TTIC 31230, Fundamentals of Deep Learning

David McAllester, Autumn 2023

The Mathematics of Diffusion Models

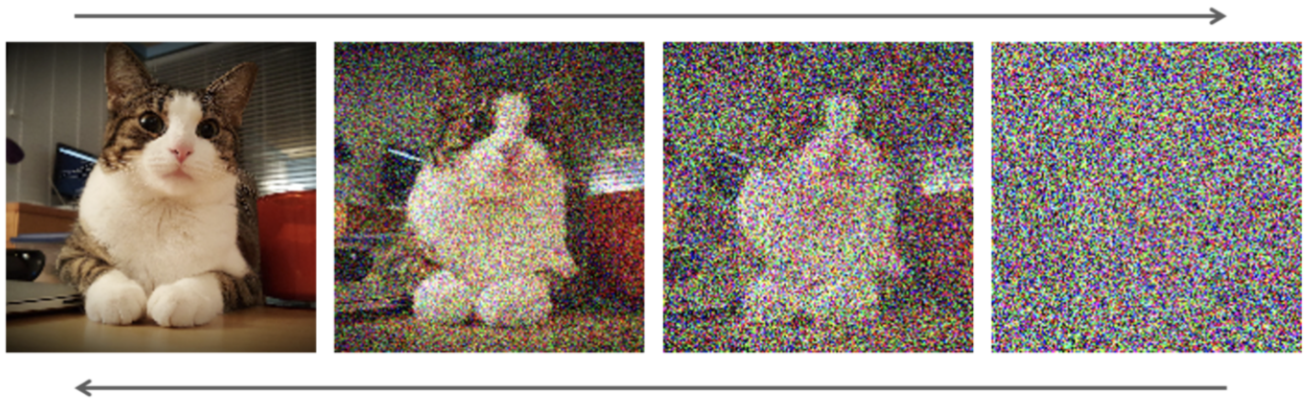
McAllester, arXiv January 2023

Denoising Diffusion Probabilistic Models (DDPM)

Ho, Jain and Abbeel, June 2020

Markovian VAEs

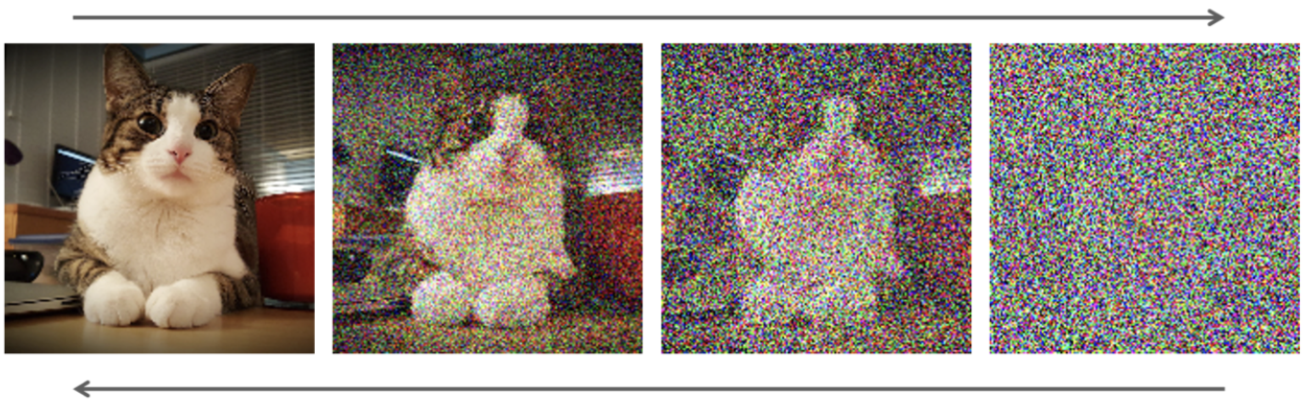
A diffusion models computes and inverts a sequence



So does an autoregressive language model

$$\text{[Sally talked to John]} \rightleftarrows \text{[Sally talked to]} \rightleftarrows \text{[Sally talked]} \rightleftarrows \text{[Sally]}$$

Markovian VAEs



[Sally talked to John] $\rightleftarrows$ [Sally talked to] $\rightleftarrows$ [Sally talked] $\rightleftarrows$ [Sally]

$$y \rightleftarrows z_1 \rightleftarrows \cdots \rightleftarrows z_N$$

Markovian VAEs

$$y \rightleftarrows z_1 \rightleftarrows \cdots \rightleftarrows z_N$$

Encoder: $\mathrm{Pop}(y)$, $P_{\mathrm{enc}}(z_1|y)$, and $P_{\mathrm{enc}}(z_{\ell+1}|z_\ell)$.

Generator: $P_{\mathrm{pri}}(z_N)$, $P_{\mathrm{gen}}(z_{\ell-1}|z_\ell)$, $P_{\mathrm{gen}}(y|z_1)$.

The encoder and the decoder define distributions $P_{\mathrm{enc}}(y, \ldots, z_N)$ and $P_{\mathrm{gen}}(y, \ldots, z_N)$ respectively.

The Markovian ELBO

$$
\begin{aligned}
H(y) &= E_{\mathrm{enc}}\left[-\ln\frac{P_{\mathrm{enc}}(y)P_{\mathrm{enc}}(z_1,\ldots,z_N|y)}{P_{\mathrm{enc}}(z_1,\ldots,z_N|y)}\right] \\
&= E_{\mathrm{enc}}\left[-\ln\frac{P_{\mathrm{enc}}(y|z_1)P_{\mathrm{enc}}(z_1|z_2)\cdots P_{\mathrm{enc}}(z_{N-1}|z_N)P_{\mathrm{enc}}(z_N)}{P_{\mathrm{enc}}(z_1|z_2,y)\cdots P_{\mathrm{enc}}(z_{N-1}|z_N,y)P_{\mathrm{enc}}(z_N|y)}\right] \\
&\leq E_{\mathrm{enc}}\left[-\ln\frac{P_{\mathrm{gen}}(y|z_1)P_{\mathrm{gen}}(z_1|z_2)\cdots P_{\mathrm{gen}}(z_{N-1}|z_N)P_{\mathrm{gen}}(z_N)}{P_{\mathrm{enc}}(z_1|z_2,y)\cdots P_{\mathrm{enc}}(z_{N-1}|z_N,y)P_{\mathrm{enc}}(z_N|y)}\right] \\
&= \left\{\begin{array}{l}
E_{\mathrm{enc}}\left[-\ln P_{\mathrm{gen}}(y|z_1)\right] \\[2ex]
+\sum_{i=2}^{N}\ E_{\mathrm{enc}}\ KL(P_{\mathrm{enc}}(z_{i-1}|z_i,y),\ P_{\mathrm{gen}}(z_{i-1}|z_i)) \\[2ex]
+E_{\mathrm{enc}}\ KL(P_{\mathrm{enc}}(Z_N|y),p_{\mathrm{gen}}(Z_N))
\end{array}\right.
\end{aligned}
$$

Markovian VAEs

$$y \overset{\rightarrow}{\leftarrow} z_1 \overset{\rightarrow}{\leftarrow} \cdots \overset{\rightarrow}{\leftarrow} z_N$$

- autoregressive models

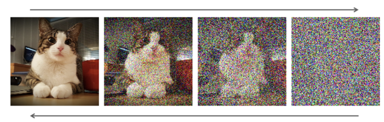
- diffusion models

- StyleGan? (layers of resolution)

- U-Nets? (layers of resolution)

A grand unified theory (GUT) of generative AI?

Diffusion Models



Consider a discrete time process $z(0), z(\Delta t), z(2\Delta t), z(3\Delta t), \ldots$

$$z(0) \;=\; y, \quad y \sim \mathrm{Pop}(y)$$

$$z(t+\Delta t) \;=\; z(t) + \epsilon\sqrt{\Delta t}, \quad \epsilon \sim \mathcal{N}(0, I)$$

A sum of two Gaussians is a Gaussian whose **variance** is the sum of the two variances.

$$z(t+n\Delta t) = z(t) + \sqrt{n\Delta t}\,\epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

Here $\sqrt{n\Delta t}$ is the **standard deviation** of the added noise.

SDE Notation

In these slides ϵ will be a random variable drawn from $\mathcal{N}(0, I)$.

This correspods to "dB" in standard notation for SDEs.

$$
\begin{aligned}
z(t + \Delta t) &= z(t) + \mu(z,t)\Delta t + \sigma(z,t)\epsilon\sqrt{\Delta t} \\
dz &= \mu(z,t)dt + \sigma(z,t)dB
\end{aligned}
$$

The first expression is longer but seems clearer to me.

The SDE denotes the limit as Δt in the first equation goes to zero.

The Diffusion SDE

For the diffusion process (Brownian motion) we have

$$\begin{aligned} z(0) &= y, \quad y \sim \mathrm{Pop}(y) \\ z(t+\Delta t) &= z(t) + \epsilon\sqrt{\Delta t} \qquad (1) \\ dz &= dB \end{aligned}$$

For diffusion we get that (1) holds for all t and Δt.

Probability Notation

In these slides unsubscripted probability notation, such as

$$P(z(t + \Delta t)|z(t)),$$

or a conditional expectation such as

$$E[f(y)|z(t)] = E_{y\sim P(y|z_t)}[f(y)],$$

refer the joint distribution on y and $z(t)$ defined by diffusion.

Markovian ELBO

For any Markovian VAE we have

$$-\ln \mathrm{Pop}(y) \;=\; -\ln \frac{P(z_N)P(z_{N-1}|z_N)\cdots P(z_1|z_2)P(y|z_1)}{P(z_N|y)P(z_{N-1}|z_N,y)\cdots P(z_1|z_2,y)}$$

$$H(y) \;=\; \begin{cases} E[KL(P(z_N|y),\;P(z_N))] \\ \\ +\sum_{i=2}^{N}\;E[KL(P(z_{i-1}|z_i,y),\;P(z_{i-1}|z_i))] \\ \\ +\;E[\ln -P(y|z_1)] \end{cases} \tag{2}$$

$$\leq \;\begin{cases} E[KL(P(z_N|y),\;P_{\mathrm{gen}}(z_N))] \\ \\ +\sum_{i=2}^{N}\;E[KL(P(z_{i-1}|z_i,y),\;P_{\mathrm{gen}}(z_{i-1}|z_i))] \\ \\ E[-\ln P_{\mathrm{gen}}(y|z_1)] \end{cases} \tag{3}$$

Reverse-Time Probabilities

In the limit of small Δt it is possible to derive the following.

$$P(z(t-\Delta t)|z(t), y) = \mathcal{N}\left(z(t) + \frac{\Delta t(y - z(t))}{t},\;\; \Delta t I \right)$$

$$P(z(t-\Delta t)|z(t)) = \mathcal{N}\left(z(t) + \frac{\Delta t(E[y|t, z(t)] - z(t))}{t},\;\; \Delta t I \right)$$

The Reverse-Diffusion SDE

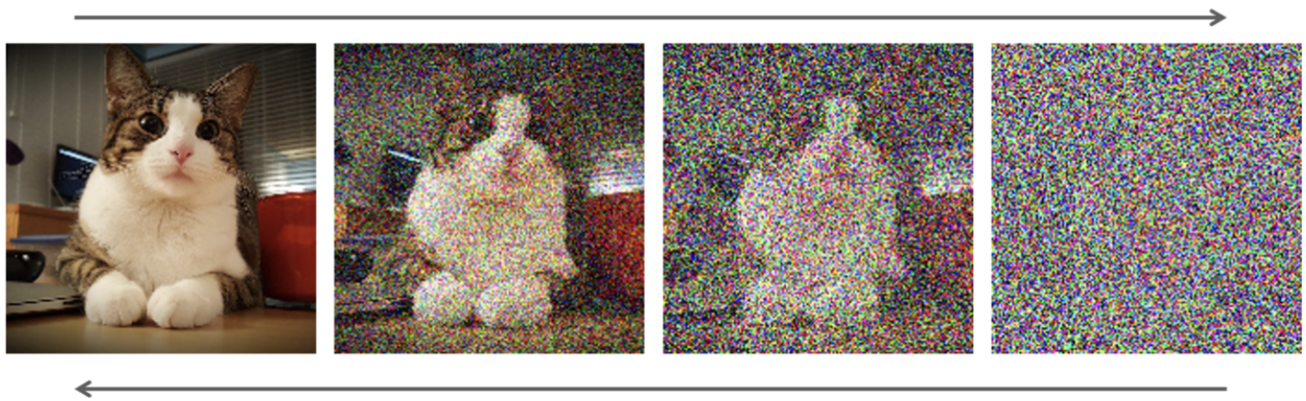
$$P(z(t-\Delta t)|z(t)) = \mathcal{N}\left(z(t) + \frac{\Delta t(E[y|t,z(t)]-z(t))}{t}, \Delta t I \right)$$

This equation defines a reverse-diffusion SDE which we can write as

$$z(t-\Delta t) = z(t) + \left(\frac{E[y|t,z(t)] - z(t)}{t}\right)\Delta t + \epsilon\sqrt{\Delta t}$$

Understanding Reverse Diffusion

$$z(t-\Delta t) = z(t) + \left(\frac{E[y|t, z(t)] - z(t)}{t}\right)\Delta t + \epsilon\sqrt{\Delta t}$$



$E[y|t, z]$ is averaging over many possible source images y.

Estimating $E[y|t, z(t)]$

$$z(t - \Delta t) = z(t) + \left(\frac{E[y|t, z(t)] - z(t)}{t}\right)\Delta t + \epsilon\sqrt{\Delta t}$$

We can train a denoising network $\hat{y}(t, z)$ to estimate $E[y|t, z(t)]$ using

$$\hat{y}^*(t, z) = \underset{\hat{y}}{\mathrm{argmin}}\;\; E\;(\hat{y}(t, z(t)) - y)^2$$

Assuming universality $\hat{y}^*(t, z) = E[y|t, z]$.

Estimating $E[y|t, z(t)]$

If the population values are scaled so as to have scale 1, then the scale of $z(t)$ is $\sqrt{1+t}$.

$$\hat{y}^* = \operatorname*{argmin}_{\hat{y}} E_{t,z(t)} \left(\hat{y}(t, z/\sqrt{1+t}) - y\right)^2$$

$$\hat{E}[y|t, z(t)] \; = \; \hat{y}^*(t, z/\sqrt{1+t}))$$

KL-Divergence

$$H(y) \; = \; \left\{ \begin{array}{l} E[KL(P(z_N|y),\; P(z_N))] \\ \\ +\sum_{i=2}^N \; E[KL(P(z_{i-1}|z_i,y),\; P(z_{i-1}|z_i))] \\ \\ +\; E[\ln -P(y|z_1)] \end{array} \right.$$

For two Gaussian distributions with the same isotropic covariance we have

$$KL\left(\,\mathcal{N}(\mu_1,\sigma^2 I),\mathcal{N}(\mu_2,\sigma^2 I)\,\right) = \frac{||u_1 - \mu_2||^2}{2\sigma^2}$$

KL-Divergence

$$H(y) \;=\; \begin{cases} E[KL(P(z_N|y),\; P(z_N))] \\ \\ +\sum_{i=2}^{N}\; E[KL(P(z_{i-1}|z_i, y),\; P(z_{i-1}|z_i))] \\ \\ +\; E[\ln - P(y|z_1)] \end{cases}$$

$$P(z(t-\Delta t)|z(t), y) \;=\; \mathcal{N}\left(\; z(t) + \frac{\Delta t(y - z(t))}{t},\;\; \Delta t I \;\right)$$

$$P(z(t-\Delta t)|z(t)) \;=\; \mathcal{N}\left(\; z(t) + \frac{\Delta t(E[y|t, z(t)] - z(t))}{t},\;\; \Delta t I \;\right)$$

KL-Divergences

$$P(z(t-\Delta t)|z(t),y) \;=\; \mathcal{N}\left(\; z(t) + \tfrac{\Delta t(y-z(t))}{t},\;\; \Delta t I \;\right)$$

$$P(z(t-\Delta t)|z(t)) \;=\; \mathcal{N}\left(\; z(t) + \tfrac{\Delta t(E[y|t,z(t)]-z(t))}{t},\;\; \Delta t I \;\right)$$

$$KL\left(\begin{array}{l} P(z(t-\Delta t)|z(t),y), \\ P(z(t-\Delta t)|z(t)) \end{array}\right) \;=\; \left(\frac{||y - E[y|t,z(t)]||^2 \Delta t^2}{2t^2 \Delta t}\right)$$

$$=\; \left(\frac{||y - E[y|t,z(t)]||^2}{2t^2}\right)\Delta t$$

KL-Divergences

$$H(y) = \begin{cases} E[KL(P(z_N|y),\ P(z_N))] \\ \\ +\sum_{i=2}^{N}\ E[KL(P(z_{i-1}|z_i, y),\ P(z_{i-1}|z_i))] \\ \\ +\ E[\ln -P(y|z_1)] \end{cases}$$

$$= \sum_{\substack{i=2 \\ t = i\Delta t}}^{N} \left(\frac{||y - E[y|t, z(t)]||^2}{2t^2} \right) \Delta t + E\left[-\ln P(y|z_1)\right]$$

Passing to the Integral

$$H(y) = \begin{cases} \int_{t_0}^{\infty} dt \;\; E_{z(t)|y} \left[\frac{||y - E[y|t, z(t)]||^2}{2t^2} \right] \\ + E_{z(t_0)|y}[-\ln P(y|z(t_0))] \end{cases}$$

$$H(y) = \begin{cases} \int_{t_0}^{\infty} dt \;\; E_{y, z(t_0)} \left[\frac{||y - E[y|t, z(t)]||^2}{2t^2} \right] \\ + H(y|z(t_0)) \end{cases}$$

Mutual Information

$$H(y) \; = \; \begin{cases} \int_{t_0}^{\infty} dt \;\; E_{y,z(t_0)} \;\; \left[\frac{||y-E[y|t,z(t)]||^2}{2t^2}\right] \\ \\ + \; H(y|z(t_0)) \end{cases}$$

$$H(y) - H(y|z(t_0)) \; = \; \int_{t_0}^{\infty} dt \;\; E_{y,z(t_0)} \;\; \left[\frac{||y - E[y|t,z(t)]||^2}{2t^2}\right]$$

$$I(y, z(t_0)) \; = \; \int_{t_0}^{\infty} dt \;\; E_{y,z(t_0)} \;\; \left[\frac{||y - E[y|t,z(t)]||^2}{2t^2}\right]$$

This is the information minimum mean squared error relation (I-MMSE) relation [Guo et al. 2005].

Computing Bits per Channel

$$I(y, z(t_0)) \;=\; \int_{t_0}^{\infty} dt \;\; E_{y,z(t_0)} \; \left[\frac{||y - E[y|t, z(t)]||^2}{2t^2} \right]$$

$$\leq \; \int_{t_0}^{\infty} dt \;\; E_{y,z(t_0)} \; \left[\frac{||y - \hat{E}[y|t, z(t)]||^2}{2t^2} \right]$$

The Fokker-Plack Anaylysis (The Score Function)

For $\epsilon \sim \mathcal{N}(0, I)$ a general SDE can be written as

$$z(t + \Delta t) = z(t) + \mu(z(t), t)\Delta t + \sigma(z(t), t)\epsilon\sqrt{\Delta t}$$

$$dz = \mu(z(t), t)dt + \sigma(z(t), t)dB$$

The diffusion process is the special case of Brownian motion

$$z(t + \Delta t) = z(t) + \epsilon\sqrt{\Delta t}$$
$$dz = dB$$

The Fokker-Planck Equation

Let $P_t(z)$ be the probability that $z(t) = z$.

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \left(\begin{array}{l} \mu(z(t), t) P_t(z) \\ \\ -\frac{1}{2}\sigma^2(z(t), t) \nabla_z P_t(z) \end{array} \right)$$

For the special case of diffusion we have

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \left(-\frac{1}{2} \nabla_z P_t(z) \right)$$

The Score Function

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \begin{pmatrix} \mu(z(t), t) P_t(z) \\ \\ -\frac{1}{2}\sigma^2(z(t), t) \nabla_z P_t(z) \end{pmatrix}$$

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \left(-\frac{1}{2} \nabla_z P_t(z) \right)$$

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \left[\left(-\frac{1}{2} \nabla_z \ln P_t(z) \right) P_t(z) \right]$$

The Score Function

$$\frac{\partial P_t(z)}{\partial t} = -\nabla \cdot \left[\left(-\frac{1}{2} \nabla_z \ln P_t(z) \right) P_t(z) \right]$$

$\ln P_t(z)$ is the score function.

The time evolution of $P_t(z)$ can be written as the result of **deterministic** flow given by

$$\frac{dz}{dt} = -\frac{1}{2} \nabla_z \ln p_t(z)$$

Deterministic Reverse Diffusion

Following the deterministic flow backward in time samples from the population!

$$z(t - \Delta t) = z(t) + \frac{1}{2} \nabla_z \ln p_t(z) \Delta t$$

No reverse diffusion noise!

Solving for the Score Function

$$
\begin{aligned}
P_t(z) &= E_y\ P_t(z|y) \\
&= E_y\ \frac{1}{Z(t)} e^{-\frac{||z-y||^2}{2t}} \\
\nabla_z P_t(z) &= E_y\ P_t(z|y)\ (y-z)/t \\
&= E_y \frac{P_t(z)P(y|t,z)}{P(y)}[(y-z)/t] \\
&= P_t(z) \int dy\ P(y|t,z)[(y-z)/t] \\
&= P_t(z) \frac{E[y|t,z]-z}{t} \\
\nabla_z \ln P_t(z) &= \frac{E[y|t,z]-z}{t}
\end{aligned}
$$

This is Tweedie's formula, Robbins 1956.

Stochastic vs. Deterministic Reverse Diffusion

$$z(t - \Delta t) \;=\; z(t) + \left(\frac{E[y|t, z(t)] - z(t)}{t}\right) \Delta t + \epsilon\sqrt{\Delta t}$$

$$z(t - \Delta t) \;=\; z(t) + \frac{1}{2}\left(\frac{E[y|t, z(t)] - z(t)}{t}\right) \Delta t$$

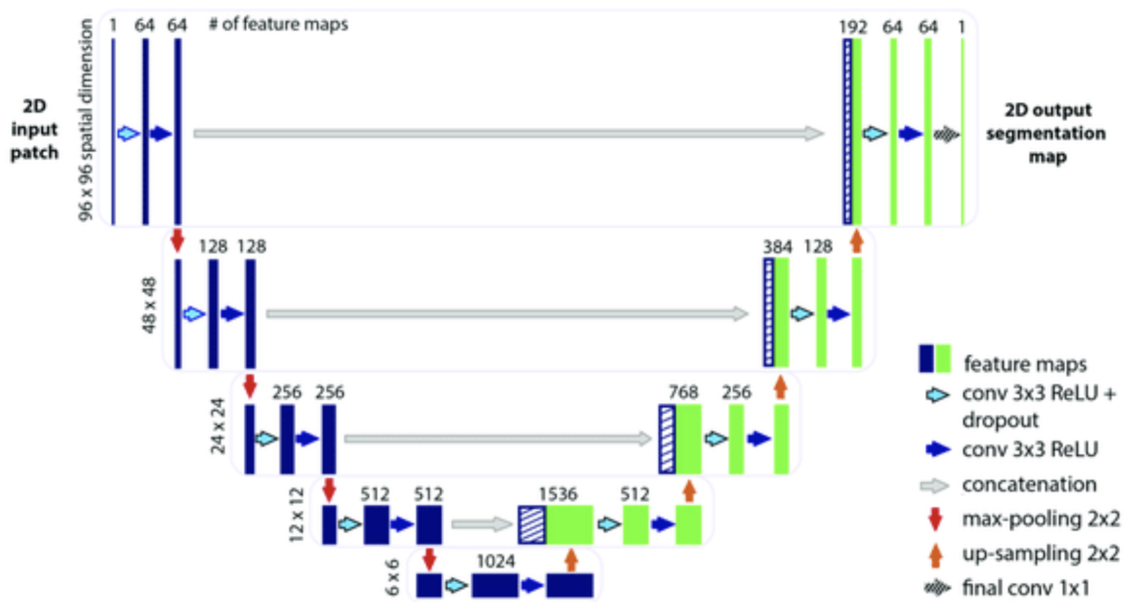
Interpolating Stochastic and Deterministic

One can show that for $\lambda \in [0, 1]$ the following also samples from the population.

$$z(t - \Delta t) = z(t) + \frac{1+\lambda}{2}\left(\frac{E[y|t, z(t)] - z(t)}{t}\right)\Delta t + \lambda\epsilon\sqrt{\Delta t}$$

$\hat{y}(t, z)$ is a U-Net

In practice $\hat{y}(t, z)$ is computed with a U-Net.



The U-Nets themselves seem closely related to Markovian VAEs.

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