DEPARTMENT OF COMPUTER SCIENCE

Video Diffusion Models for Climate Simulations

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Abstract

Dedication and Acknowledgements

Declaration

I declare that the work in this dissertation was carried out in accordance with the requirements of the University's Regulations and Code of Practice for Taught Programmes and that it has not been submitted for any other academic award. Except where indicated by specific reference in the text, this work is my own work. Work done in collaboration with, or with the assistance of others, is indicated as such. I have identified all material in this dissertation which is not my own work through appropriate referencing and acknowledgement. Where I have quoted or otherwise incorporated material which is the work of others, I have included the source in the references. Any views expressed in the dissertation, other than referenced material, are those of the author.

George Herbert, Sunday 26$^{\text{th}}$ March, 2023

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2.1 Diffusion Models

Diffusion models are

Given observed datapoints $\mathbf{x}$, the goal of a generative model is to learn to model its true data distribution $p(\mathbf{x})$.

2.1.1 Forward Diffusion Process

The *forward process* is a Gaussian diffusion process that defines a sequence of increasingly noisy versions of $\mathbf{x}$, which we call the *latent variables*:

$$\mathbf{z} = \{\mathbf{z}_t \mid t \in [0,1]\} \tag{2.1}$$

The forward process forms a conditional joint distribution $q(\mathbf{z}|\mathbf{x})$, whose marginal distributions of latent variables $\mathbf{z}_t$ given $\mathbf{x} \sim p(\mathbf{x})$ are given by:

$$q(\mathbf{z}_t|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}_t; \alpha_t \mathbf{x}, \sigma_t^2 \mathbf{I}\right) \tag{2.2}$$

where α_t and σ_t are strictly positive scalar-valued functions of t.

A notable aspect of the forward process is that the joint distribution of latent variables $\mathbf{z}_r, \mathbf{z}_s, \mathbf{z}_t$ at subsequent timesteps $0 \leq r < s < t \leq 1$ is Markovian:

$$q(\mathbf{z}_t|\mathbf{z}_s, \mathbf{z}_r) = q(\mathbf{z}_t|\mathbf{z}_s) = \mathcal{N}\left(\mathbf{z}_t; \alpha_{t|s}\mathbf{z}_s, \sigma_{t|s}^2 \mathbf{I}\right) \tag{2.3}$$

where $\alpha_{t|s} = \alpha_t \alpha_s^{-1}$ and $\sigma_{t|s}^2 = \sigma_t^2 - \alpha_{t|s}^2 \sigma_s^2$. A full derivation of $q(\mathbf{z}_t|\mathbf{z}_s)$ is given in Appendix A.1.

2.1.2 Reverse Generative Model

The generative model is a learned hierarchical model that matches the forward process running in reverse-time: we sequentially generate latent variables $\mathbf{z}_t$ starting from $t = 1$ and working backwards to $t = 0$.

Assuming our diffusion model is variance preserving (i.e. $\alpha_t = \sqrt{1 - \sigma_t^2}$) and $\alpha_1 \approx 0$, we can model the marginal distribution of $\mathbf{z}_1$ as the multivariate standard Gaussian:

$$p(\mathbf{z}_1) \approx \mathcal{N}(\mathbf{z}_1; \mathbf{0}, \mathbf{I}) \tag{2.4}$$

2.1.3 Noise Schedule

We formalise the notion that $\mathbf{z}_t$ is increasingly noisy by defining a log signal-to-noise ratio $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ as a strictly monotonically decreasing function of time $t \in [0,1]$.

$$\lambda(t) = \log\left(\frac{\alpha_t^2}{\sigma_t^2}\right) \tag{2.5}$$

The *noise schedule* is a critical aspect of the diffusion model. It maps the time variable $t \in [0,1]$ to a log-signal-to-noise ratio $\lambda \in [\lambda_{\min}, \lambda_{\max}]$.

2.2 Climate Simulations

Bibliography

Appendix A

Diffusion Models

A.1 Derivation of $q(\mathbf{z}_t|\mathbf{z}_s)$

From Equation 2.2, we know $q(\mathbf{z}_t|\mathbf{x})$ is an isotropic Gaussian probability density function. As such, we can sample $\mathbf{z}_t \sim q(\mathbf{z}_t|\mathbf{x})$ by sampling $\boldsymbol{\epsilon}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ from the multivariate standard Gaussian distribution and computing:

$$\mathbf{z}_t = \alpha_t \mathbf{x} + \sigma_t \boldsymbol{\epsilon}_t \tag{A.1}$$

With some algebraic manipulation, we can show that:

$$\begin{align}
\mathbf{z}_t &= \alpha_t \mathbf{x} + \sqrt{\sigma_t^2} \boldsymbol{\epsilon}_t \tag{A.2}\\
&= \alpha_t \mathbf{x} + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2 + \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t \tag{A.3}\\
&= \alpha_t \mathbf{x} + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2 + \left(\frac{\alpha_t}{\alpha_s}\sigma_s\right)^2} \boldsymbol{\epsilon}_t \tag{A.4}
\end{align}$$

The sum of two independent Gaussian random variables with mean μ_1 and μ_2 and variance σ_1^2 and σ_2^2 is a Gaussian random variable with mean $\mu_1 + \mu_2$ and variance $\sigma_1^2 + \sigma_2^2$. As such, we can manipulate the above equation further to show that:

$$\begin{align}
\mathbf{z}_t &= \alpha_t \mathbf{x} + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t^* + \frac{\alpha_t}{\alpha_s}\sigma_s \boldsymbol{\epsilon}_s \tag{A.5}\\
&= \alpha_t \mathbf{x} + \frac{\alpha_t}{\alpha_s}\sigma_s \boldsymbol{\epsilon}_s + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t^* \tag{A.6}\\
&= \frac{\alpha_s}{\alpha_s}\alpha_t \mathbf{x} + \frac{\alpha_t}{\alpha_s}\sigma_s \boldsymbol{\epsilon}_s + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t^* \tag{A.7}\\
&= \frac{\alpha_t}{\alpha_s}(\alpha_s \mathbf{x} + \sigma_s \boldsymbol{\epsilon}_s) + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t^* \tag{A.8}\\
& \tag{A.9}
\end{align}$$

where $\boldsymbol{\epsilon}_t^*, \boldsymbol{\epsilon}_s \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ are similarly both sampled from the multivariate standard Gaussian distribution. We can substitute $\mathbf{z}_s = \alpha_s \mathbf{x} + \sigma_s \boldsymbol{\epsilon}_s$ into the above equation to show that:

$$\begin{align}
\mathbf{z}_t &= \frac{\alpha_t}{\alpha_s}\mathbf{z}_s + \sqrt{\sigma_t^2 - \frac{\alpha_t^2}{\alpha_s^2}\sigma_s^2} \boldsymbol{\epsilon}_t^* \tag{A.10}\\
&= \alpha_{t|s}\mathbf{z}_s + \sigma_{t|s}\boldsymbol{\epsilon}_t^* \tag{A.11}\\
&\sim \mathcal{N}\left(\mathbf{z}_t; \alpha_{t|s}\mathbf{z}_s, \sigma_{t|s}^2 \mathbf{I}\right) \tag{A.12}
\end{align}$$

The subscript $t|s$ relates to the fact that $\alpha_{t|s}$ and $\sigma_{t|s}$ define the parameters of the Gaussian probability density function $q(\mathbf{z}_t|\mathbf{z}_s)$.