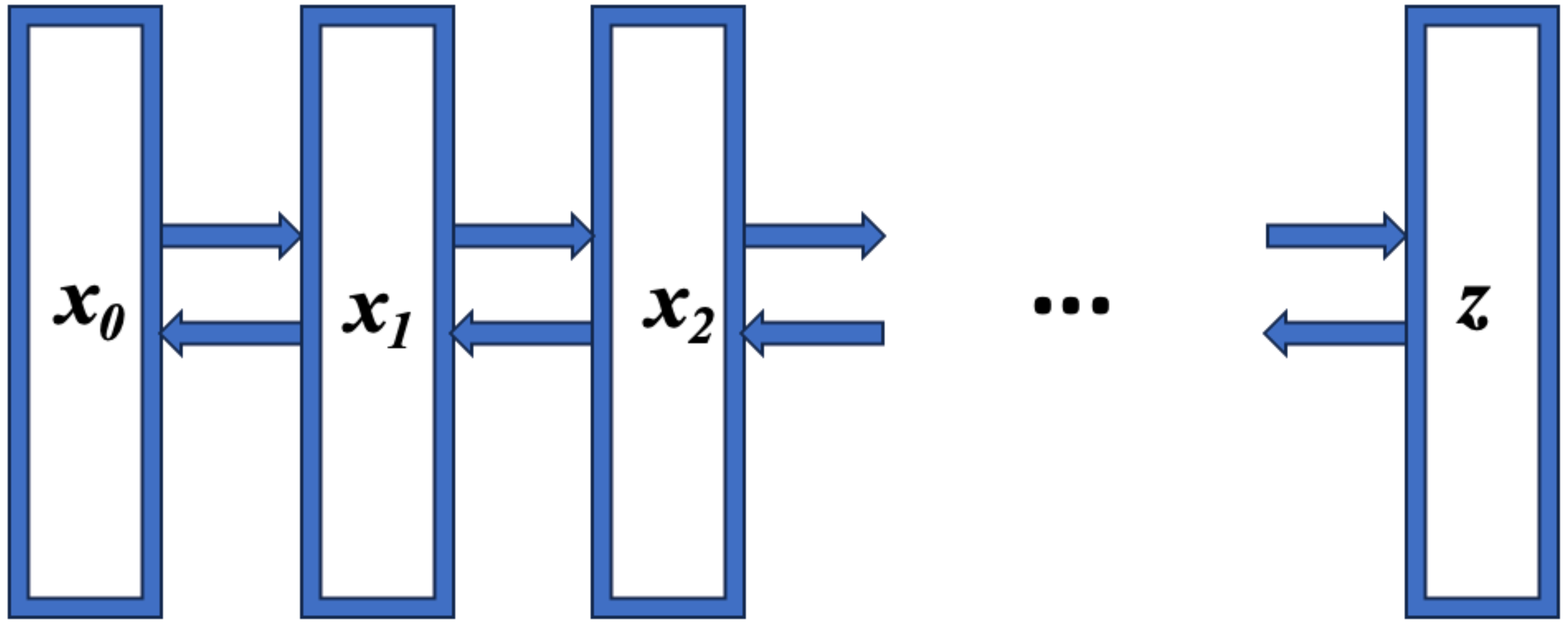
Lecture 2. Diffusion models

Introduction to Bayesian statistical Learning II

04.06.2024 Instructors: Alina Bazarova, Oleg Filatov, Sabrina Benassou

Denoising Diffusion Probabilistic Models (DDPM)

Another type of generative models. What do they have to do with Bayes?



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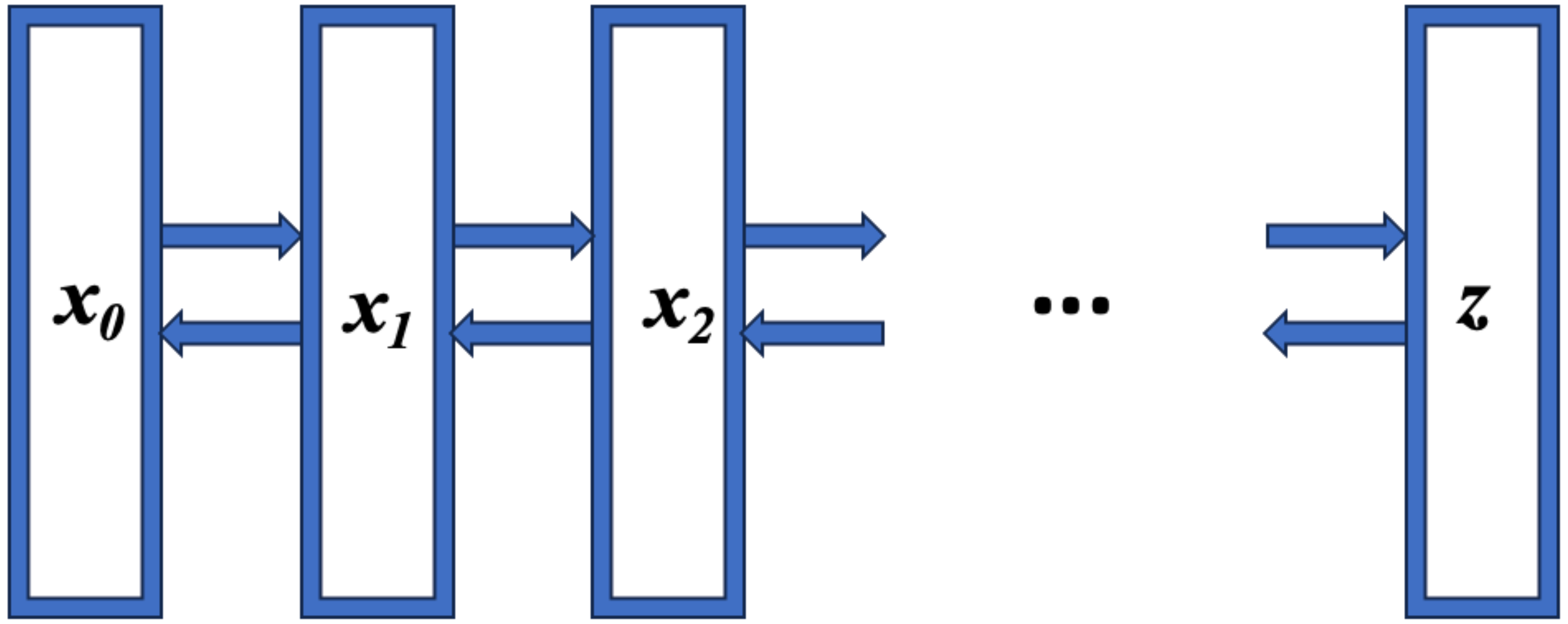

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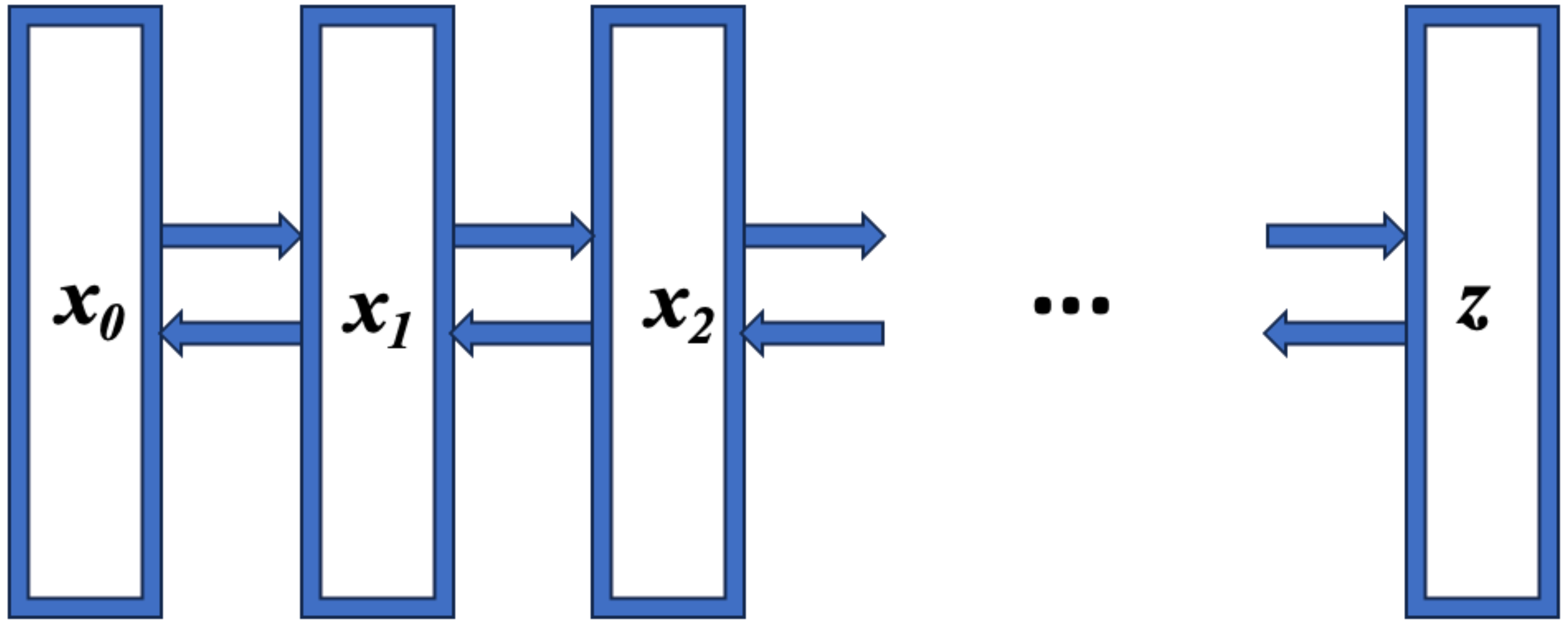

1. Forward diffusion process: gradually **adding noise** to samples
2. Reverse diffusion process: **recreating** the sample **from noise**
3. Heavily relying on conditional probability and **Bayes theorem** in particular

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As $T \rightarrow \infty$, x_T is equivalent to a **Gaussian distribution**

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Larger update step when the sample gets noisier: $\beta_1 < \beta_2 < \ldots < \beta_T$,

and therefore $\bar{\alpha}_1 > \ldots > \bar{\alpha}_T$

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If we reverse the above process and sample from $q(x_{t-1} | x_t)$,

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Important: $q(x_{t-1} | x_t, x_0) \sim \mathcal{N}(x_{t-1}; \tilde{\mu}(x_t, x_0), \tilde{\beta}\mathbf{I})$ **tractable!**

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We can reparametrise it further! —> $= \dfrac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}x_t + \dfrac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}x_0$

Remember! $x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1 - \bar{\alpha}_t}\varepsilon,\qquad x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1 - \bar{\alpha}_t}\varepsilon_t)$

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Recap! We need to learn the distributions $p_\theta(x_{t-1} \mid x_t) \sim \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

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Kullback-Leibler divergence ≥ 0

$$-\log p_\theta(x_0) \leq -\log p_\theta(x_0) + D_{KL}(q(x_{1:T} \,|\, x_0) \,||\, p_\theta(x_{1:T} \,|\, x_0)) =$$

$$-\log p_\theta(x_0) + E_{x_{1:T} \sim q(x_{1:T}|x_0)}[\log \frac{q(x_{1:T} \,|\, x_0)}{p_\theta(x_{0:T})/p_\theta(x_0)}] = -\log p_\theta(x_0) + E_q[\log \frac{q(x_{1:T} \,|\, x_0)}{p_\theta(x_{0:T})}] + \log p_\theta(x_0)$$

Remember! $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon, \qquad x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\varepsilon_t)$

Substitute this into expression of $\tilde{\mu}_t$ and get $\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_t)$

Recap! We need to learn the distributions $p_\theta(x_{t-1} | x_t) \sim \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

So we will train μ_θ to predict $\tilde{\mu}_t$

How are we going to do that? Minimise negative log-likelihood $-\log p_\theta(x_0)$

$$-\log p_\theta(x_0) \leq -\log p_\theta(x_0) + \underbrace{D_{KL}(q(x_{1:T} | x_0) || p_\theta(x_{1:T} | x_0))}_{\textbf{Kullback-Leibler divergence } \geq 0} =$$

$$-\log p_\theta(x_0) + E_{x_{1:T} \sim q(x_{1:T}|x_0)}[\log \frac{q(x_{1:T} | x_0)}{p_\theta(x_{0:T})/p_\theta(x_0)}] = -\log \cancel{p_\theta(x_0)} + E_q[\log \frac{q(x_{1:T} | x_0)}{p_\theta(x_{0:T})}] + \log \cancel{p_\theta(x_0)} = E_q[\log \frac{q(x_{1:T} | x_0)}{p_\theta(x_{0:T})}]$$

Let $L_{VLB} = E_{q(x_{0:T})}[\log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}] \geq -E_{q(x_0)} \log p_\theta(x_0)$

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We used that $E_{q(x_0)} E_{q(x_{1:T}|x_0)} f(x_{0:T}) = E_{q(x_{0:T})} f(x_{0:T})$ for any f of our interest

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$$= E_q[\underbrace{D_{KL}(q(x_T|x_0)||p_\theta(x_T))}_{L_T} + \sum_{t=2}^{T} \underbrace{D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))]}_{L_{t-1}} - \underbrace{\log p_\theta(x_0|x_1)}_{L_0}$$

Simplifying the loss further

$$L_{VLB} = L_T + L_{T-1} + \ldots + L_0$$

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Remember again! We need to learn the distributions $p_\theta(x_{t-1} | x_t) \sim \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

That is for L_t !

Parametrisation of L_t for Training Loss

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

We would like to train μ_θ to predict $\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_t)$

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$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}}\varepsilon_\theta(x_t, t))$$

Parametrisation of L_t for Training Loss

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$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t, t)) \qquad x_{t-1} \sim \mathcal{N}(x_{t-1}; \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t, t)), \Sigma_\theta(x_t, t))$$

Parametrisation of L_t for Training Loss

$$L_t = E_{x_0,\varepsilon}\left[\frac{1}{2||\Sigma_\theta(x_t, t)||_2^2}||\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)||^2\right]$$

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$$= E_{x_0,\varepsilon}\left[\frac{1}{2||\Sigma_\theta||_2^2}||\frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_t) - \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t,t))||^2\right]$$

Parametrisation of L_t for Training Loss

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$$= E_{x_0,\varepsilon}[\frac{1}{2||\Sigma_\theta||_2^2}||\frac{1}{\sqrt{\alpha_t}}(\cancel{x_t} - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_t) - \frac{1}{\sqrt{\alpha_t}}(\cancel{x_t} - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t,t))||^2]$$

$$= E_{x_0,\varepsilon}[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)||\Sigma_\theta||_2^2}||\varepsilon_t - \varepsilon_\theta(x_t,t)||^2]$$

Parametrisation of L_t for Training Loss

$$L_t = E_{x_0,\varepsilon}[\frac{1}{2||\Sigma_\theta(x_t,t)||_2^2}||\tilde{\mu}_t(x_t,x_0) - \mu_\theta(x_t,t)||^2]$$

$$= E_{x_0,\varepsilon}[\frac{1}{2||\Sigma_\theta||_2^2}||\frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_t) - \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t,t))||^2]$$

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Bottom line: what we are doing is predicting the noise!

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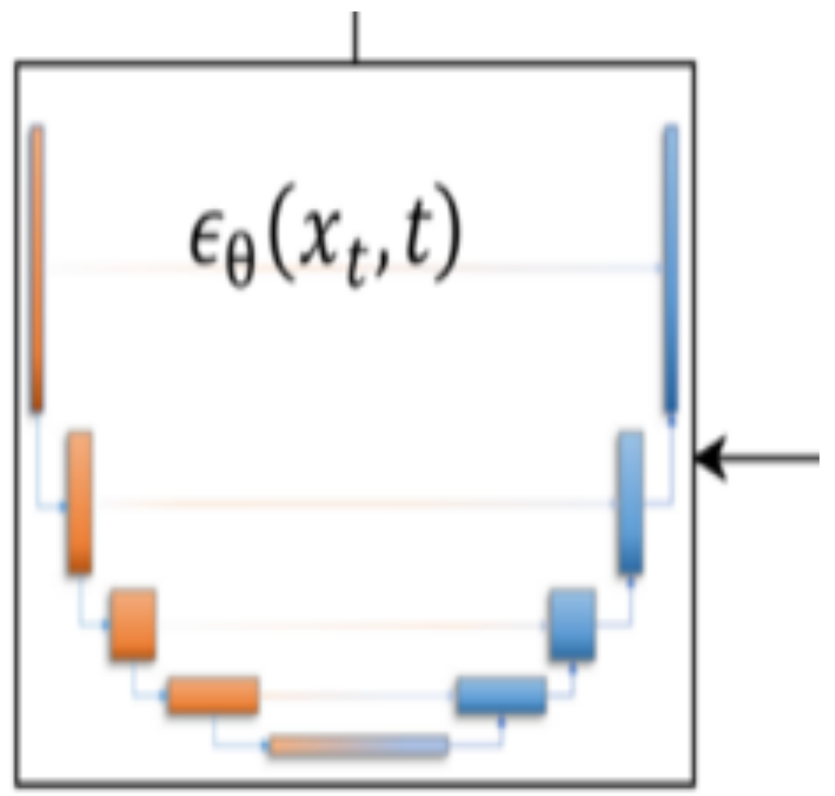

Bottom line: what we are doing is predicting the noise!

Unet architecture is used for that

Parametrization of β_t

Typically a sequence of linearly increasing constants: e.g. from $\beta_1 = 10^{-4}$ to $\beta_T = 0.02$

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Hence, the loss $L = L_{simple} + \lambda L_{VLB}$, λ is small ~ 0.001 and L_{VLB} only guides the training of Σ_θ

(In L_{VLB} stop gradient with respect to μ_θ)

Bonus! Score networks and guided diffusion

The score of each sample's x probability density function is defined as $\nabla_x \log q(x)$

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$$q(x_t | x_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t} x_0, (1-\bar{\alpha}_t)\mathbf{I})$$

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And therefore $s_\theta(x_t, t) \approx \nabla_{x_t} \log q(x_t) = E_{q(x_0)} \nabla_{x_t} q(x_t \mid x_0) = E_{q(x_0)}\left[-\frac{\varepsilon_\theta(x_t, t)}{\sqrt{1-\bar{\alpha}_t}}\right] = -\frac{\varepsilon_\theta(x_t, t)}{\sqrt{1-\bar{\alpha}_t}}$

Guided diffusion

- We have additional input y (a class label in classifier guided diffusion)
- We want to model a conditional distribution $p(x \mid y)$ instead

Conditioned on dogs

Classifier guided diffusion

We separately train a classifier $f_\phi(y \mid x_t, t)$ on a noisy image x_t, and use gradients $\nabla_x \log f_\phi(y \mid x_t)$

to guide the diffusion. Let us have a joint distribution $q(x_t, y)$, y is e.g. the image label

Classifier guided diffusion

We separately train a classifier $f_\phi(y|x_t, t)$ on a noisy image x_t, and use gradients $\nabla_x \log f_\phi(y|x_t)$

to guide the diffusion. Let us have a joint distribution $q(x_t, y)$, y is e.g. the image label

$$\nabla_{x_t} \log q(x_t|y) = \nabla_{x_t} \log q(x_t) + \nabla_{x_t} \log q(y|x_t) - \nabla_{x_t} \log q(y)$$

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Where w is the strength of the guidance

Classifier guided diffusion

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $f_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + s\Sigma\,\nabla_{x_t} \log f_\phi(y|x_t), \Sigma)$
end for
return x_0

Downsides:

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Downsides:

- The classifier has to cope with noise, might need to be trained separately
- If noise-robust might be inefficient: most of the information on x is irrelevant to y

Classifier free guidance

- Train a diffusion model $p(x \mid y)$ with conditioning dropout: conditional information is removed some percentage of the time

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Classifier free guidance

- Train a diffusion model $p(x|y)$ with conditioning dropout: conditional information is removed some percentage of the time
- Resulting model can be conditional $p(x|y)$ and unconditional $p(x)$
- No need for a separate classifier!

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Guide the diffusion without an independent classifier f_ϕ

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Classifier free guidance

$$\nabla_{x_t} \log p(x_t, y) = \nabla_{x_t} \log p(x_t \mid y) + \nabla_{x_t} \log p(y \mid x_t)$$

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Hence, analogously to the case of classifier guided diffusion

Classifier free guidance

$$\nabla_{x_t} \log p(x_t, y) = \nabla_{x_t} \log p(x_t \,|\, y) + \nabla_{x_t} \log p(y \,|\, x_t)$$

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Hence, analogously to the case of classifier guided diffusion

$\bar{\varepsilon}_\theta(x_t, t, y) = \varepsilon_\theta(x_t, t, y) - \sqrt{1-\bar{\alpha}_t}\, w \nabla_{x_t} \log p(y \,|\, x_t)$, where $\varepsilon_\theta(x_t, t, y)$ parametrises $p(x_t \,|\, y)$

Classifier free guidance

$$\nabla_{x_t} \log p(x_t, y) = \nabla_{x_t} \log p(x_t | y) + \nabla_{x_t} \log p(y | x_t)$$

$$\nabla_{x_t} \log p(y | x_t) = -\frac{1}{\sqrt{1 - \bar{\alpha}_t}} (\varepsilon_\theta(x_t, t, y) - \varepsilon_\theta(x_t, t))$$

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$$= \varepsilon_\theta(x_t, t, y) + w(\varepsilon_\theta(x_t, t, y) - \varepsilon_\theta(x_t, t))$$