the amount of energy

I have left this school year
Energy-Based Models and 🟢🟢🟢 Score Modeling 🟢🟢🟢
Diffusion Models: a TLDR

**An observation:** adding steady amounts of Gaussian noise eventually corrupts an image into something indistinguishable from a standard Gaussian sample.

- Diffusion models simply learn to **reverse** this procedure over many timesteps
Diffusion Models: a TLDR

\[ p(x_0|x_1) \quad p(x_1|x_2) \quad p(x_{T-1}|x_T) \]

\[ q(x_1|x_0) \quad q(x_2|x_1) \quad q(x_T|x_{T-1}) \]
Diffusion Models: A Quick Review

A Diffusion Model is:

- One NN that predicts a clean image from a noisy version of the image
Diffusion Models: A Quick Review

A Diffusion Model is:

- One NN that predicts a clean image from a noisy version of the image
Sampling

\[ \hat{x}_\theta(x_{t+1}, t + 1) \]

\[ x_0 \quad \ldots \quad x_{t-1} \quad x_t \quad x_{t+1} \quad \ldots \quad x_T \]
Sampling

\[ \hat{x}_\theta(x_{t+1}, t + 1) \]

\[ q(x_t|x_0) \]
Sampling

\[ \hat{x}_\theta(x_{t+1}, t + 1) \]

\[ p(x_t|x_{t+1}) \]

\[ q(x_t|x_0) \]
Sampling

\[ \hat{x}_\theta(x_t, t) \quad p(x_t|x_{t+1}) \]
Sampling

$x_0$ \ldots $x_{t-1}$ $x_t$ $x_{t+1}$ \ldots $x_T$

$\hat{x}_\theta(x_t, t)$

$p(x_t|x_{t+1})$

$q(x_{t-1}|x_0)$
Sampling

\[ \hat{x}_\theta(x_t, t) \quad p(x_{t-1}|x_t) \quad p(x_t|x_{t+1}) \]

\[ q(x_{t-1}|x_0) \]
Sampling

$p(x_0|x_1) \quad p(x_{t-1}|x_t) \quad p(x_t|x_{t+1}) \quad p(x_{T-1}|x_T)$
Diffusion Models: A Quick Review

A Diffusion Model is:

- One NN that predicts a clean image from a noisy version of the image

A naive question: Why don’t we just predict one step and be done?
Diffusion Models: A Quick Review

We have learned that a diffusion model is simply one neural network that predicts a clean image from a noisy image.

Objective: \( \arg\min_\theta \left\| x_0 - \hat{x}_\theta(x_t, t) \right\|^2 \)

Sampling:

\[ x_0 \rightarrow p(x_0|x_1) \rightarrow x_1 \rightarrow p(x_1|x_2) \rightarrow x_2 \rightarrow p(x_2|x_{t+1}) \rightarrow x_{t+1} \rightarrow \ldots \rightarrow p(x_T|x_T) \rightarrow x_T \rightarrow \hat{x}_0 \]
Diffusion Models as a Noise Predictor 🎧

Recall that our objective is to predict $\hat{x}_\theta(x_t, t) \approx x_0$
Image 🖼 and Noise 🎧? They are the same!

What does it mean intuitively?

For arbitrary $\mathbf{x}_t \sim q(\mathbf{x}_t \mid \mathbf{x}_0)$, we can rewrite it as $\mathbf{x}_t = \mathbf{x}_0 + \alpha_t \mathbf{\epsilon}_0$

Predicting $\mathbf{x}_0$ determines $\mathbf{\epsilon}_0$ and vice-versa, since they sum to the same thing!
Score Functions 💯

What are score functions?

\[ \nabla_x \log p(x) \]

Intuitively, they describe how to move in data space to improve the (log) likelihood.
Tweedie’s Formula

Mathematically, for a Gaussian variable \( z \sim \mathcal{N}(z; \mu_z, \Sigma_z) \), Tweedie’s formula states:

\[
\mathbb{E}[\mu_z | z] = z + \Sigma_z \nabla_z \log p(z)
\]

Then, since we have previously shown that:

\[
q(x_t | x_0) = \mathcal{N}(x_t; x_0, \alpha_t^2 I)
\]

By Tweedie’s Formula, we derive:

\[
\mathbb{E}[\mu_{x_t} | x_t] = x_t + \alpha_t^2 \nabla_{x_t} \log p(x_t)
\]

The best estimate for the true mean is \( \mu_{x_t} = x_0 \)

\[
x_0 = x_t + \alpha_t^2 \nabla_{x_t} \log p(x_t)
\]
Tweedie’s Formula

There exists a mathematical formula that states that:

$$x_0 \approx x_t + \alpha_t^2 \nabla_x \log p(x_t)$$

Due to the fact that the distribution is Gaussian:

$$q(x_t|x_0) = \mathcal{N}(x_t | x_0, \alpha_t^2 I)$$
Recall that our objective is to predict $\hat{x}_\theta(x_t, t) \approx x_0$
Score 💯 and Noise 📻?

There is a relationship between the score and the noise, which we can derive by equating Tweedie’s formula with the Reparameterization Trick.

\[
\mathbf{x}_0 = \mathbf{x}_t + \alpha_t^2 \nabla \log p(\mathbf{x}_t) = \mathbf{x}_t - \alpha_t \epsilon_0
\]

\[
\therefore \alpha_t^2 \nabla \log p(\mathbf{x}_t) = -\alpha_t \epsilon_0
\]

\[
\nabla \log p(\mathbf{x}_t) = -\frac{1}{\alpha_t} \epsilon_0
\]

Intuitively, the direction to move in data space towards a natural image is the negative noise term that was added.
Three Different Interpretations

Last class we learned that a DiffModel can be implemented as a neural net that:

- ![Predicts original image](image)
  \( \hat{x}_\theta(x_t, t) \approx x_0 \)

- ![Predicts noise epsilon](image)
  \( \hat{\epsilon}_\theta(x_t, t) \approx \epsilon_0 \)

- ![Predicts score function](image)
  \( \hat{s}_\theta(x_t, t) \approx \nabla_{x_t} \log p(x_t) \)

\[
\begin{align*}
x_0 & \approx x_t + \alpha_t^2 \nabla_{x_t} \log p(x_t) \\
x_t & = x_0 + \alpha_t \epsilon_0 \\
& \text{Decoder NN} \quad \hat{x}_0 \\
& \text{Decoder NN} \quad \hat{\epsilon}_0 \\
& \text{Decoder NN} \quad \nabla_{x_t} \log p(x_t)
\end{align*}
\]
Three Different Interpretations

Last class we learned that a DiffModel can be implemented as a neural net that:

- ![Image] Predicts original image $\hat{x}_\theta(x_t, t) \approx x_0$

- 🔊 Predicts noise epsilon $\hat{\epsilon}_\theta(x_t, t) \approx \epsilon_0$

- 💯 Predicts score function $s_\theta(x_t, t) \approx \nabla_{x_t} \log p(x_t)$
Recap: Generative Modeling

Data distribution (unknown)

Model distribution

Deep Neural Network

source: Learning to Generate Data by Estimating Gradients of the Data Distribution
Probability-based Generative Modeling

Why is modeling the **probability** hard in GenMo?
Probability-based **Discriminative** Modeling

What about modeling the **probability** for classifiers?

Probabilities, and therefore model outputs, have to be:

- Non-negative: \( 0 \leq p_\theta(x) \)
- Less than or equal to 1: \( p_\theta(x) \leq 1 \)
- Sum to 1 for the entire space: \( \int_x p_\theta(x) \, dx = 1 \)

How did we do this for discriminative modeling?
Probability-based Generative Modeling

Why is modeling the **probability** hard in GenMo?

Probabilities, and therefore model outputs, have to be:

- Non-negative: \( 0 \leq p_\theta(x) \)

- Less than or equal to 1: \( p_\theta(x) \leq 1 \)

- Sum to 1 for the **entire** space: \( \int_x p_\theta(x) \, dx = 1 \)

In GenMo we do not model the probability over all labels for an image…

We model the **probability of all possible images** - there’s no way we can pass everything through our model and softmax over the result!
Probability-based Generative Modeling

Why is modeling the **probability** hard in GenMo?

Probabilities, and therefore model outputs, have to be:

- Non-negative: \( 0 \leq p_\theta(x) \)
- Less than or equal to 1: \( p_\theta(x) \leq 1 \)
- Sum to 1 for the entire space: \( \int_x p_\theta(x) \, dx = 1 \)

This puts a lot of architectural burden on our network, to output **valid** probabilities!
A simple observation…

All probability distributions can be written as:

$$p_\theta(x) = \frac{1}{Z_\theta} e^{-f_\theta(x)}$$

This is a concept from thermodynamics, where the $f_\theta(x)$ is a flexible, unconstrained value called the energy.

$Z_\theta$ is a normalization constant, computed as: $Z_\theta = \int_x e^{-f_\theta(x)} \, dx$
Energy-based Generative Modeling

Idea: Let’s just model the energy function \( f_\theta(x) \) using a flexible neural network!

\( f_\theta(x) \) is called an energy-based model (EBM) or unnormalized probabilistic model.

How do we train our energy function?

- We can try interpreting it as a probability: \( p_\theta(x) = \frac{1}{Z_\theta} e^{-f_\theta(x)} \)

- Then we can maximize log likelihood as before: \( \max_\theta \sum_{i=1}^{N} \log p_\theta(x_i) \)

What is the problem with this?

\( Z_\theta = \int_{x} e^{-f_\theta(x)} dx \)

Intractable for complex parameterizations!
Another simple observation…

How do we avoid calculating the normalization constant?

Remember that $\mathcal{Z}_\theta$ is a constant that only depends on parameters $\theta$

Then, if we take the input gradient of the log of the probability:

\[
p_\theta(x) = \left(\frac{1}{\mathcal{Z}_\theta} e^{-f_\theta(x)}\right)
\]
Score Functions 🆙

What are score functions?

$$\nabla_x \log p(x)$$

Intuitively, it describes how to move in data space to improve the (log) likelihood.
What are score functions?

\[ \nabla_x \log p(x) \]

Intuitively, it describes how to move in **data space** to improve the (log) likelihood.
Score-based Generative Modeling

Idea: Let’s just model the score function $s_\theta(x)$ using a flexible neural network!

The score is still an unconstrained value, which is attractive to model directly.

How do we train our score function?

- Minimize the Fisher Divergence between the ground truth and predicted score

$$\mathbb{E}_{p(x)} \left[ \| \nabla \log p(x) - s_\theta(x) \|^2_2 \right]$$

- Intuitively this is simply minimizing the L2-distance between our score model and the ground truth score
Score-based Generative Modeling

[Diagram showing various plots and graphs related to score-based generative modeling.]
Score-based Generative Modeling

To drive the point home, score-based generative modeling is a way to implicitly model the energy function $f_\theta(x)$.

We can visualize the learned energy along with the score estimate below:
Score-based Generative Modeling

Once we have trained a score-based model $s_\theta(x) \approx \nabla_x \log p_\theta(x)$, we can use an iterative procedure called Langevin dynamics to draw samples from it:

$$x_{i+1} \leftarrow x_i + c \nabla_x \log p(x) + \sqrt{2c} \epsilon_i, \quad i = 0, 1, \cdots, K,$$

source: Generative Modeling by Estimating Gradients of the Data Distribution
Score-based Generative Modeling

Once we have trained a score-based model \( s_\theta(x) \approx \nabla_x \log p_\theta(x) \), we can use an iterative procedure called Langevin dynamics to draw samples from it:

\[
x_{i+1} \leftarrow x_i + c \nabla_x \log p(x) + \sqrt{2c} \, \epsilon_i, \quad i = 0, 1, \cdots, K,
\]

source: Generative Modeling by Estimating Gradients of the Data Distribution
Score-based Generative Modeling
Score-based Generative Modeling

What is the problem with this optimization objective?

$$E_{p(x)} \left[ \left\| \nabla \log p(x) - s_\theta(x) \right\|_2^2 \right]$$

This is not generally assumed to be known.

The score tells how to change each element of the input to increase its likelihood.
For images, this is like saying how we can change each pixel to make each image more image-like. We don't really have access to this function!
Score Matching

Fortunately, there are a class of methods called score matching that minimize the Fisher Divergence without needing to know the ground-truth score!

**Ground Truth Score Matching:**  
\[ \mathbb{E}_{p(x)} \left[ \left\| \nabla \log p(x) - s_\theta(x) \right\|^2 \right] \]

**Hyvarinen Score Matching:**  
\[ \mathbb{E}_{p(x)} \left[ \text{tr} \left( \nabla_x s_\theta(x) \right) + \frac{1}{2} \left\| s_\theta(x) \right\|^2 \right] \]

**Sliced Score Matching:**  
\[ \mathbb{E}_{p_\nu} \mathbb{E}_{p(x)} \left[ \mathbf{v}^T \nabla_x s_\theta(x) \mathbf{v} + \frac{1}{2} \left\| s_\theta(x) \right\|^2 \right] \]

**Denoising Score Matching:**  
\[ \mathbb{E}_{q_\sigma(\tilde{x}|x)p(x)} \left[ \left\| \nabla_{\tilde{x}} \log q_\sigma(\tilde{x}|x) - s_\theta(\tilde{x}) \right\|^2 \right] \]
Hyvarinen Score Matching

Hyvarinen (2005) utilized integration by parts to remove the unknown $\nabla \log p(\mathbf{x})$:

$$
\mathbb{E}_{p(\mathbf{x})} \left[ \| \nabla \log p(\mathbf{x}) - s_\theta(\mathbf{x}) \|^2 \right]
$$

$$
L(\theta) = \frac{1}{2} \int p(\mathbf{x}) \left[ s_\theta(\mathbf{x})^\top s_\theta(\mathbf{x}) - 2 s_\theta(\mathbf{x})^\top \nabla \log p(\mathbf{x}) + \nabla \log p(\mathbf{x})^\top \nabla \log p(\mathbf{x}) \right] d\mathbf{x}
$$

$$
= \frac{1}{2} \int p(\mathbf{x}) \left[ s_\theta(\mathbf{x})^\top s_\theta(\mathbf{x}) - 2 s_\theta(\mathbf{x})^\top \nabla \log p(\mathbf{x}) \right] d\mathbf{x}
$$

log-deriv trick: $p(\mathbf{x}) \nabla \log p(\mathbf{x}) = \nabla p(\mathbf{x})$

$$
\int p(\mathbf{x}) s_\theta(\mathbf{x})^\top \nabla \log p(\mathbf{x}) d\mathbf{x} = \int s_\theta(\mathbf{x})^\top \nabla p(\mathbf{x}) d\mathbf{x}
$$

$$
= [p(\mathbf{x}) s_\theta(\mathbf{x})]_{-\infty}^\infty - \int p(\mathbf{x}) \nabla_x s_\theta(\mathbf{x}) d\mathbf{x}
$$

$$
\mathbb{E}_{p(\mathbf{x})} \left[ \text{tr}(\nabla_x s_\theta(\mathbf{x})) + \frac{1}{2} \| s_\theta(\mathbf{x}) \|^2 \right]
$$
Hyvarinen Score Matching

\[ \mathbb{E}_{p(x)} \left[ \text{tr} (\nabla_x s_\theta (x)) + \frac{1}{2} \| s_\theta (x) \|_2^2 \right] \]

We have gotten rid of unknown \( \nabla \log p(x) \) 🎉

But now we have to compute \( \text{tr} (\nabla_x s_\theta (x)) \)

When our data has high dimensionality, this is not cheap - many nested backprops!

\[
\nabla_x s_\theta (x) = \begin{pmatrix}
\frac{\partial s_{\theta,1}(x)}{\partial x_1} & \frac{\partial s_{\theta,1}(x)}{\partial x_2} & \frac{\partial s_{\theta,1}(x)}{\partial x_3} \\
\frac{\partial s_{\theta,2}(x)}{\partial x_1} & \frac{\partial s_{\theta,2}(x)}{\partial x_2} & \frac{\partial s_{\theta,2}(x)}{\partial x_3} \\
\frac{\partial s_{\theta,3}(x)}{\partial x_1} & \frac{\partial s_{\theta,3}(x)}{\partial x_2} & \frac{\partial s_{\theta,3}(x)}{\partial x_3}
\end{pmatrix}
\]
Sliced Score Matching

Song (2019) utilized random projections to estimate the expensive $\text{tr}(\nabla_x s_\theta(x))$.

Hyvarinen: $\mathbb{E}_{p(x)} \left[ \text{tr}(\nabla_x s_\theta(x)) + \frac{1}{2} \| s_\theta(x) \|^2_2 \right]$.

Sliced Score Matching: $\mathbb{E}_{p_\mathbf{v}} \mathbb{E}_{p(x)} \left[ \mathbf{v}^\top \nabla_x s_\theta(x) \mathbf{v} + \frac{1}{2} \| s_\theta(x) \|^2_2 \right]$.

Intuition - when we project to a lower dimension, the problem becomes tractable.

- $p_\mathbf{v}$ is a simple distribution of random vectors, e.g. the multivariate std. normal.
Sliced Score Matching

Song (2019) utilized random projections to estimate the expensive $\text{tr}(\nabla_x s_\theta(x))$

$$\mathbb{E}_{p_v} \mathbb{E}_{p(x)} \left[ v^T \nabla_x s_\theta(x) v + \frac{1}{2} \| s_\theta(x) \|_2^2 \right]$$

\(\nabla_x \log p_{\text{data}}(x)\) \(
\approx\)

\(s_\theta(x)\) \(
\approx\)

\(\approx\)
Denoising Autoencoders

Denoising Autoencoders work as follows:

The rationale is that this minimizes “memorization” - the input is corrupted from the start!
Denoising Score Matching

Vincent (2010) proved that matching the score for a noisy perturbation of the input can also minimize the score for the ground truth estimator.

The intuition is that following the gradient of some simple Gaussian perturbation of an input should move us towards the original clean input.

\[
\mathbb{E}_{q_\sigma}(\tilde{x} | x)p(x) \left[ \left\| \nabla_{\tilde{x}} \log q_\sigma(\tilde{x} | x) - s_\theta(\tilde{x}) \right\|_2^2 \right]
\]

With a simple Gaussian for \( q_\sigma(\tilde{x} | x) = \mathcal{N}(\tilde{x}; x, \sigma^2) \)

We know that indeed: \( \nabla_{\tilde{x}} \log q_\sigma(\tilde{x} | x) = \frac{1}{\sigma^2}(\tilde{x} - x) \)
Denoising Score Matching

\[ \mathbb{E}_{q_\sigma}(\tilde{x}|x)p(x)[\| \nabla_{\tilde{x}} \log q_\sigma(\tilde{x}|x) - s_\theta(\tilde{x}) \|^2_2] \]

A simple algorithm:

- Take in your input sample
- Perturb it with some Gaussian noise
- Compute the score estimate for the noisy sample
- Compare it with the ground truth score computed by the noising Gaussian

\[ \nabla_{\tilde{x}} \log q_\sigma(\tilde{x}|x) = \frac{1}{\sigma^2}(\tilde{x} - x) \]
Score Matching
Score-based Generative Modeling

Data samples
\[ \{x_1, x_2, \cdots, x_N\} \overset{\text{i.i.d.}}{\sim} p(x) \]

Scores
\[ s_\theta(x) \approx \nabla_x \log p(x) \]

Langevin dynamics

source: Generative Modeling by Estimating Gradients of the Data Distribution
Score-based Generative Modeling

What is the problem with vanilla score-matching?

\[
\mathbb{E}_{p(x)}[\| \nabla_x \log p(x) - s_\theta(x) \|^2_2] = \int p(x) \| \nabla_x \log p(x) - s_\theta(x) \|^2_2 \, dx
\]

Our model of the score will not learn the low-density regions well.
Score-based Generative Modeling

What is the solution for vanilla score-matching?

- Adding Gaussian noise!

source: Generative Modeling by Estimating Gradients of the Data Distribution
Score-based Generative Modeling 🟢

How do we choose an appropriate noise scale for the perturbation process?
Score-based Generative Modeling

\[ \sigma_1 < \sigma_2 < \sigma_3 \]

source: Generative Modeling by Estimating Gradients of the Data Distribution
Score-based Generative Modeling

Now, we estimate the score function of each noise-perturbed distribution

\[ s_\theta(x, t) \approx \nabla_{x_t} \log p_{\sigma_t}(x_t) \]

for all \( t = 1, 2, \cdots, T \)

We model it as a neural network, called the **Noise Conditional Score Network**

The training objective is a weighted sum of Fisher divergences for all noise scales:

\[ \arg \min_\theta \sum_{t=1}^{T} \lambda(t) \mathbb{E}_{p_{\sigma_t}(x_t)} \left[ \left\| \nabla \log p_{\sigma_t}(x_t) - s_\theta(x, t) \right\|_2^2 \right] \]

source: *Generative Modeling by Estimating Gradients of the Data Distribution*
Score-based Generative Modeling

Sampling is done using annealed Langevin Dynamics

- Running Langevin dynamics for each noise level in sequence, initializing the next noise level with the results of the previous one.

source: Generative Modeling by Estimating Gradients of the Data Distribution
Examples!

source: Generative Modeling by Estimating Gradients of the Data Distribution
Review: Variational Diffusion Models

We want to learn a denoising decoder:

\[ \hat{x}_{t-1} = \hat{x}_0 + \alpha_{t-1} \epsilon \]

But what is the form of \( x_{t-1} \)?

Recall that:

\[ q(x_{t-1} | x_0) = \mathcal{N}(x_{t-1} | x_0, \alpha_{t-1}^2 I) \]

\[ \therefore x_{t-1} = x_0 + \alpha_{t-1} \epsilon \]

Do we really need to predict \( \sigma_{dec} \)?

What is the ground truth signal for \( \mu_{dec} \)?
Review: Variational Diffusion Models

We want to learn a denoising decoder:

\[ \mathbf{x}_t \xrightarrow{\text{Decoder NN}} \hat{x}_0 \xrightarrow{\text{reparam. trick!}} \mathbf{x}_{t-1} \]

where ground truth denoising sample is:

\[ \mathbf{x}_{t-1} = \mathbf{x}_0 + \alpha_{t-1} \ast \epsilon \quad \epsilon \sim \mathcal{N}(0, \mathbf{I}) \]

Loss Objective:

\[ \arg\min_{\theta} \sum_{t=1}^{T} \| \mathbf{x}_0 - \hat{x}_\theta(\mathbf{x}_t, t) \|_2^2 \]
Review: Variational Diffusion Models

We want to learn a denoising decoder:

\[
\begin{align*}
\mathbf{x}_t & 
\rightarrow \mathbf{\hat{e}}_0 
\rightarrow \mathbf{x}_{t-1}
\end{align*}
\]

where ground truth denoising sample is:

\[
\mathbf{x}_{t-1} = \mathbf{x}_0 + \alpha_{t-1} \times \mathbf{\epsilon}
\]

which is equivalent to:

\[
\mathbf{x}_{t-1} = \mathbf{x}_t - \alpha_t \times \mathbf{\epsilon}_0 + \alpha_{t-1} \times \mathbf{\epsilon}
\]

(reparam. trick!)

\[\mathbf{\epsilon} \sim \mathcal{N}(0, \mathbf{I})\]

Loss Objective:

\[
\arg \min_{\theta} \sum_{t=1}^{T} \| \mathbf{\epsilon}_0 - \mathbf{\hat{e}}_{\theta}(\mathbf{x}_t, t) \|^2_2
\]
Review: Score 💯 and Noise 🔊?

There is a relationship between the score and the noise, which we can derive by equating Tweedie’s formula with the Reparameterization Trick.

\[ x_0 = x_t + \alpha_t^2 \nabla \log p(x_t) = x_t - \alpha_t \epsilon_0 \]

\[ \therefore \alpha_t^2 \nabla \log p(x_t) = -\alpha_t \epsilon_0 \]

\[ \nabla \log p(x_t) = -\frac{1}{\alpha_t} \epsilon_0 \]

Intuitively, the direction to move in data space towards a natural image is the negative noise term that was added.
We want to learn a denoising decoder:

\[
\begin{align*}
    x_t \quad \text{Decoder NN} \\
    \nabla x_t \log p(x_t) \quad \rightarrow \quad x_{t-1}
\end{align*}
\]

where ground truth denoising sample is:

\[
x_{t-1} = \boxed{x_0} + \alpha_{t-1} \epsilon
\]

which is equivalent to:

\[
x_{t-1} = x_t - \alpha_t \epsilon_0 + \alpha_{t-1} \epsilon
\]

which is equivalent to:

\[
x_{t-1} = \boxed{x_t + \alpha_t^2 \nabla x_t \log p(x_t)} + \alpha_{t-1} \epsilon
\]

(score prediction)

**Loss Objective:**

\[
\arg \min_{\theta} \sum_{t=1}^{T} \left\| \nabla x_t \log p(x_t) - \hat{s}_\theta(x_t, t) \right\|_2^2
\]
Unifying Two Interpretations - Training Objective

The Hierarchical VAE interpretation of diffusion models shows that we can use a network to model the score function at arbitrary noise corruptions, learned by:

$$\arg \min_\theta \sum_{t=1}^T \left\| \nabla_{x_t} \log p(x_t) - \hat{s}_\theta(x_t, t) \right\|_2^2$$

Score-based generative modeling also uses a network to model the score function at arbitrary levels of Gaussian noise corruption, learned by:

$$\arg \min_\theta \sum_{t=1}^T \lambda(t) \mathbb{E}_{p_{\sigma_t}(x_t)} \left[ \left\| \nabla \log p_{\sigma_t}(x_t) - s_\theta(x, t) \right\|_2^2 \right]$$
We want to learn a denoising decoder:

\[
\begin{align*}
x_t & \xrightarrow{\text{Decoder NN}} \nabla x_t \log p(x_t) \rightarrow x_{t-1} \\
\end{align*}
\]

where ground truth denoising sample is:

\[
x_{t-1} = x_0 + \alpha_{t-1} * \epsilon
\]

which is equivalent to:

\[
x_{t-1} = x_t - \alpha_t * \epsilon_0 + \alpha_{t-1} * \epsilon
\]

which is equivalent to:

\[
x_{t-1} = x_t + \alpha_t^2 * \nabla x_t \log p(x_t) + \alpha_{t-1} * \epsilon
\]

(score prediction)

Loss Objective:

\[
\arg \min_\theta \sum_{t=1}^{T} \left\| \nabla x_t \log p(x_t) - \hat{s}_\theta(x_t, t) \right\|_2^2
\]
Unifying Two Interpretations - Sampling Procedure

Let's take a closer look at Langevin Dynamics:

\[ x_{i+1} \leftarrow x_i + \frac{\alpha}{2} \nabla_x \log p(x) + \sqrt{2 \alpha} \epsilon_i, \quad i = 0, 1, \ldots, K, \]

Recall our denoising transition from the Hierarchical VAE formulation:

\[ x_{t-1} = x_t + \alpha_t^2 \nabla_x \log p(x_t) + \alpha_{t-1} \epsilon_t \]

Annealed Langevin Dynamics sampling is analogous to Markov Chain procedure.
Sampling

$\mathbf{HVAEs}$

$\mathbf{NCSNs}$
Unifying Two Interpretations

We have shown two equivalently valid ways to describe a diffusion model!

- One takes the perspective of a Markovian Hierarchical VAE, where samples are steadily denoised through “hierarchies”

- Another takes the perspective of energy-based models and score matching where we iteratively refine an input through noise levels.

*they are two sides of the same coin!*
Conditional Diffusion Models

So far we have been learning an unconditional diffusion model \( p_\theta(x) \).
Conditional Diffusion Models

How do we incorporate conditional information, to control data generation?

“a painting of a fox sitting in a field at sunrise in the style of Claude Monet”

Parti (but pretend it is ImageN)  |  StableDiffusion  |  Dall-E 2.0

source: ImageN, StableDiffusion, Dall-E 2.0
Conditional Diffusion Models

How do we incorporate conditional information, to control data generation?

Suppose we have conditioning information $y$ and now want to learn $p_\theta(x \mid y)$

Well an unconditional diffusion model $p_\theta(x)$ really is just:

$$
\begin{align*}
\text{Decoder NN} & \quad \hat{x}_0 \\
\end{align*}
$$
Three Different Interpretations

It turns out, training a DiffModel can be implemented as a neural net that:

- ![Image] Predicts original image $\hat{x}_\theta(x_t, t) \approx x_0 \rightarrow \hat{x}_\theta(x_t, t, y) \approx x_0$

- ![Image] Predicts noise epsilon $\hat{\epsilon}_\theta(x_t, t) \approx \epsilon_0 \rightarrow \hat{\epsilon}_\theta(x_t, t, y) \approx \epsilon_0$

- ![Image] Predicts score function $s_\theta(x_t, t) \approx \nabla_{x_t} \log p(x_t) \rightarrow s_\theta(x_t, t, y) \approx \nabla \log p(x_t | y)$

Caveat: A conditional diffusion model trained by this simple conditioning may ignore or downplay the given conditioning information.
Guidance

Guidance provides more explicit control on the amount of weight the model gives to the conditioning information, at the cost of sample diversity.

- How much should our generated $x$ match $y$?

Let us take the score-based perspective of diffusion models.

Now, we are interested in learning $\nabla \log p(x_t | y)$ rather than unconditional score function $\nabla \log p(x_t)$.
Classifier Guidance

Score of a conditional diffusion model:

\[ \nabla \log p(x_t | y) = \nabla \log \left( \frac{p(x_t)p(y | x_t)}{p(y)} \right) \]

\[ P(A|B) = \frac{P(B|A)P(A)}{P(B)} \]
Classifier Guidance

Score of a conditional diffusion model:

$$\nabla \log p(x_t | y) = \nabla \log \left( \frac{p(x_t)p(y | x_t)}{p(y)} \right)$$

$$= \nabla \log p(x_t) + \nabla \log p(y | x_t) - \nabla \log p(y)$$

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$
Classifier Guidance

Score of a conditional diffusion model:

\[ \nabla \log p(x_t \mid y) = \nabla \log \left( \frac{p(x_t)p(y \mid x_t)}{p(y)} \right) \]

\[ = \nabla \log p(x_t) + \nabla \log p(y \mid x_t) - \nabla \log p(y) \]

\[ = \nabla \log p(x_t) + \nabla \log p(y \mid x_t) \]

unconditional score  adversarial gradient
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\[ = \underbrace{\nabla \log p(x_t)} + \underbrace{\nabla \log p(y | x_t)} \]

unconditional score \hspace{1cm} adversarial gradient

It turns out that training a conditional diffusion model is as simple as training an unconditional diffusion model (as before) along with a classifier \( p(y | x_t) \)!
Classifier Guidance

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\nabla \log p(x_t | y) = \nabla \log \left( \frac{p(x_t)p(y | x_t)}{p(y)} \right) \\
= \nabla \log p(x_t) + \nabla \log p(y | x_t) - \nabla \log p(y) \\
= \text{unconditional score} + \text{adversarial gradient}
\]

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\[ = \nabla \log p(x_t) + \nabla \log p(y | x_t) - \nabla \log p(y) \]

\[ = \underbrace{\nabla \log p(x_t)}_{\text{unconditional score}} + \underbrace{\nabla \log p(y | x_t)}_{\text{adversarial gradient}} \]

It turns out that training a conditional diffusion model is as simple as training an unconditional diffusion model (as before) along with a classifier \( p(y | x_t) \)!

Sampling is then done by querying the learned unconditional score function as well as the adversarial gradient of a classifier.

\[ \nabla_{x_t} \log p(x_t) + \left( \text{dog} - \text{blueberry muffin} \right) \]
Classifier Guidance

Score of a conditional diffusion model:

\[ \nabla \log p(x_t | y) = \nabla \log \left( \frac{p(x_t)p(y | x_t)}{p(y)} \right) \]

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- The classifier attempts to tell us how good the noisy image matches the conditional label. It must be trained for arbitrary noise levels, however!

\[ \nabla \log p(x_t | y) = \nabla \log p(x_t) + \gamma \nabla \log p(y | x_t) \]
Classifier Guidance

Sampling is then done by querying the learned unconditional score function as well as the adversarial gradient of a classifier.

\[ \nabla \log p(x_t \mid y) = \nabla \log p(x_t) + \gamma \nabla \log p(y \mid x_t) \]
Classifier Guidance

Sampling is then done by querying the learned unconditional score function as well as the adversarial gradient of a classifier.

\[
\nabla \log p(x_t \mid y) = \nabla \log p(x_t) + \gamma \nabla \log p(y \mid x_t)
\]
Classifier Guidance

Sampling is then done by querying the learned unconditional score function as well as the adversarial gradient of a classifier.

Why not just use $\nabla \log p(x_t \mid y) = \nabla \log p(y \mid x_t)$?
Classifier-Free Guidance

Let’s revisit the score of a conditional diffusion model:

\[ \nabla \log p(x_t \mid y) = \nabla \log p(y \mid x_t) + \nabla \log p(x_t) \]
Classifier-Free Guidance

$$\nabla \log p(x_t | y) = \gamma \nabla \log p(x_t | y) + (1 - \gamma) \nabla \log p(x_t)$$

**Questions:**

- What happens if $\gamma$ is 1?
- What happens if $\gamma$ is larger than 1?
- How many diffusion models do we need to train?

$$s_\theta(x_t, t, y) \approx \nabla \log p(x_t | y)$$

$$s_\theta(x_t, t) \approx \nabla \log p(x_t)$$
Classifier-Free Guidance

\[
\nabla \log p(x_t \mid y) = \gamma \nabla \log p(x_t \mid y) + (1 - \gamma) \nabla \log p(x_t)
\]

Questions:

- What happens if \( \gamma \) is 1?
- What happens if \( \gamma \) is larger than 1?
- How many diffusion models do we need to train?

\[

s_\theta(x_t, t, y) \approx \nabla \log p(x_t \mid y)
\]

\[

s_\theta(x_t, t, 0) \approx \nabla \log p(x_t)
\]

Just one - as long as we train it with dropout on the conditioning info!
Classifier-Free Guidance

(source: 画像生成AI「Stable Diffusion」でどれぐらいプロンプト・呪文の指示に従うかを決めるCFG(classifier-free guidance)とは一体何なのか？)
Classifier-Free Guidance

- A bald eagle made of chocolate powder, mango, and whipped cream.
- A photo of a Corgi dog riding a bike in Times Square. It is wearing sunglasses and a beach hat.
- A bucket bag made of blue suede. The bag is decorated with intricate golden paisley patterns. The handle of the bag is made of rubies and pearls.
- Three spheres made of glass falling into ocean. Water is splashing. Sun is setting.
- A photo of a raccoon wearing an astronaut helmet, looking out of the window at night.
- The Toronto skyline with Google brain logo written in fireworks.

source: ImageN
Models in Practice

Let’s explore some of the state-of-the-art diffusion models in practice:

- DALL-E 2
- ImageN
- StableDiffusion
DALL-E 2

“a corgi playing a flame throwing trumpet”

“where is the diffusion model?”

source: Hierarchical Text-Conditional Image Generation with CLIP Latents
ImageN

“A Golden Retriever dog wearing a blue checkered beret and red dotted turtleneck.”

source: Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding
StableDiffusion

Remember this?

- In a VAE we learn two networks: an encoder and a decoder.
- How many do we need to learn for a Hierarchical VAE?

...what if we assume all latent dimensions are the same?
StableDiffusion

It turns out that this is exactly what Stable/Latent Diffusion is doing!

- We model the latent distribution using a diffusion model

source: High-Resolution Image Synthesis with Latent Diffusion Models
StableDiffusion

It turns out that this is exactly what Stable/Latent Diffusion is doing!

- Projects the image into a smaller latent space
- Learns the diffusion model for **only the latent**
- Re-projects the denoised latents back to image space
- Benefits?

[source: High-Resolution Image Synthesis with Latent Diffusion Models]
Summarization

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Summarization

- We show that a Diffusion Model is simply a special case of a Hierarchical VAE.
- We show that optimization boils down to learning a network to either predict the original image, the source noise, or the score function at arbitrary Gaussian noise corruption levels.
- We draw an explicit connection to score-based generative modeling and show they are equivalent in what they model, their objective, and sampling process.
- We showcase how to build a conditional diffusion model, and apply guidance.
Is it Good?

Diffusion models have amazing generative performance!
- Probably state of the art generative model right now
- Absolutely incredible at learning conditional distributions
Fin