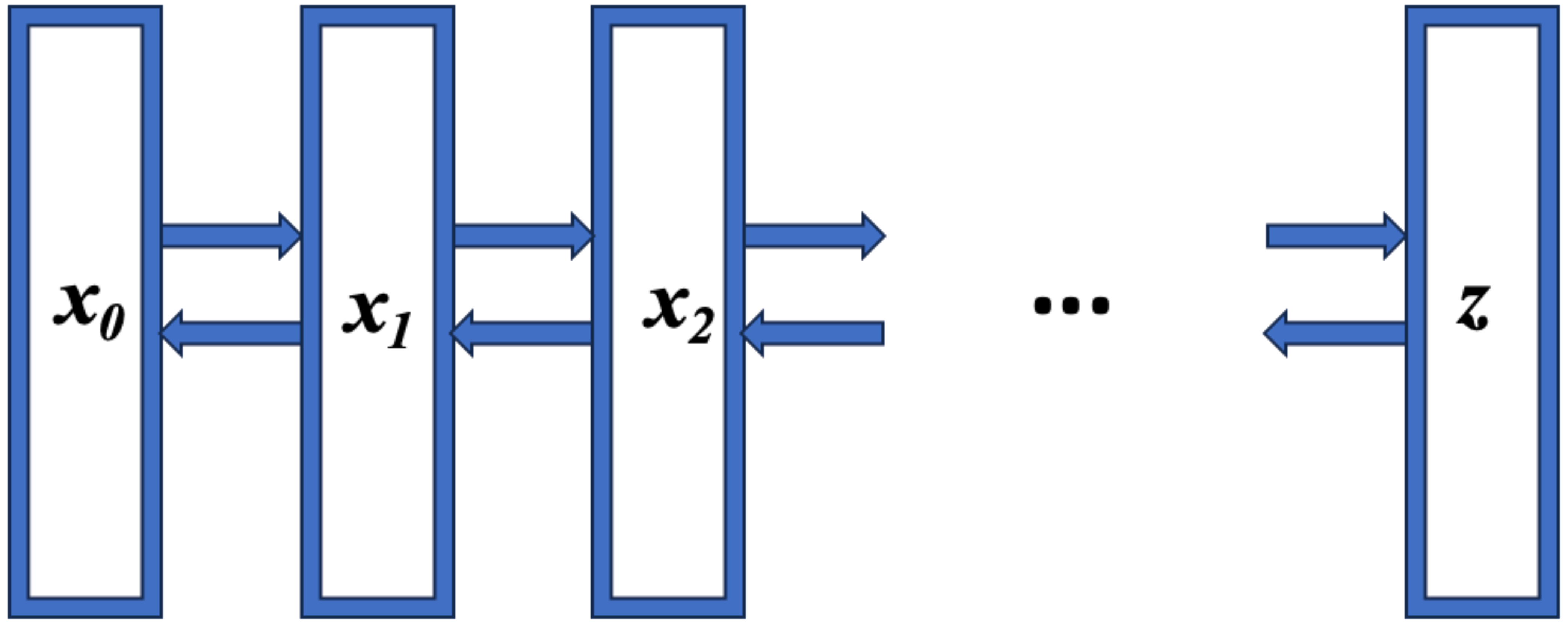
Lecture 2. Diffusion models

Introduction to Bayesian statistical Learning II

04.06.2024 Instructors: Alina Bazarova, Oleg Filatov

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



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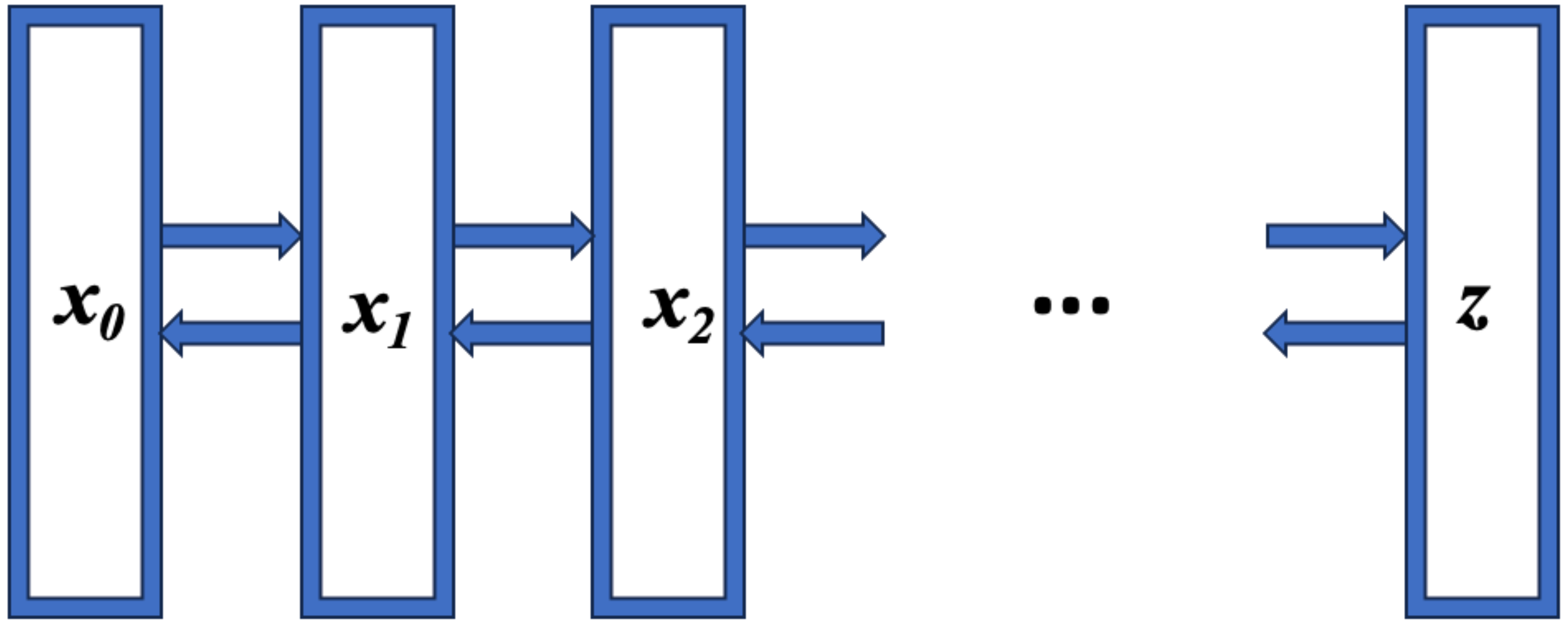

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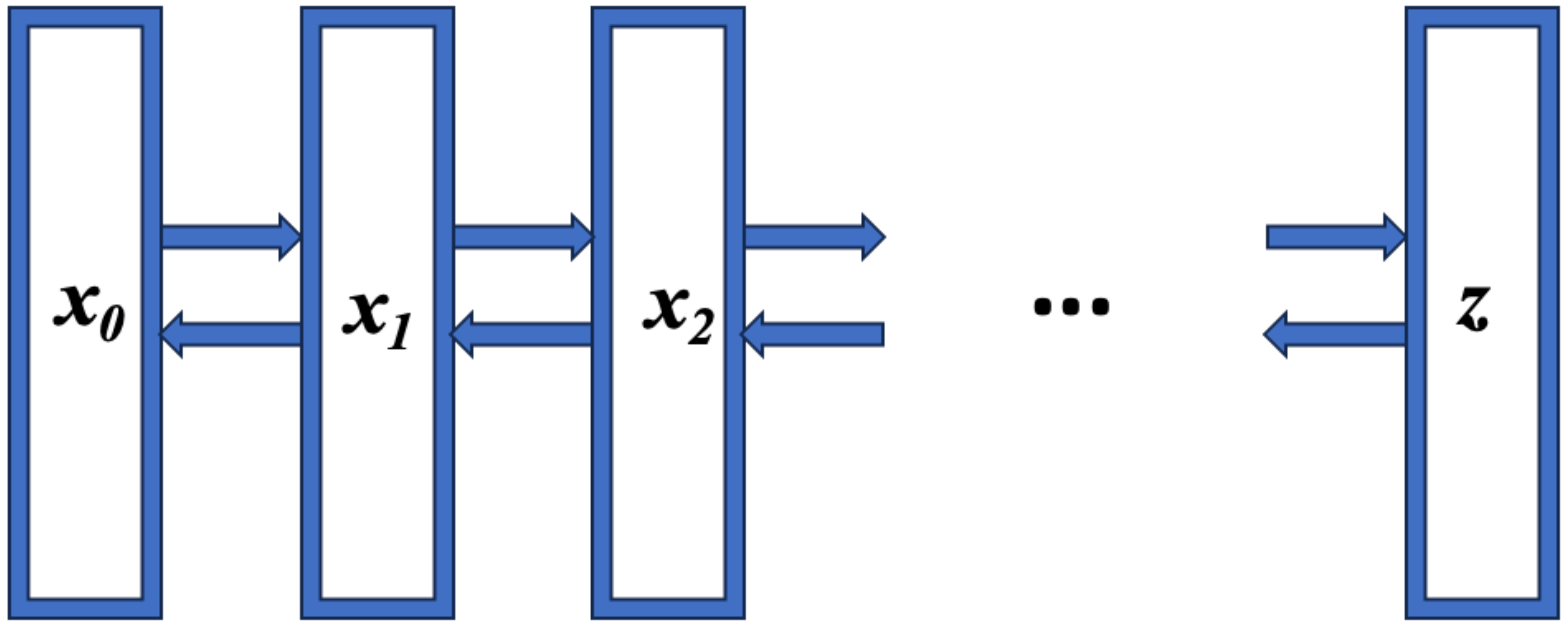

1. Forward diffusion process: gradually **adding noise** to samples
2. Reverse diffusion process: **recreating** the sample **from noise**
3. Heavily relying on conditional probability and **Bayes theorem** in particular

Forward diffusion process

Let $x_0 \sim q(x)$ be a real data distribution.

We produce a sequence of **noisy samples** $x_1, \ldots, x_T$

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

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$$x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1 - \alpha_t} \varepsilon_{t-1} = \sqrt{\alpha_t \alpha_{t-1}} x_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \bar{\varepsilon}_{t-2}$$

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Following the same argument

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

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

Reverse diffusion process

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

we can recreate a sample from $x_T \sim \mathcal{N}(0,\mathbf{I})$

We need to estimate $q(x_{t-1} | x_t)$. We do it with another probability density function p_θ

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1} | x_t), \quad p_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

Which is learned via a neural network (θ are the parameters of NN)!

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! —>

$$= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}x_0$$

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

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

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Kullback-Leibler divergence ≥ 0

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

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

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 $-\log p_\theta(x_0)$

Kullback-Leibler divergence ≥ 0

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

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

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

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

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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

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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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But x_t is available during training time!

Hence, let us **predict the noise term instead**!

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

Parametrisation of L_t for Training Loss

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

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$$L_t^{simple} = E_{t,x_0,\varepsilon}[||\varepsilon_t - \varepsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon_t, t)||^2$$

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

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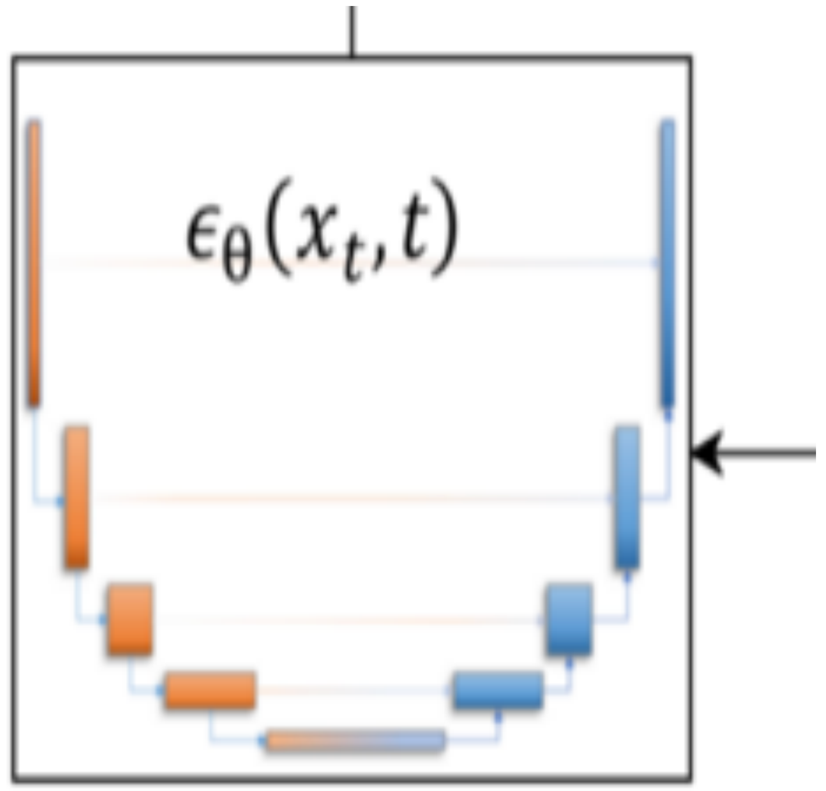

Bottom line: what we are doing is predicting the noise! Unet architecture is used for that

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

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Alternative $\Sigma_\theta(x_t, t) = \exp(v \log \beta_t + (1 - v) \log \tilde{\beta}_t)$, $\quad \tilde{\beta}_t = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}$, v is learnable

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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

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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Langevin dynamics can sample data points from a probability density distribution using only the score $\nabla_x \log q(x)$ in an iterative process.

Score network $s_\theta(x_t, t) \approx \nabla_x \log q(x)$ If $x \sim \mathcal{N}(\mu, \sigma^2 \mathbf{I})$, $\nabla_x \log p(x) = \nabla_x(-\frac{1}{2\sigma^2}(x-\mu)^2)$

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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 $\nabla_x \log f_\phi(y \mid x_t)$

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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 ve inefficient: most of the information on x is irrelevant to y

Classifier free guidance

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Guide the diffusion without an independent classifier f_ϕ

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- Unconditional denoising diffusion model $p_\theta(x)$, parametrised through a score estimator $\varepsilon_\theta(x_t, t)$

- Conditional model $p_\theta(x \mid y)$ parametrised through $\varepsilon_\theta(x_t, t, y)$

- Conditional model is trained on paired data (x, y)

- Conditional information y gets discarded periodically: $\varepsilon_\theta(x_t, t) = \varepsilon_\theta(x_t, t, y = \emptyset)$

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

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

Classifier free guidance

Guide the diffusion without an independent classifier f_ϕ

- Unconditional denoising diffusion model $p_\theta(x)$, parametrised through a score estimator $\varepsilon_\theta(x_t, t)$

- Conditional model $p_\theta(x \mid y)$ parametrised through $\varepsilon_\theta(x_t, t, y)$

- Conditional model is trained on paired data (x, y)

- Conditional information y gets discarded periodically: $\varepsilon_\theta(x_t, t) = \varepsilon_\theta(x_t, t, y = \varnothing)$

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

$$\begin{aligned}\bar{\varepsilon}_\theta(x_t, t, y) &= \varepsilon_\theta(x_t, t, y) - \sqrt{1-\bar{\alpha}_t}\, w \nabla_{x_t} \log p(y \mid x_t) = \varepsilon_\theta(x_t, t, y) + w(\varepsilon_\theta(x_t, t, y) - \varepsilon_\theta(x_t, t)) \\ &= (w+1)\varepsilon_\theta(x_t, t, y) - w\varepsilon_\theta(x_t, t)\end{aligned}$$