Diffusion Model

Machine Learning pour Physicien - Projet

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January 16, 2025

Modèle de diffusion

Présentation générale

Les modèles de diffusion permettent de générer des images distribuées de la même manière qu'un dataset donnée.

Dataset

Images générées

Figure 1: Source : Denoising Diffusion Probabilistic Models, Ho. and Al.

Application en physique

Eliot si tu peux rajouter quelques trucs ici, genre des exemples avec des images

Denoising Diffusion Probabilistic Models, théorie

General Idea

Consider the set of hand-written digits D. Can you give a probability distribution q such that $x \sim q(x)$?

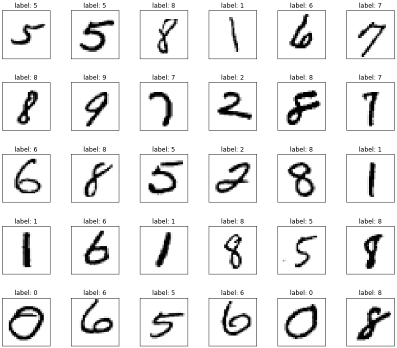

Figure 2: Source: ludwig.ai

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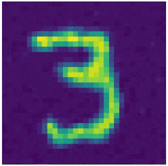
Consider the set of hand-written digits D. It is hard to find q such that $x \sim q(x)$, we need a clever way to sample hand-written digits. Consider the following process:



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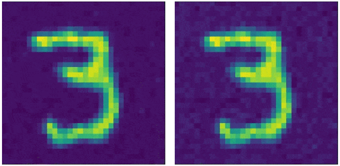

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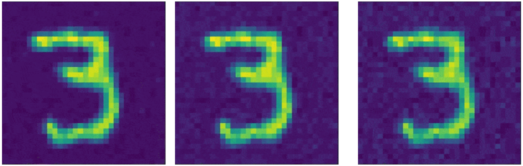

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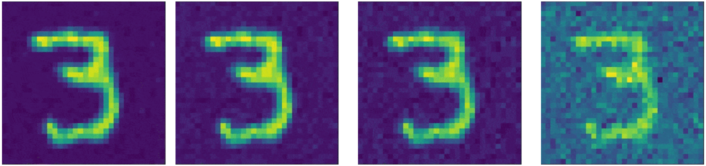

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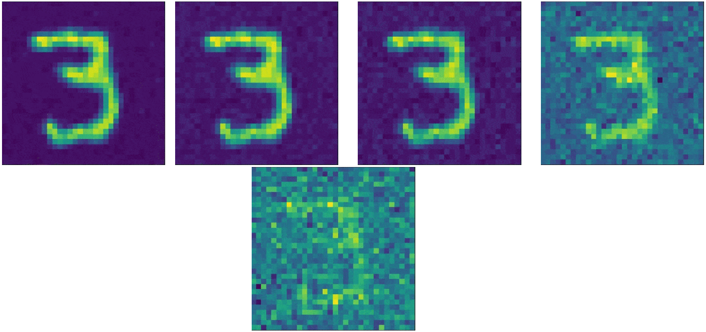

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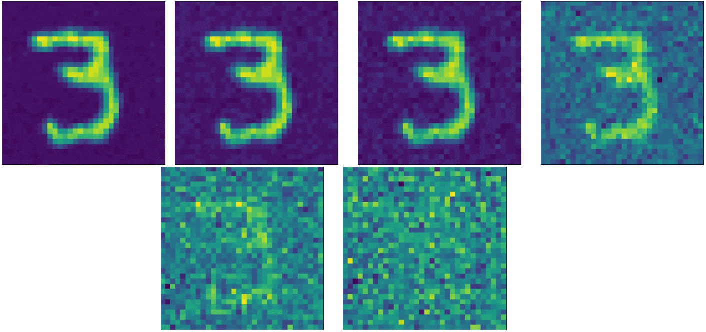

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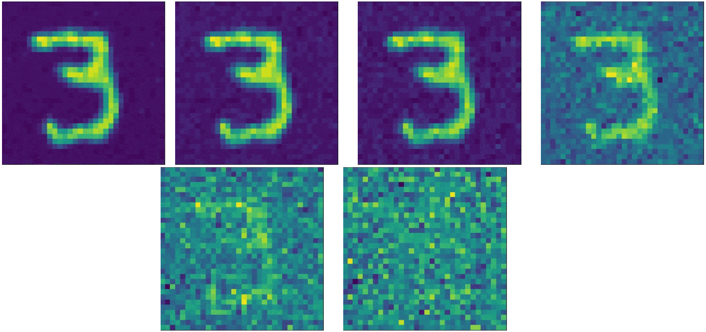
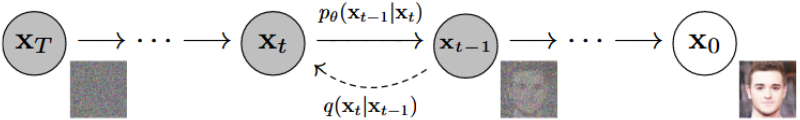


Formally: $q(x_{t+1} \mid x_t) := \mathcal{N}(x_{t+1}; \sqrt{1-\beta_t} x_t, \beta_t I)$ for some schedule $(\beta_t)_t$. Can we learn to reverse this process ?

What we want to learn

Given a noisy image x_t, we train a model to predict x_{t-1}.



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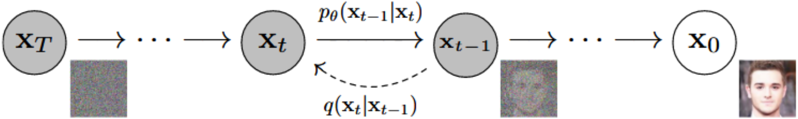

- Given a data image x_0, we sample $(x_t)_{1:T}$ according to $q(x_{1:T} \mid x_0) := \prod_{t=1}^{T} q(x_t \mid x_{t-1})$,

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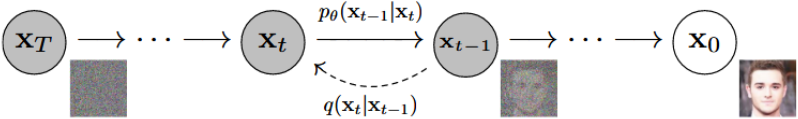

- Given a data image x_0, we sample $(x_t)_{1:T}$ according to $q(x_{1:T} \mid x_0) := \prod_{t=1}^{T} q(x_t \mid x_{t-1})$,
- Given a noisy image x_t and t, we sample according to $p_\theta(x_{t-1} \mid x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$.

Decreasing training data generation cost

Given a data image x_0, compute x_t takes t sampling on q. But a simple trick, allows to do only one.

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Remember that $q(x_{t+1} \mid x_t) := \mathcal{N}(x_{t+1}; \sqrt{1-\beta_t}x_t, \beta_t I)$. Let $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$.

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$$x_t = \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1}$$

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Let $G_1 \sim \mathcal{N}(0, \sigma_1^2 I)$, $G_2 \sim \mathcal{N}(0, \sigma_2^2 I)$, the sum of them gives $g_2 \sim \mathcal{N}(0, (\sigma_1^2 + \sigma_2^2)I)$.

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We have $x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$.

Training

For now, our model is learning μ and Σ, i.e. we sample according to

$$p_\theta(x_{t-1} \mid x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

They've found that fixing Σ_θ to a constant gives the same result. So,

$$p_\theta(x_{t-1} \mid x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t I)$$

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The probability for our model to generate x_0 is $p_\theta(x_0) := \int p_\theta(x_{0:T}) dx_{1:T}$.

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$$E_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2 \right]$$

where $\tilde{\mu}$ is the optimal mean that depends on x_0 which we don't know.

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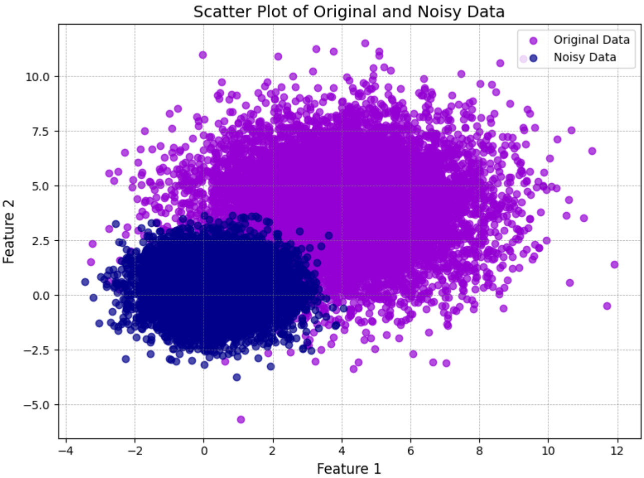
where $\tilde{\mu}$ is the optimal mean that depends on x_0. Using $x_t(x_0, \epsilon) = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$ we have a loss we can train on.

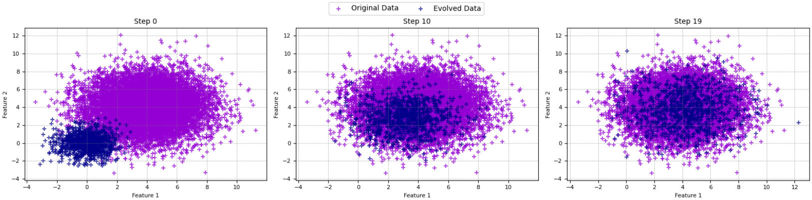
Our results - Gaussian

We have started with Gaussian generation:



Our results - Gaussian

We have started with Gaussian generation and got satisfying results:

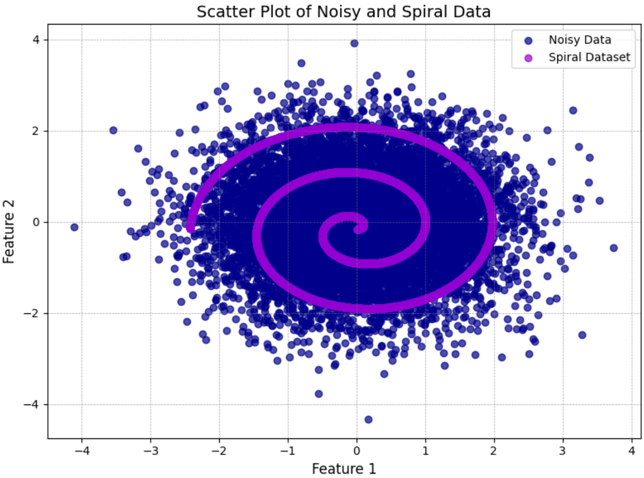


Our results - Deux gaussiennes

A ajouter

Our results - Spirale

Then we moved to a more complicated dataset, Spirale generation:



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