

# 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  $\ln \text{pop}(y)$  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  $\Delta t$  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  $\Delta t$ . 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  $\Delta t$ .

## 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

# Mathematics Of Diffusion

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