Diffusion Models

Tweedie's formula

Let σ be a constant and consider a random variable X with probability density function f_X as well as a random Gaussian noise $\mathcal{E} \sim \mathcal{N}(0, 1)$ that is independent from X. If $Y = X + \sigma\mathcal{E}$ then

$$\mathbb{E}[X|Y = y] = y + \sigma^2 \nabla_y \log f_Y(y) \qquad \mathbb{E}[\mathcal{E}|Y = y] = -\sigma \nabla_y \log f_Y(y).$$

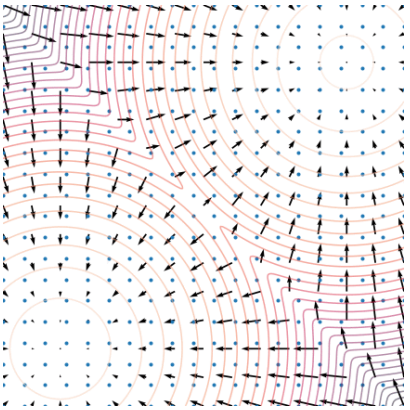
▶ **Proof**

From Tweedie's formula, ϵ is estimated to be $-\sigma\nabla_y \log f_Y(y)$.

Sampler *Langevin dynamics*:

$$y_{k+1} = y_k + \delta_k \nabla_y \log f_Y(y_k) + \sqrt{2\delta_k} w_k \quad \text{where } w_k \sim \mathcal{N}(0, 1)$$

Image source.



Score matching

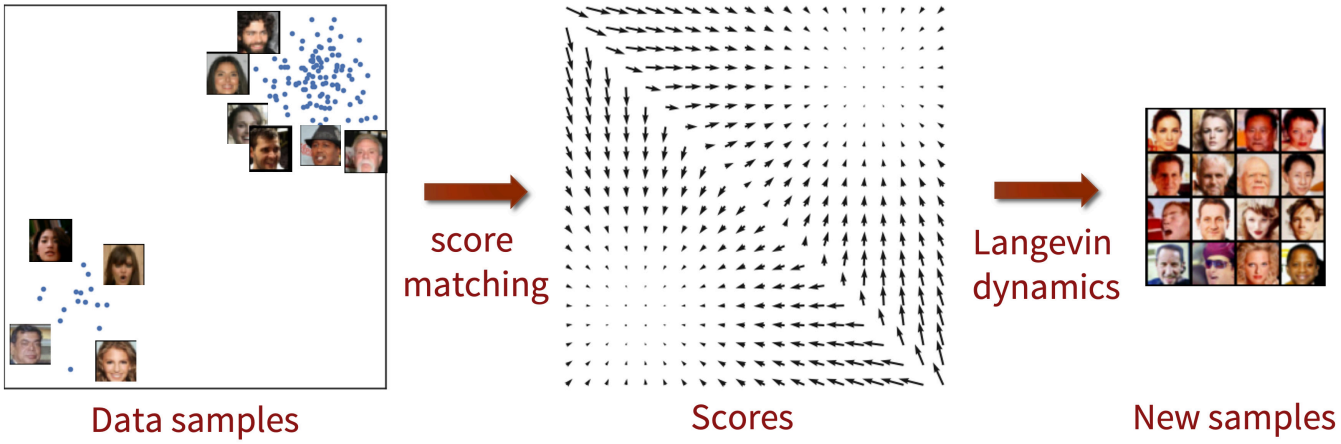
Diffusion models are also known as *energy-based models* and then *score-matching*.

For **fixed** σ, the matching is $\epsilon_\theta(y) \approx \mathbb{E}[\mathcal{E}|X+\sigma\mathcal{E}=y] = -\sigma\nabla_y \log f_{X+\sigma\mathcal{E}}(y)$.

Training: sample x / pick x in dataset, sample ε, update θ to minimize (e.g., using gradient descent), the loss:

$$\mathbb{E}[\|\epsilon_\theta(X+\sigma\mathcal{E}) - \mathcal{E}\|^2]$$

Image source.

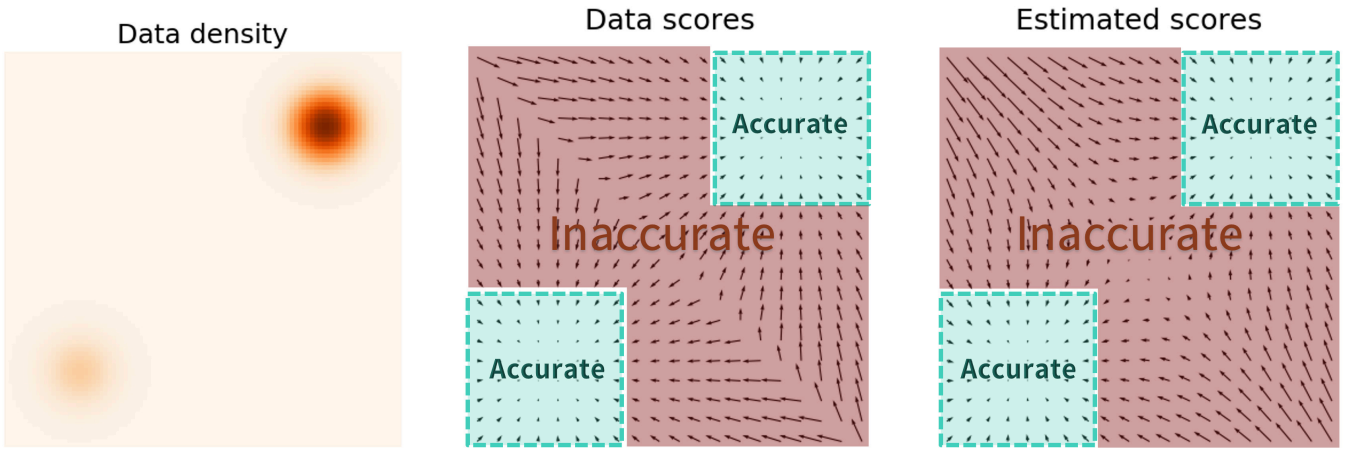


Issue with small variance

If σ is too small then the support of $X + \sigma\mathcal{E}$ may not cover the whole state space → inaccurate $\epsilon_\theta(y)$ in these parts. More formally, the loss is the Fisher divergence:

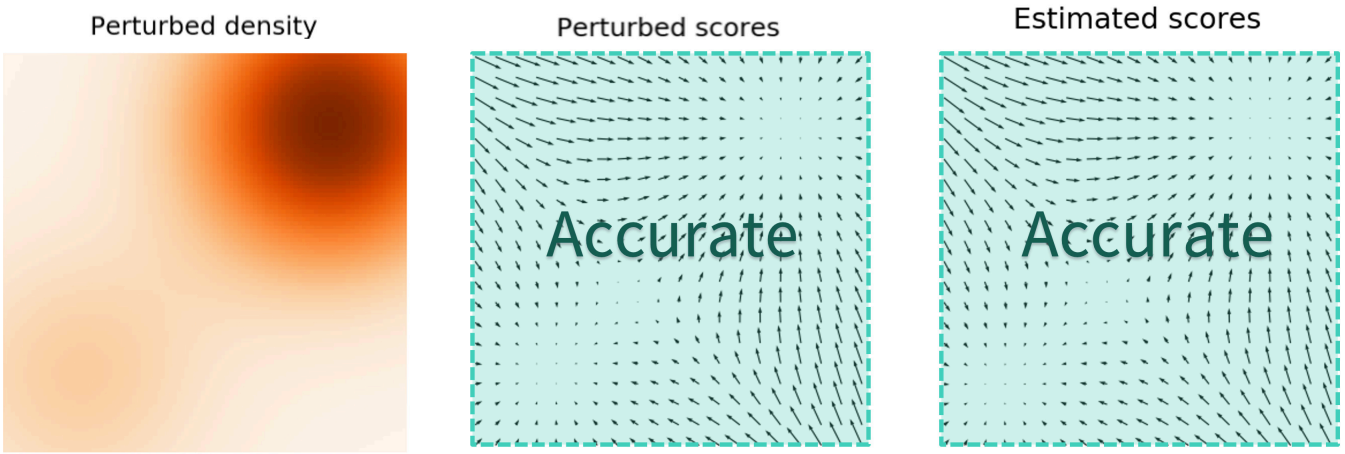
$$\mathbb{E}[\|\epsilon_\theta(y) + \sigma\nabla_y \log f_Y(y)\|^2] = \int_y f_Y(y)\|\epsilon_\theta(y) + \sigma\nabla_y \log f_Y(y)\|^2 \, \mathrm{d}y$$

so it is inaccurate for y such that $f_Y(y)$ is too small. Image source.



Issue with large variance

If σ is too large then $\epsilon_\theta(y) \approx -\sigma \nabla_y \log f_{X+\sigma\mathcal{E}}(y)$ everywhere but the distribution $Y \sim X + \sigma\mathcal{E}$ is too noisy, less specific to X (small signal to noise ratio). Image source.



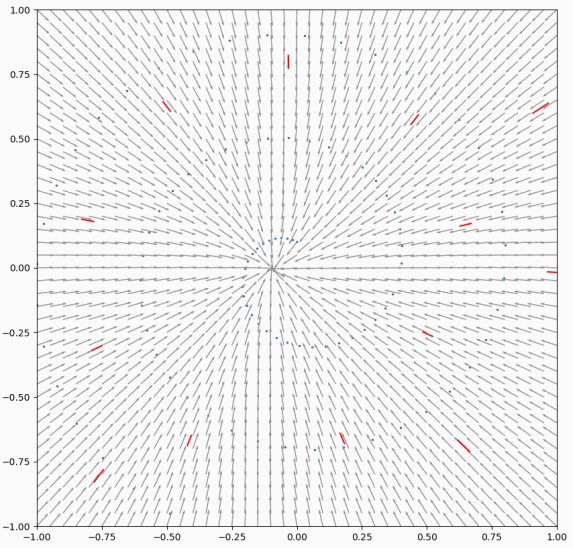
Variance-dependent score

The matching is $\epsilon_\theta(y, \sigma) \approx -\sigma \nabla_y \log f_{X+\sigma\mathcal{E}}(y)$.

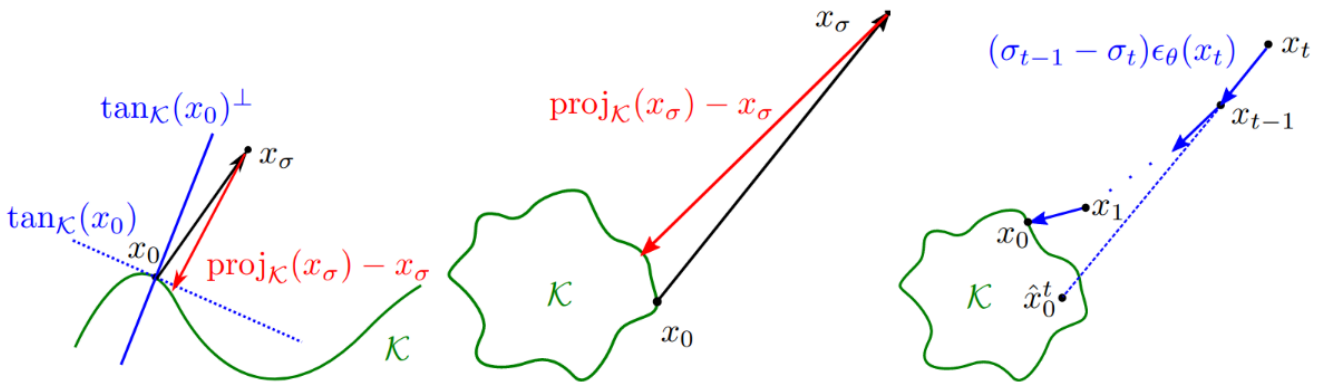
Training: sample x / pick x in dataset, sample σ, ε, update θ to minimize (e.g., using gradient descent), the loss:

$$\mathbb{E}[\|\epsilon_\theta(X + \sigma\mathcal{E}, \sigma) - \mathcal{E}\|^2]$$

Animation generated with `smalldiffusion` using a deterministic (i.e. $w_k = 0$) sampler.



Sampling



(a) Low noise (b) High noise (c) Denoising process (DDIM)

Image from [PY24; Figure 1]. Deterministic DDIM : move from a variance estimate $\boldsymbol{\sigma_t}$ to $\boldsymbol{\sigma_{t-1}}$:

$$
\begin{aligned}
X_t &= X_0 + \sigma_t \mathcal{E} \\
\mathbb{E}[X_{t-1} | X_t = x_t] &= \mathbb{E}[X_0 | X_t = x_t] + \sigma_{t-1} \mathbb{E}[\mathcal{E} | X_t = x_t] \\
&= \mathbb{E}[X_t | X_t = x_t] - \sigma_t \mathbb{E}[\mathcal{E} | X_t = x_t] + \sigma_{t-1} \mathbb{E}[\mathcal{E} | X_t = x_t] \\
&= x_t + (\sigma_{t-1} - \sigma_t) \mathbb{E}[\mathcal{E} | X_t = x_t]
\end{aligned}
$$

Denoising with randomness

Given $0 \leq \mu < 1$, pick $\sigma_{t'}$ such that $\sigma_{t-1} = \sigma_t^{\mu}\sigma_{t'}^{1-\mu}$ we have the following sampler of [PY24]:

$$x_{t-1} = x_t + (\sigma_{t'} - \sigma_t)\epsilon_\theta(x_t, \sigma_t) + \eta w_t \qquad w_t \sim \mathcal{N}(0, I)$$

For $\mu = 0$, $\sigma_{t'} = \sigma_{t-1}$ and we recover deterministic DDIM. For $\mu = 1/2$, we have DDPM of [HJA20]

▶ **What is the order between σ_{t-1}, σ_t and $\sigma_{t'}$?**

▶ **What should η be ?**

[HJA20] J. Ho, A. Jain and P. Abbeel. *Denoising Diffusion Probabilistic Models*. In: *Proceedings of the 34th International Conference on Neural Information Processing Systems, NIPS '20* (Curran Associates Inc., Red Hook, NY, USA, Dec 2020); pp. 6840–6851. Accessed on Nov 26, 2024.

[PY24] F. Permenter and C. Yuan. *Interpreting and Improving Diffusion Models from an Optimization Perspective* (Jun 2024), arXiv:2306.04848. Accessed on Nov 26, 2024.

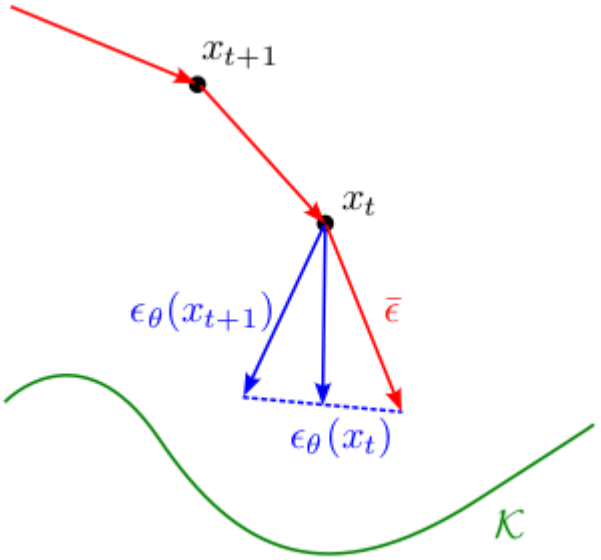
Acceleration

As $\epsilon_\theta(x_t, \sigma_t)$ is more accurate than $\epsilon_\theta(x_{t+1}, \sigma_{t+1})$, [PY24; Section 5] suggests to accelerate the convergence by correcting part of the previous step. That is, we take:

$$\bar{\epsilon}_t = \gamma \epsilon_\theta(x_t, \sigma_t) + (1-\gamma)\epsilon_\theta(x_{t+1}, \sigma_{t+1})$$

with $\gamma > 1$.

Image is [PY24; Figure 3].



[PY24] F. Permenter and C. Yuan. *Interpreting and Improving Diffusion Models from an Optimization Perspective* (Jun 2024), arXiv:2306.04848. Accessed on Nov 26, 2024.

Auto-Encoder

Find encoder E and decoder D that minimize the loss:

$$\mathbb{E}[\|X - D(E(X))\|_2^2]$$

The *code* (aka *latent variable*) $z = E(x)$ typically has smaller size compared to x to force the model to only keep essential features.

▶ **What is the solution if E and D were linear (i.e. matrices) ?**

Variational Auto-Encoder

We add artificial noise to improve learning:

$$\mathbb{E}[\|X - D(E_\mu(X) + \mathcal{E} \odot E_\sigma(X))\|_2^2]$$

An insightful way to model this is as follows.

- Assume our dataset come from a distribution X that is obtained from a latent space Z using a decoder $X = D(Z)$.
- If we knew the latent variable z, we would search for a decoder D that maximizes $\mathbb{E}[\log(f_{X|Z}(x|z))]$.
- Since we do not know z, we make an estimate of y using an encoder $Y = E(X)$.
- The validity of these encoder and decoder models can now be measure with a Maximum Likelihood Estimator that search for the encoder and decoder models that maximizes $\mathbb{E}[\log(f_X(X))]$.

Evidence Lower BOund (ELBO)

For any random variables X, Y and Z, we have

$$\log(f_X(x)) = D_{\mathrm{KL}}((Y|X=x) \parallel (Z|X=x)) + \mathcal{L}(x)$$

where the *evidence lower bound* [KW13]

$$\mathcal{L}(x) = -D_{\mathrm{KL}}((Y|X=x) \parallel Z) + \mathbb{E}[\log(f_{X|Z}(x|Y))]]$$

▶ **Proof**

$\mathcal{L}(x)$ is a **lower bound** to $\log(f_X(x))$ as the Kullback-Leibler divergence $D_{\mathrm{KL}}((Y|X=x) \parallel (Z|X=x))$ is always nonnegative.

In the context of VAEs, Z represents the actual latent variable and Y represents the estimated random variables so $D_{\mathrm{KL}}((Y|X=x) \parallel (Z|X=x))$ is a measure of the error made by our estimator.

[KW13] D. P. Kingma and M. Welling. *Auto-Encoding Variational Bayes* (Dec 2013). Accessed on Nov 26, 2024.

Gaussian ELBO

Consider two deterministic functions $E_\mu, E_\sigma : \mathbb{R}^n \to \mathbb{R}^r$ and $D_\mu, D_\sigma : \mathbb{R}^r \to \mathbb{R}^n$. Suppose $X = D_\mu(Z) + \mathcal{E}_1 \odot D_\sigma(Z)$ and $Y = E_\mu(X) + \mathcal{E}_2 \odot E_\sigma(X)$ with $\mathcal{E}_1, \mathcal{E}_2 \sim \mathcal{N}(0, I)$. We have (see [KW13; Appendix B] for a proof):

$$2D_{\mathrm{KL}}((Y|X=x) \parallel Z) = \|E_\mu(X)\|_2^2 + \|E_\sigma(X)\|_2^2 - r - \sum_{i=1}^{r} \log((E_\sigma(X))_i^2)$$

For the second part of the ELBO, we have

$$\begin{aligned}
&\mathbb{E}[\log(f_{X|Z}(x|Y))]] \\
&= \mathbb{E}[\log(f_{X|Z}(x|E_\mu(x) + \mathcal{E}_2 \odot E_\sigma(x)))]] \\
&= \mathbb{E}[\log(f_{\mathcal{E}_1}(\mathbf{Diag}(D_\sigma(E_\mu(x) + \mathcal{E}_2 \odot E_\sigma(x)))^{-1}(x - D_\mu(E_\mu(x) + \mathcal{E}_2 \odot E_\sigma(x)))))]] \\
&= -\frac{\log(2\pi)}{2} + \mathbb{E}[\|\mathbf{Diag}(D_\sigma(E_\mu(x) + \mathcal{E}_2 \odot E_\sigma(x)))^{-1}(x - D_\mu(E_\mu(x) + \mathcal{E}_2 \odot E_\sigma(x)))\|_2^2]]
\end{aligned}$$

[KW13] D. P. Kingma and M. Welling. *Auto-Encoding Variational Bayes* (Dec 2013). Accessed on Nov 26, 2024.

Monte-Carlo sampling

This can be approximated using Monte-Carlo given L samples $\epsilon_1, \dots \epsilon_L$ from the distribution $\mathcal{N}(0, I)$ as

$$\mathbb{E}[\log(f_{X|Z}(x|Y))]] \approx \frac{1}{L} \sum_{i=1}^{L} \log(f_{X|Z}(x|E_\mu(x) + \epsilon_i \odot E_\sigma(x))).$$

In the simpler case where $D_\sigma(z) = \mathbf{1}$, we recognize the classical L2 norm:

$$\mathbb{E}[\log(f_{X|Z}(x|Y))]] \approx -\frac{\log(2\pi)}{2} + \frac{1}{L} \sum_{i=1}^{L} \|x - D_\mu(E_\mu(x) + \epsilon_i\|_2^2.$$

Variational AutoEncoders (VAEs)

- We want to learn the distribution of our data represented by the random variable $\boldsymbol{X}$.
- The encoder maps a data point $\boldsymbol{x}$ to a Gaussian distribution $\boldsymbol{Y} \sim \mathcal{N}(\boldsymbol{E}_\mu(\boldsymbol{x}), \boldsymbol{E}_\Sigma(\boldsymbol{x}))$ over the latent space
- The decoder maps a latent variable $\boldsymbol{z} \sim \boldsymbol{Z}$ to a the Gaussian distribution $\mathcal{N}(\boldsymbol{D}_\mu(\boldsymbol{z}), \boldsymbol{D}_\sigma(\boldsymbol{Z}))$

The Maximum Likelyhood Estimator (MLE) maximizes the following sum over our datapoints $\boldsymbol{x}$ with its ELBO:

$$\sum_{\boldsymbol{x}} \log(\boldsymbol{f}_{\boldsymbol{X}}(\boldsymbol{x})) \geq \sum_{\boldsymbol{x}} -D_{\mathrm{KL}}((\boldsymbol{Y}|\boldsymbol{X}=\boldsymbol{x}) \parallel \boldsymbol{Z}) + \mathbb{E}[\log(\boldsymbol{f}_{\boldsymbol{X}|\boldsymbol{Z}}(\boldsymbol{x}|\boldsymbol{Y}))]$$

So the MLE minimizes the loss

$$-\mathbb{E}[\log(\boldsymbol{f}_{\boldsymbol{X}|\boldsymbol{Z}}(\boldsymbol{x}|\boldsymbol{Y}))].$$

with the KL-regularizer

$$D_{\mathrm{KL}}((\boldsymbol{Y}|\boldsymbol{X}=\boldsymbol{x}) \parallel \boldsymbol{Z})$$

Denoising Auto-Encoder

Auto-Encoder	$D(E(X))$
Variational Auto-Encoder	$D(E(X) + \mathcal{E})$
Denoising Auto-Encoder	$D(E(X + \sigma\mathcal{E}))$

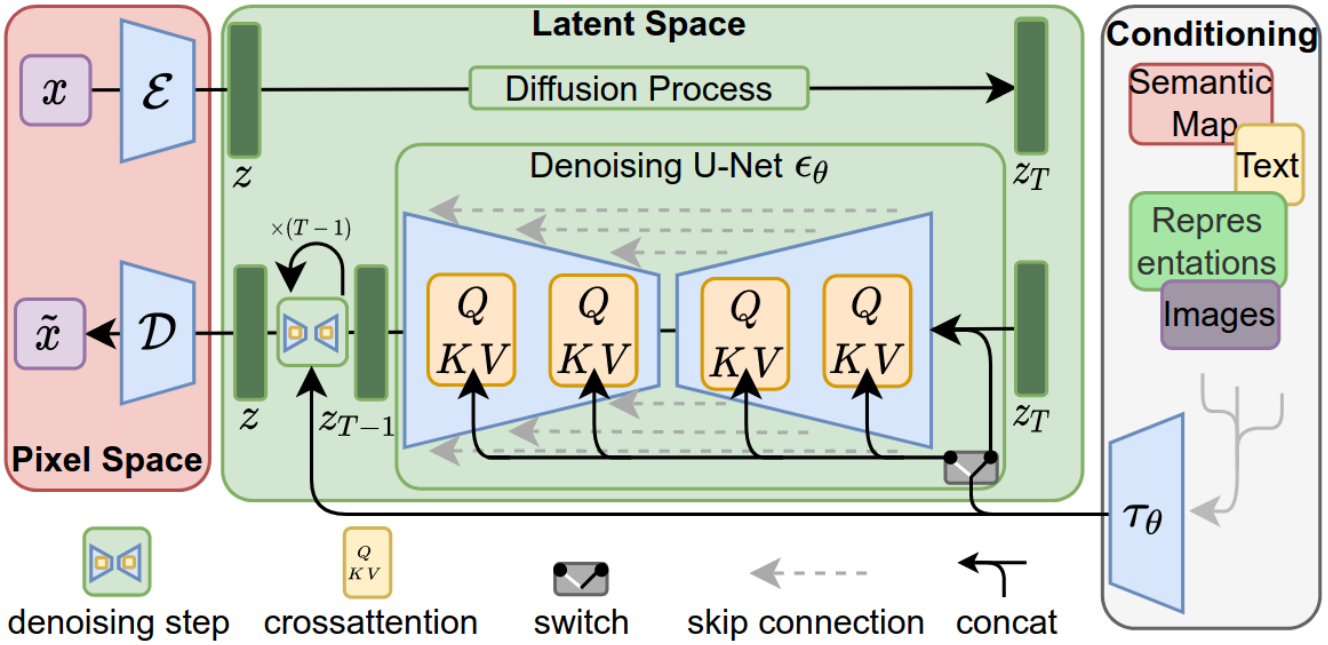
The goal of the diffusion model is, given a noisy image $Y = X + \sigma\mathcal{E}$ and σ, to find the noise $\mathcal{E}$. The denoising Auto-Encoder instead attempts to find the original image X. At the limit $\sigma \to 0$, the denoising Auto-Encoder $D(E(X + \sigma\mathcal{E}))$ is a classical Auto-Encoder, hence the name.

To train the denoising Auto-Encoder, we can use the Evidence Lower-Bound with $Y = X + \sigma\mathcal{E}$ and Z such that $X = D(E(Z))$ [HJA20]:

$$-\log(f_X(x)) \leq \mathbb{E}[-\log(f_{X|Z}(x|Y))] + D((Y|X = x) \parallel Z)$$

[HJA20] J. Ho, A. Jain and P. Abbeel. *Denoising Diffusion Probabilistic Models*. In: *Proceedings of the 34th International Conference on Neural Information Processing Systems, NIPS '20* (Curran Associates Inc., Red Hook, NY, USA, Dec 2020); pp. 6840–6851. Accessed on Nov 26, 2024.

Conditioned diffusion



Source : [RBL+22; Figure 3]

[RBL+22] R. Rombach, A. Blattmann, D. Lorenz *et al.* *High-Resolution Image Synthesis With Latent Diffusion Models*. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition* (2022); pp. 10684–10695. Accessed on Aug 26, 2024.

Classifier-Free Guidance

Improvement for conditioned diffusion for multi-modal distributions : use classifier [DN24]. **Issue**: need to train a classifier...

This classifier-guided strategy was replaced in [HS22] by a simpler trick: Train both a conditioned (with condition τ) and unconditioned diffusion model and combine then with:

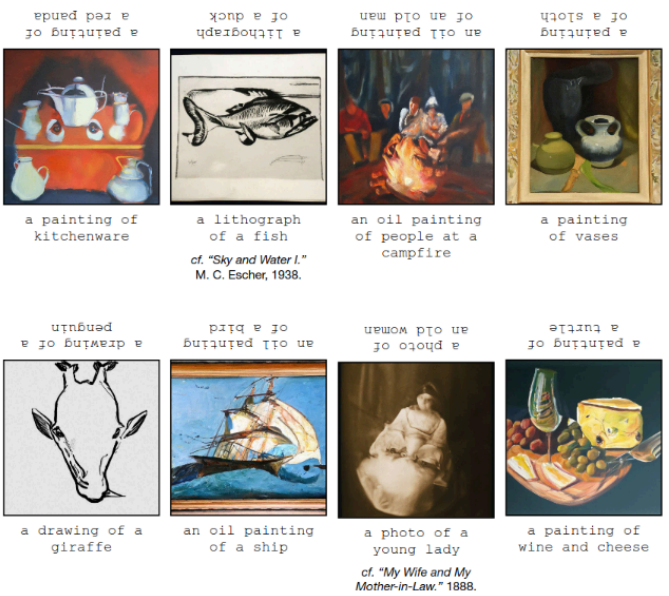
$$\bar{\epsilon}_t = \lambda \epsilon_\theta(x_t, \sigma_t, \tau) + (1-\lambda)\epsilon_\theta(x_t, \sigma_t) \qquad \text{with } \lambda > 1$$

[DN24] P. Dhariwal and A. Nichol. *Diffusion Models Beat GANs on Image Synthesis*. In: *Proceedings of the 35th International Conference on Neural Information Processing Systems, NIPS '21* (Curran Associates Inc., Red Hook, NY, USA, Jun 2024); pp. 8780–8794. Accessed on Nov 26, 2024.
[HS22] J. Ho and T. Salimans. *Classifier-Free Diffusion Guidance* (Jul 2022), arXiv:2207.12598. Accessed on Nov 26, 2024.

Optical illusions

It was shown in [BLL+23] how to train a diffusion model to generate illusions. Suprisingly, [GPO24] showed that you don't need a specialized model and you can use a pre-trained diffusion model. Given N transformations $v_1, \ldots, v_N$ [GPO24; Equation (2)]:

$$\bar{\epsilon}_t = \frac{1}{N} \sum_{i=1}^{N} v_i^{-1}(\epsilon_\theta(v_i(x_t), \sigma_t, \tau))$$



[BLL+23] R. Burgert, X. Li, A. Leite *et al*. *Diffusion Illusions: Hiding Images in Plain Sight* (Dec 2023), arXiv:2312.03817. Accessed on Nov 27, 2024.

[GPO24] D. Geng, I. Park and A. Owens. *Visual Anagrams: Generating Multi-View Optical Illusions with Diffusion Models* (Apr 2024), arXiv:2311.17919. Accessed on Nov 27, 2024.

Utils

```
using PlutoUI, DataFrames, PrettyTables, LinearAlgebra, Luxor, LaTeXStrings, MathTeXEngine
```

```
import DocumenterCitations, CSV, Logging
```

```
qa (generic function with 2 methods)
```

```
include("utils.jl")
```

```
biblio =
```

▸ CitationBibliography("/home/runner/work/LINMA2472/LINMA2472/Lectures/biblio.bib", AlphaSt

```
biblio = load_biblio!()
```

```
ⓘ Loading bibliography from `/home/runner/work/LINMA2472/LINMA2472/Lectures/biblio.bib`...
```

```
ⓘ Loading completed.
```

```
cite (generic function with 1 method)
```

```
cite(args...) = bibcite(biblio, args...)
```

```
refs (generic function with 1 method)
```

```
refs(args...) = bibrefs(biblio, args...)
```