gaussian-like distribution.

$$x_t = \sqrt{\bar{a}(t)}x_0 + \sqrt{1 - \bar{a}(t)}z, z \sim N(0, I)$$

(NOTE: x_0 is the original data, x_t is the perturbed data at time t, and z is the Gaussian noise. The term $\bar{a}(t)$ controls the amount of noise added at each time slice.)

• In the reverse diffusion process, the goal of the scored-based diffusion model is to learn how to reverse the forward diffusion process to generate new data samples from noise. This reverse diffusion process is an SDE or a discrete-time Markov chain. The model learns the score function at each time step:

$$\nabla_{x_t} \log p(x_t) \approx s_{\theta}^*(x_t, t)$$

APPROXIMATION OF THE LIKELIHOOD: The approximation technique here utilizes "Bayesian Net' and "Monte-Carlo" random process. Noting that approximations are made to simplify calculations:

$$p(y|x_t) \approx p(y|\hat{x}_0), \text{ where } \hat{x}_0 := E[x_0|x_t]$$

The expectation \hat{x}_0 is the proxy for most likely original data given the noisy observation. In further mathematical proof, the diffusion model applied "Jensen's Inequality" and "Jensen gap" to quantify the approximation value for validity and higher accuracy.

OPTIMIZATION ALGORITHM: For score-based model training, the article is aimed at minimizing a score-matching loss function that encourages the NNs to learn the true score function $\nabla_{x_t} \log p(x_t)$ of the data distribution at each time step.

$$\theta^* = \arg\min_{\theta} E_{t,x(t),x(0)} \left[\| s_{\theta}(x(t),t) - \nabla_{x_t} \log p(x(t)|x(0)) \|_2^2 \right]$$

The article aims to minimize the expectation of differences based on the random variables on the set parameters θ : t (time from a certain distribution), x(t) (The noisy data sample at time t, generated by the forward diffusion process), x(0) (The original clean data sample at time before any noise is added).

The differences is calculated between $s_{\theta}(x(t), t)$, the neural network parameterized by θ to approximate the score function (i.e. "true distribution"); and $\nabla_{x_t} \log p(x(t)|x(0))$, the score function aims to approximate)

Suggested In-Course Beneficial Mathematical Content

Partial Derivatives, Differential Equation, \cdots : Might be beneficial for diffusion model and optimization algorithm understanding.

Matrix Operations, Eigenvalues, and Eigenvectors, Taylor Expansions, gra: Might be useful to understand the TensorFlow after linear transformation of the data and analyzing the convergence path for the iterative model behind the suggested score-based diffusion model.

Gaussian and Poisson Distribution, Posterior Distribution: Might be crucial to understanding such probabilistic reasoning and proofs behind the diffusion model.

Monte Carlo Methods: Might be important to understand the sampling configurations on the dataset (e.g. ImageNet). In some respect, they can be combined with "Molecular Dynamics" simulations to enhance sampling efficiency.