

On the Mathematics of Diffusion Models

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Abstract

This paper attempts to present the stochastic differential equations of diffusion models in a manner that is accessible to a broad audience. The diffusion process is defined over a population density $\text{pop}(y)$ for $y \in \mathcal{R}^d$. Of particular interest is a population of images. In a diffusion model one first defines a diffusion process that starts from a sample $y \in \mathcal{R}^d$ and gradually adds noise until only noise remains. The fundamental idea is to sample from the population by a reverse-diffusion process mapping pure noise to a population sample. The diffusion process is defined independent of any “interpretation” but can be analyzed using the mathematics of variational auto-encoders (the “VAE interpretation”) or the Fokker-Planck equation (the “score matching interpretation”). Both analyses yield reverse-diffusion methods involving the score function $\nabla_z \log p_t(z) = (E[y|t, z(t)] - z)/t$. The Fokker-Planck analysis yields a family of reverse-diffusion SDEs parameterized by any desired reverse-diffusion noise level including zero (deterministic reverse-diffusion). The VAE analysis yields the reverse-diffusion SDE at the same noise level as the diffusion SDE. The VAE analysis also yields a useful expression for $\log \text{pop}(y)$ for any given y which does not seem to follow naturally from the Fokker-Planck analysis. Most, but apparently not all, of the mathematics presented here can be found in the literature. Attributions are given at the end of the paper.

1 The Diffusion Stochastic Differential Equation (SDE)

We assume a population density $\text{pop}(y)$ for $y \in \mathcal{R}^d$. Of particular interest is a population of images. For a given time resolution Δt we consider the discrete-time process $z(0), z(\Delta t), z(2\Delta t), z(3\Delta t), \dots$ defined by

$$\begin{aligned} z(0) &= y, \quad y \sim \text{pop}(y) \\ z(t + \Delta t) &= z(t) + \sqrt{\Delta t} \epsilon, \quad \epsilon \sim \mathcal{N}(0, I) \end{aligned} \tag{1}$$

Taking (1) to the limit of $\Delta t \rightarrow 0$ is the diffusion SDE. For $\epsilon \sim \mathcal{N}(0, I)$ each coordinate of the random variable $\sqrt{\Delta t} \epsilon$ has standard deviation $\sqrt{\Delta t}$ and variance Δt . A sum of Gaussians is a Gaussian with variance equal to the sum of the variances. This implies that the variance of the coordinates of $z(n\Delta t)$ conditioned on $z(0)$ is $n\Delta t$. Taking this to limit as $\Delta t \rightarrow 0$ we get that the variance of the coordinates of $z(t)$ given $z(0)$ is t . More generally in the limit of $\Delta t \rightarrow 0$ equation (1) holds for sampling $z(t + \Delta t)$ given $z(t)$ for any (continuous) non-negative t and Δt .

2 The VAE Analysis

We first review general variational auto-encoders (VAEs). Let $\text{pop}(y)$ be any population distribution or density on any set \mathcal{Y} . Let $p(z|y)$ be any distribution or density on any set \mathcal{Z} conditioned on $y \in \mathcal{Y}$. For the joint distribution defined by $\text{pop}(y)$ and $p(z|y)$ we have the following for $p(y, z) > 0$ and where $p_{\text{pop}}(z)$ and

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