# TTIC 31230, Fundamentals of Deep Learning

David McAllester, Autumn 2023

The Mathematics of Diffusion Models

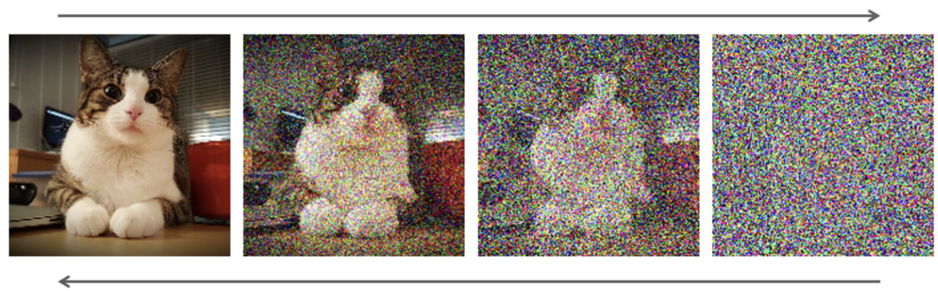
McAllester, arXiv January 2023

## Diffusion Models

Deep unsupervised learning using nonequilibrium thermodynamics
Sohl-Dickstein et al., 2015.

Denoising Diffusion Probabilistic Models (DDPM)
Ho, Jain and Abbeel, June 2020

# Diffusion Models

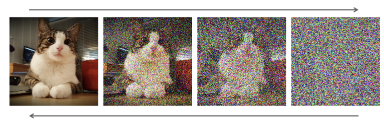


Consider a discrete time process $z(0), z(\Delta t), z(2\Delta t), z(3\Delta t), \ldots$

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

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

# Diffusion Models



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

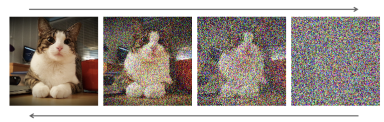
$$z(t+\Delta t) \;=\; z(t) + \epsilon\sqrt{\Delta t}, \quad \epsilon \sim \mathcal{N}(0, I)$$

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

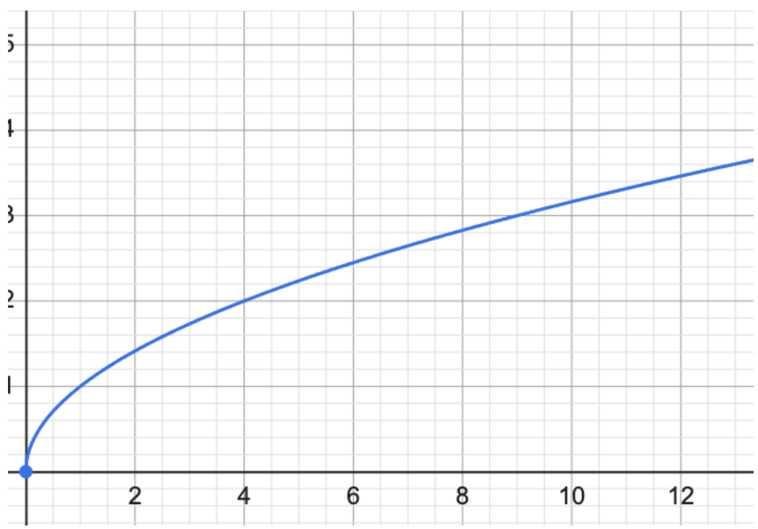
$$z(t+n\Delta t) = z(t) + \sqrt{n\Delta t}\,\epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

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

# Diffusion Models



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




$z(t)$ $z(t) + n\Delta t$

## SDE Notation

In these slides $\epsilon$ 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 $\Delta t$ 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 $\Delta t$.

## 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.

# The Hierarchical ELBO

$$H(y) = E_{\text{enc}}\left[-\ln \frac{P(y)P_{\text{enc}}(z|y)}{P_{\text{enc}}(z|y)}\right] = E_{\text{enc}}\left[-\ln \frac{P(y)P_{\text{enc}}(z_1,\ldots,z_N|y)}{P_{\text{enc}}(z_1,\ldots,z_N|y)}\right]$$

$$= E_{\text{enc}}\left[-\ln \frac{P(y)P_{\text{enc}}(z_1|y)P_{\text{enc}}(z_2|z_1)\cdots P_{\text{enc}}(z_N|z_{N-1})}{P_{\text{enc}}(z_1|y)P_{\text{enc}}(z_2|z_1)\cdots P_{\text{enc}}(z_N|z_{N-1})}\right]$$

$$= E_{\text{enc}}\left[-\ln \frac{P_{\text{enc}}(y|z_1)P_{\text{enc}}(z_1|z_2)\cdots P_{\text{enc}}(z_{N-1}|z_N)P_{\text{enc}}(z_N)}{P_{\text{enc}}(z_1|z_2,y)\cdots P_{\text{enc}}(z_{N-1}|z_N,y)P_{\text{enc}}(z_N|y)}\right]$$

$$\leq E_{\text{enc}}\left[-\ln \frac{P_{\text{gen}}(y|z_1)P_{\text{gen}}(z_1|z_2)\cdots P_{\text{gen}}(z_{N-1}|z_N)P_{\text{gen}}(z_N)}{P_{\text{enc}}(z_1|z_2,y)\cdots P_{\text{enc}}(z_{N-1}|z_N,y)P_{\text{enc}}(z_N|y)}\right]$$

$$= \left\{\begin{array}{l} E_{\text{enc}}\left[-\ln P_{\text{gen}}(y|z_1)\right] \\ \\ +\sum_{i=2}^{N} E_{\text{enc}}\; KL(P_{\text{enc}}(z_{i-1}|z_i,y),\;\; P_{\text{gen}}(z_{i-1}|z_i)) \\ \\ +E_{\text{enc}}\; KL(P_{\text{enc}}(Z_N|y), p_{\text{gen}}(Z_N)) \end{array}\right.$$

## Reverse-Time Probabilities

In the limit of small $\Delta t$ it is possible to derive the following.

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

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

## The Reverse-Diffusion SDE

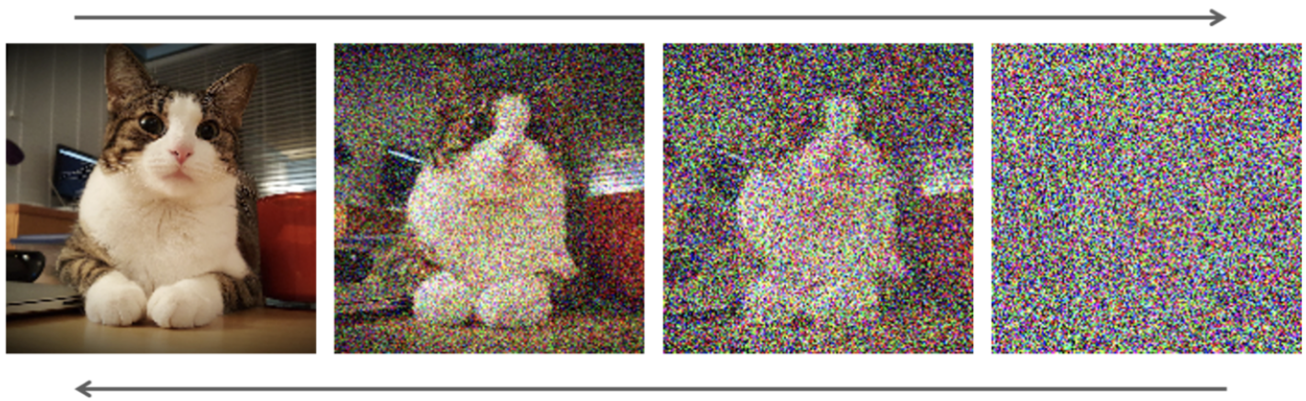
$$P(z(t-\Delta t)|z(t)) = \mathcal{N}\left( z(t) + \frac{\Delta t(E[y|t,z(t)]-z(t))}{t}, \Delta t I \right)$$

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

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

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

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

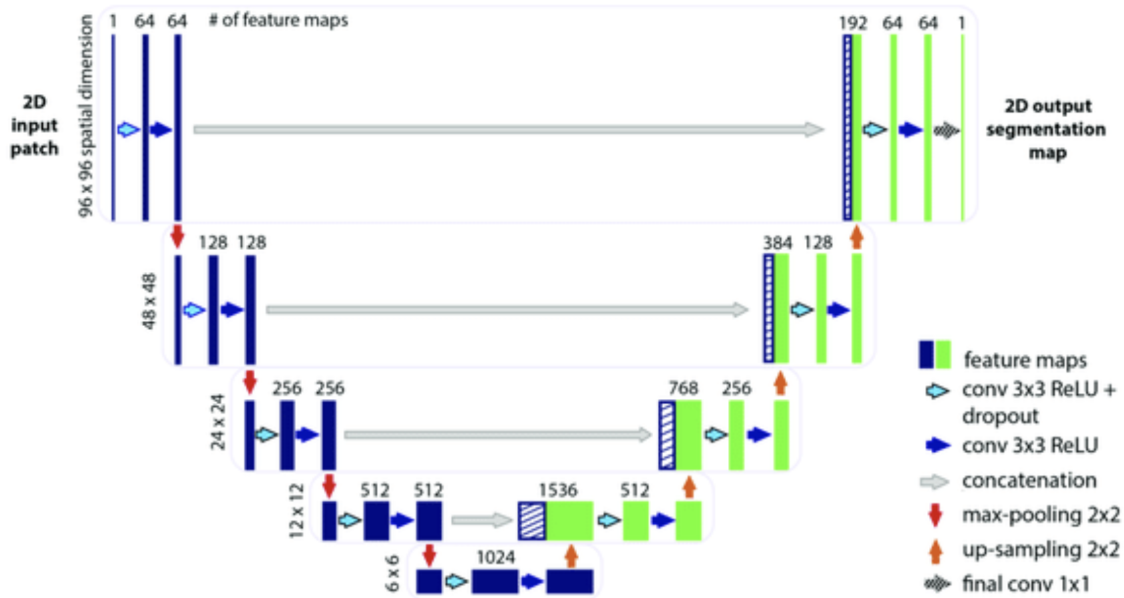
If the population values are scaled so as to have scale 1, then the scale of $z(t)$ is $\sqrt{1+t}$.

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

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

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

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




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

## Computing (or Bounding) Entropy

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

For two Gaussian distributions with the same isotropic covariance we have

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

# Computing (or Bounding) Entropy

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

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

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

# Computing (or Bounding) Entropy

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

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

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

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

## Computing (or Bounding) Entropy

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

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

$$t = i\Delta t$$

# Passing to the Integral

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

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

# Mutual Information

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

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

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

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

# Bounding Entropy

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

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

## 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 $z(t) = z$.

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

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.

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

**END**