Introduction to Deep Generative Modeling

Lecture #13

HY-673 – Computer Science Dep., University of Crete

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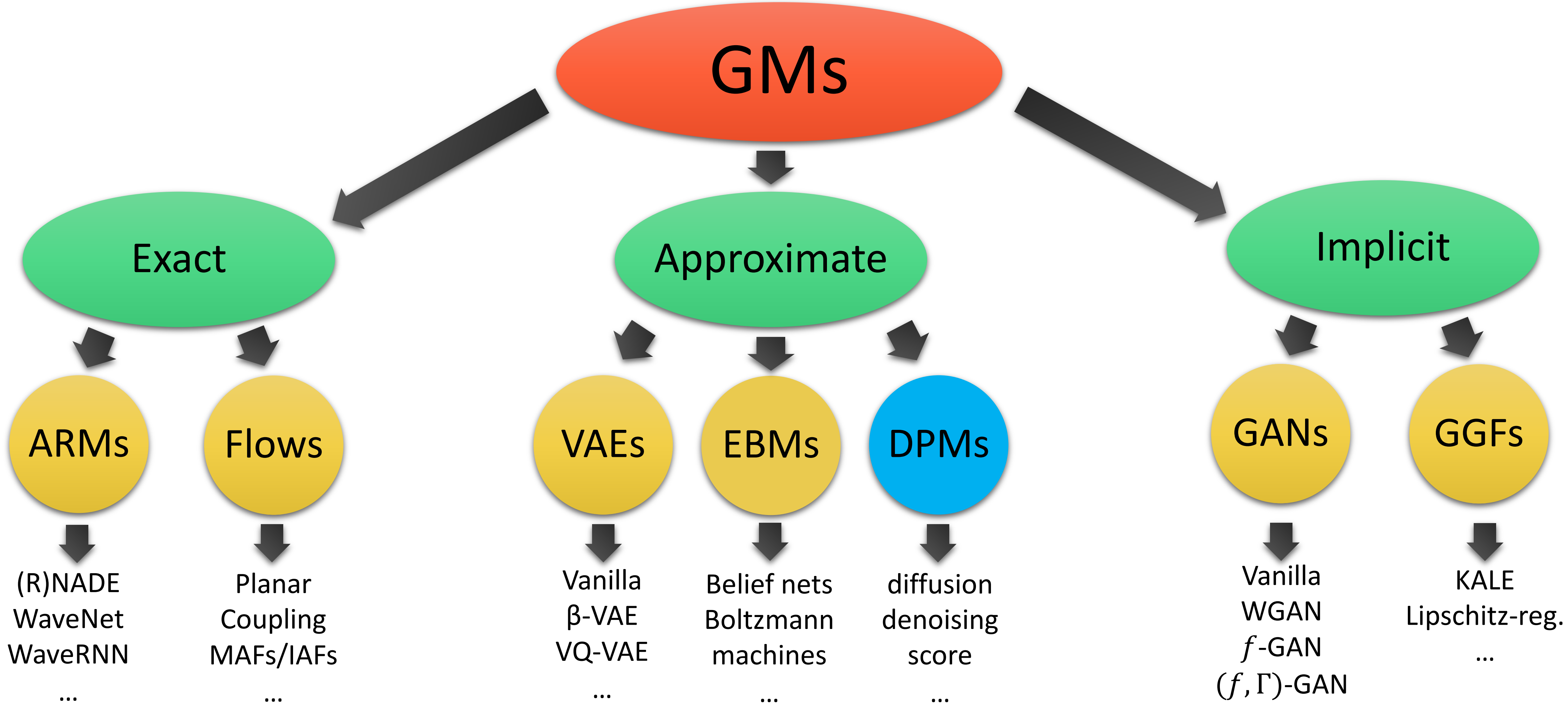
Taxonomy of GMs



Denoising Diffusion Models

Emerging as powerful generative models, outperforming GANs

https://arxiv.org/abs/2105.05233

https://arxiv.org/abs/2106.15282

Image Super-resolution

Successful applications - SR3 Mode

https://arxiv.org/abs/2104.07636

Text-to-Image Generation

DALL·E 2

“a teddy bear on a skateboard in times square”

Imagen

“A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk”.

https://arxiv.org/abs/2204.06125

https://arxiv.org/abs/2205.11487

Learning to generate by denoising

Denoising diffusion models consist of two processes:

- Forward diffusion process that gradually adds noise to input
- Reverse denoising process that learns to generate data by denoising

Forward diffusion process (fixed)

Data

Noise

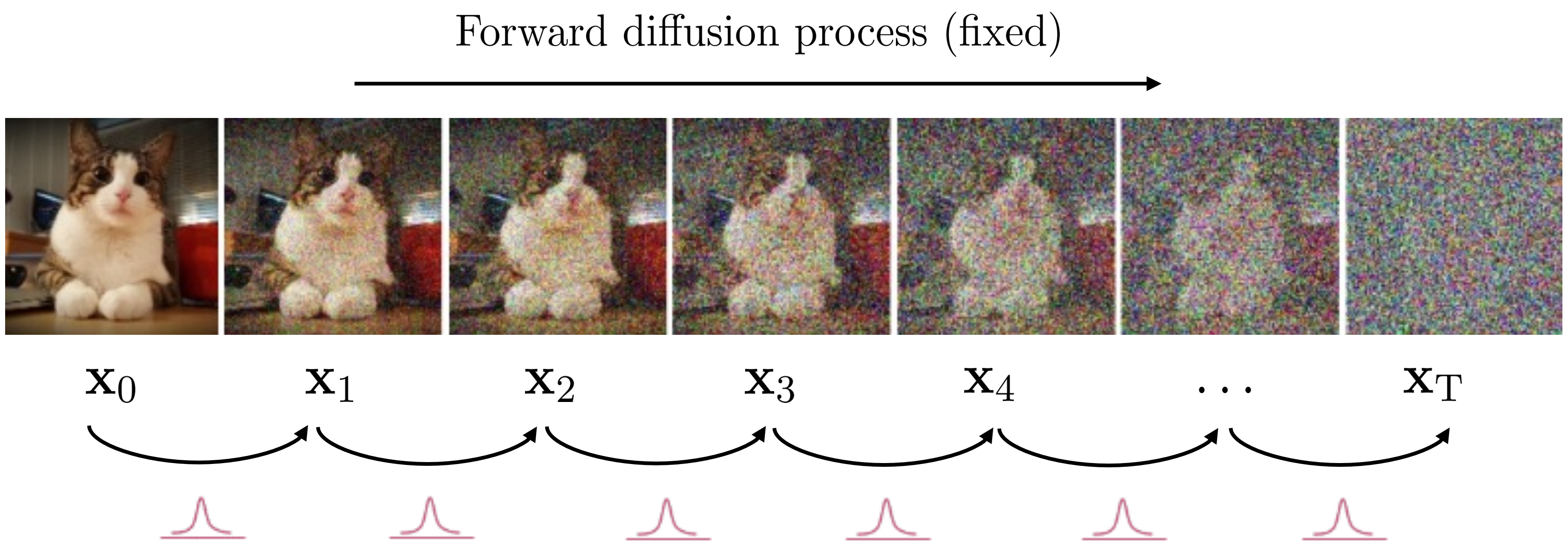
Reverse denoising process (generative)

https://arxiv.org/abs/2011.13456
https://arxiv.org/abs/2006.11239
https://arxiv.org/abs/1503.03585

Forward Diffusion Process

The formal definition of the forward process in T steps:

Data

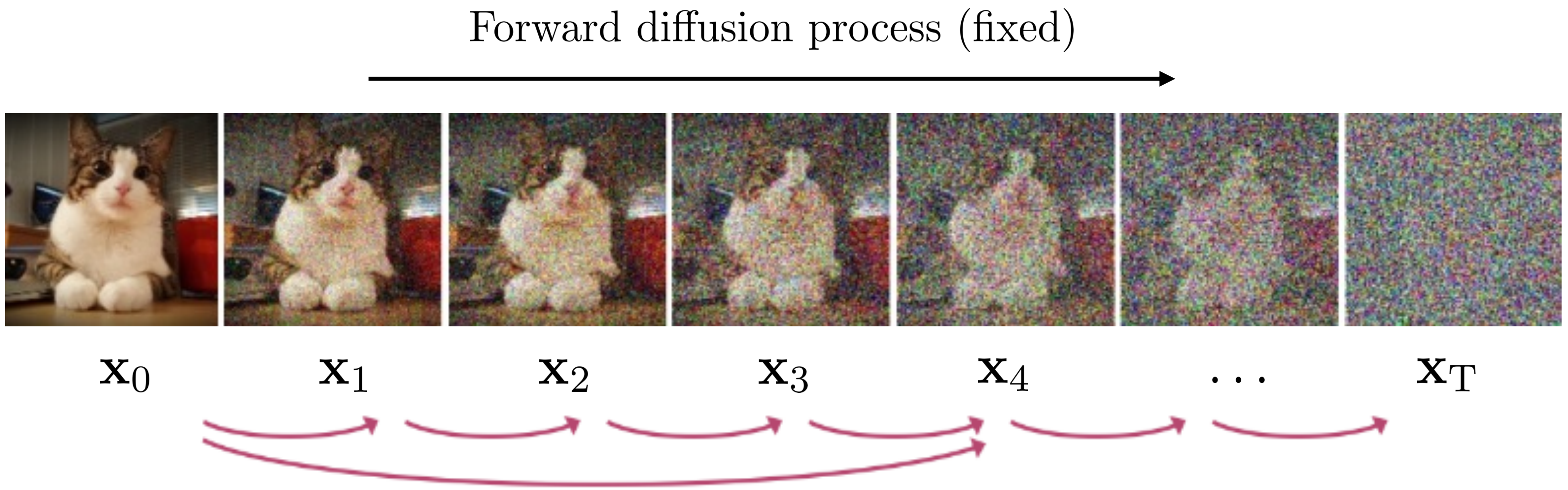


Noise

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \mathbf{I}) \quad \Rightarrow \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}). \qquad \text{(joint)}$$

Diffusion Kernel

Data



Noise

(Diffusion Kernel)

Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$.

For sampling: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

β_t values schedule (i.e., the noise schedule) is designed such that $\bar{\alpha}_T \rightarrow 0$ and $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

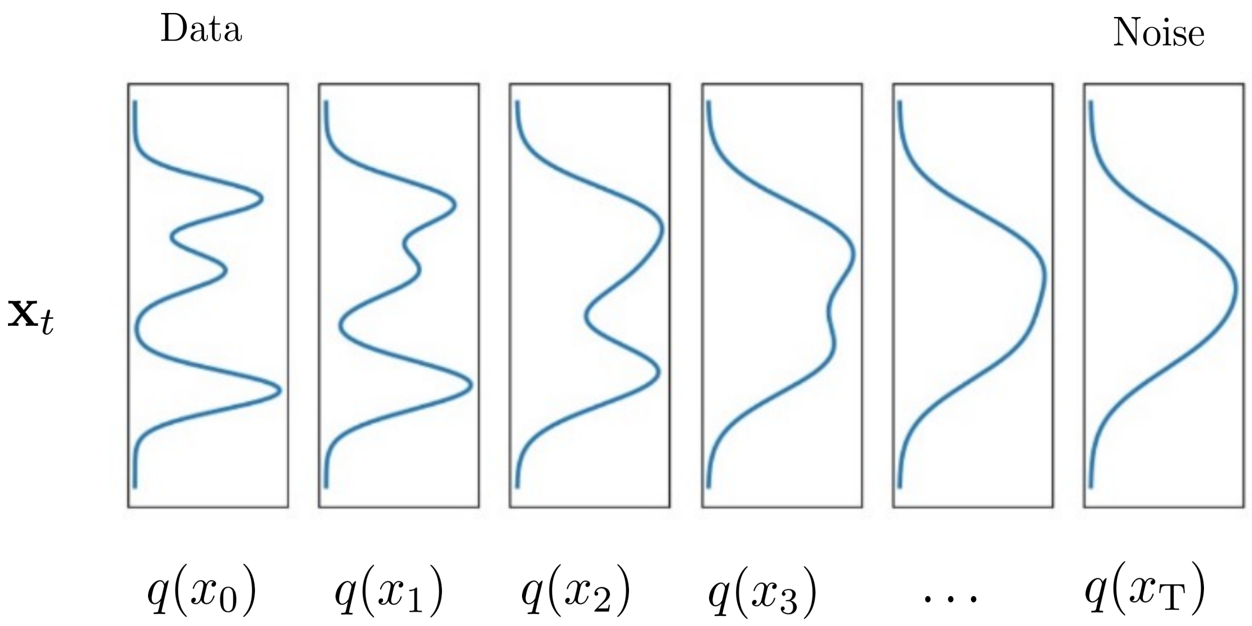
What happens to a distribution in the forward diffusion?

So far, we discussed the diffusion kernel $q(\mathbf{x}_t|\mathbf{x}_0)$ but what about $q(\mathbf{x}_t)$?

$$\underbrace{q(\mathbf{x}_t)}_{\text{Diffused data dist.}} = \int \underbrace{q(\mathbf{x}_0, \mathbf{x}_t)}_{\text{Joint dist.}} d\mathbf{x}_0 = \int \underbrace{q(\mathbf{x}_0)}_{\text{Input data dist.}} \underbrace{q(\mathbf{x}_t|\mathbf{x}_0)}_{\text{Diffusion kernel}} d\mathbf{x}_0.$$

The diffusion kernel is Gaussian convolution.

Diffused Data Distributions



We can sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ by first sampling $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ and then sampling $\mathbf{x}_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$ (i.e., ancestral sampling).

Generative Learning by Denoising

Recall, that the diffusion parameters are designed such that $q(\mathbf{x}_\mathrm{T}) \approx \mathcal{N}(\mathbf{x}_\mathrm{T}; \mathbf{0}, \mathbf{I})$

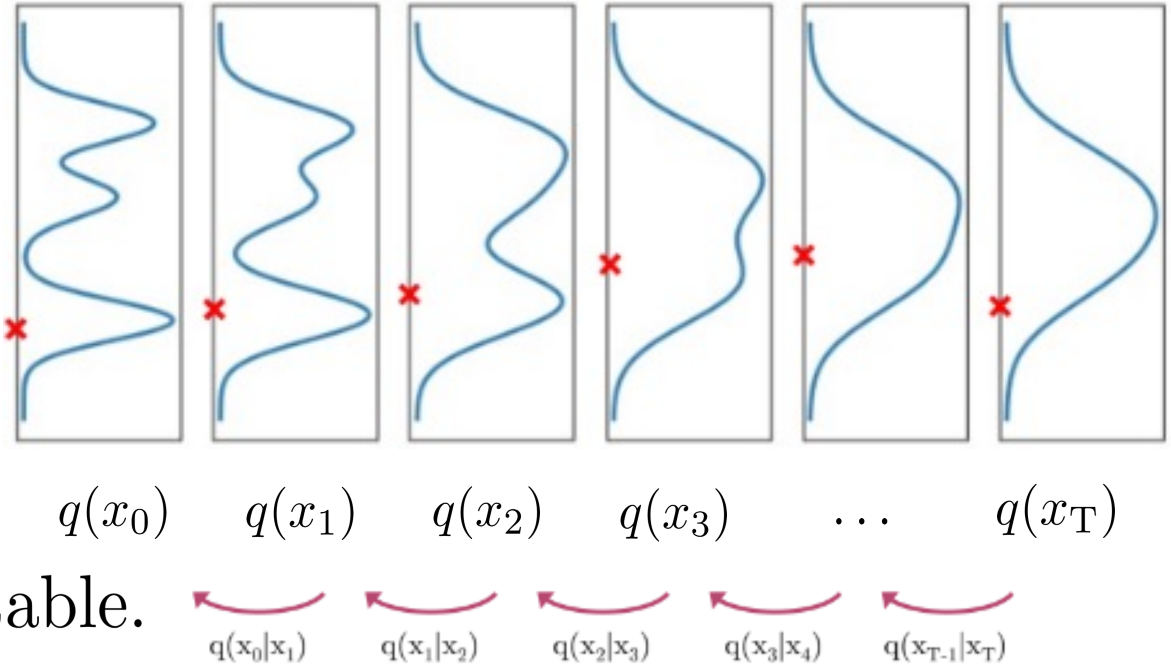
Generation:

Diffused Data Distributions

Sample $\mathbf{x}_\mathrm{T} \sim \mathcal{N}(\mathbf{x}_\mathrm{T}; \mathbf{0}, \mathbf{I})$

$$\text{Iteratively sample } \mathbf{x}_{t-1} \sim \underbrace{q(\mathbf{x}_{t-1}|\mathbf{x}_t)}_{\text{True Denoising Dist.}}$$

$\mathbf{x}_t$

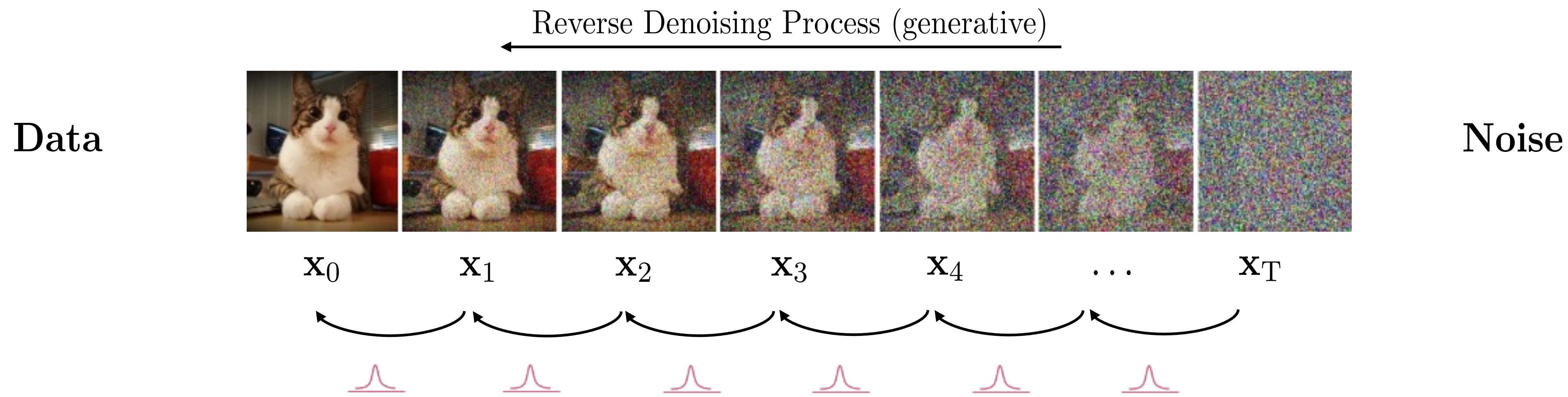


In general, $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \propto q(\mathbf{x}_t|\mathbf{x}_{t-1})$ is intractable.

Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$? Yes, we can use a Normal distribution if β_t is small in each forward diffusion step.

Reverse Denoising Process

The formal definition of the reverse process in T steps:



$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu(\mathbf{x}_t, t)}_{\text{Trainable network}}, \sigma_t^2 \mathbf{I})$$

Trainable network
(U-net, Denoising Autoencoder)

$$\Rightarrow \quad p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t).$$

Learning Denoising Model

For training, we can form variational upper bound that is commonly used for training variational autoencoders:

$$\mathbb{E}_{q(\mathbf{x}_0)}\Big[-\log p_\theta(\mathbf{x}_0)\Big] \leq \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:\mathrm{T}}|\mathbf{x}_0)}\left[-\log \frac{p_\theta(\mathbf{x}_{0:\mathrm{T}})}{q(\mathbf{x}_{1:\mathrm{T}}|\mathbf{x}_0)}\right] =: \mathrm{L}.$$

Sohl-Dickstein et al. ICML 2015 and Ho et al. NeurlPs 2020 show that:

$$\mathrm{L} = \mathbb{E}_q\Bigg[\underbrace{\mathrm{D_{KL}}(q(\mathbf{x}_\mathrm{T}|\mathbf{x}_0)||p(\mathbf{x}_\mathrm{T}))}_{\mathrm{L_T}} + \sum_{t>1} \underbrace{\mathrm{D_{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathrm{L_{t-1}}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{\mathrm{L}_\theta}\Bigg].$$

where $q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)$ is the tractable posterior distribution:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1};\tilde{\mu}_t(\mathbf{x}_t,\mathbf{x}_0),\tilde{\beta}_t\mathbf{I}),$$

$$\text{where } \tilde{\mu}_t(\mathbf{x}_t,\mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{1-\beta_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \text{ and } \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t.$$

Sohl-Dickstein et al. ICML 2015: https://arxiv.org/abs/1503.03585
Ho et al. NeurlPs 2020: ttps://arxiv.org/abs/2006.11239

Parameterizing the Denoising Model

Since both $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ and $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ are Normal distributions, the KL divergence has a simple form:

$$\mathrm{L}_{t-1} = \mathrm{D}_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{t}, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) = \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}||\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)||^2\right] + \mathrm{C}$$

Recall that $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon$. Ho et al. NeurIPS 2020 observe that:

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{1-\beta_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right)$$

They propose to represent the mean of the denoising model using a noise-prediction network:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{1-\beta_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x}_t, t)\right)$$

With this parameterization:

$$\mathrm{L}_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})}\left[\frac{\beta_t^2}{2\sigma_t^2(1-\beta_t)(1-\bar{\alpha}_t)}||\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon}_{\mathbf{x}_t}, t)||^2\right] + \mathrm{C}.$$

https://arxiv.org/abs/2006.11239

Training Objective Weighting

Trading likelihood for perceptual quality

$$\mathrm{L}_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\underbrace{\frac{\beta_t^2}{2\sigma_t^2 (1-\beta_t)(1-\bar{\alpha}_t)}}_{\lambda_t} ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2 \right].$$

The time dependent λ_t ensures that the training objective is weighted properly for the maximum data likelihood training.

However, this weight is often very large for small t's.

Ho et al. NeurIPS 2020 observer that simply setting $\lambda_t = 1$ improves sample quality. So, they propose to use:

$$\mathrm{L}_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, \mathrm{T})} \left[||\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon}_{\mathbf{x}_t}, t)||^2 \right].$$

For more advanced weighting see Choi et al., Perception Prioritized Training of Diffusion Models, CVPR 2022 (https://arxiv.org/abs/2204.00227)

https://arxiv.org/abs/2204.00227
https://arxiv.org/abs/2006.11239

Summary

Training and Sample Generation

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0) = p_{\text{data}}(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(1, \ldots, \text{T})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on

$$\nabla_\theta ||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t)||^2$$

6: **until** converged

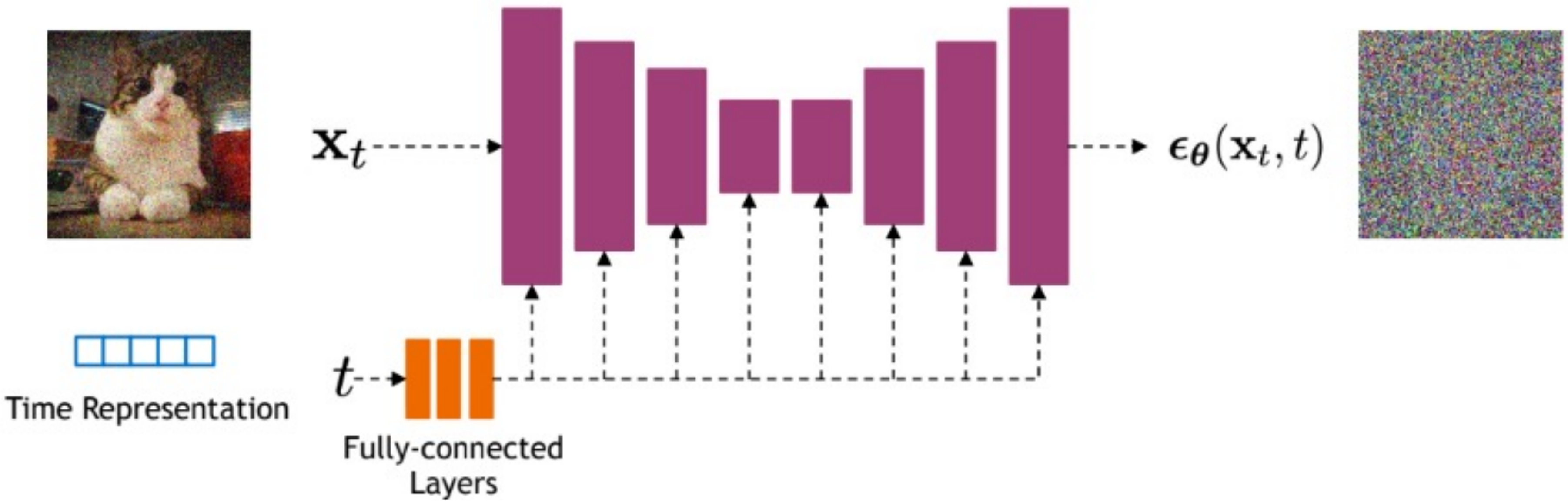
Algorithm 2 Sampling

1: $\mathbf{x}_\text{T} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = \text{T}, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

Implementation Considerations

Network Architectures

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_\theta(\mathbf{x}_t, t)$



Time representation: sinusoidal positional embeddings or random Fourier features.

Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see Dharivwal and Nichol NeurIPS 2021)

https://arxiv.org/abs/2105.05233

Diffusion Parameters

Noise Schedule

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

Data

Noise

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2\mathbf{I})$$

Above, β_t and σ_t^2 control the variance of the forward diffusion and reverse denoising processes respectively.

Often a linear schedule is used for β_t, and σ_t^2 is set equal to β_t.

Kingma et al.NeurIPS 2022 introduce a new parameterization of diffusion models using signal-to-noise ratio (SNR), show how to learn the noise schedule by minimizing the variance of the training objective.

We can also train σ_t^2 while training diffusion model by minimizing the variational bound (Improved DPM by Nichol and Dhariwal ICLM 2021) or after training the diffusion model (Analytic-DPM by Bao et al. ICLR 2022).

https://arxiv.org/abs/2201.06503

https://arxiv.org/abs/2107.00630
https://arxiv.org/abs/2102.09672

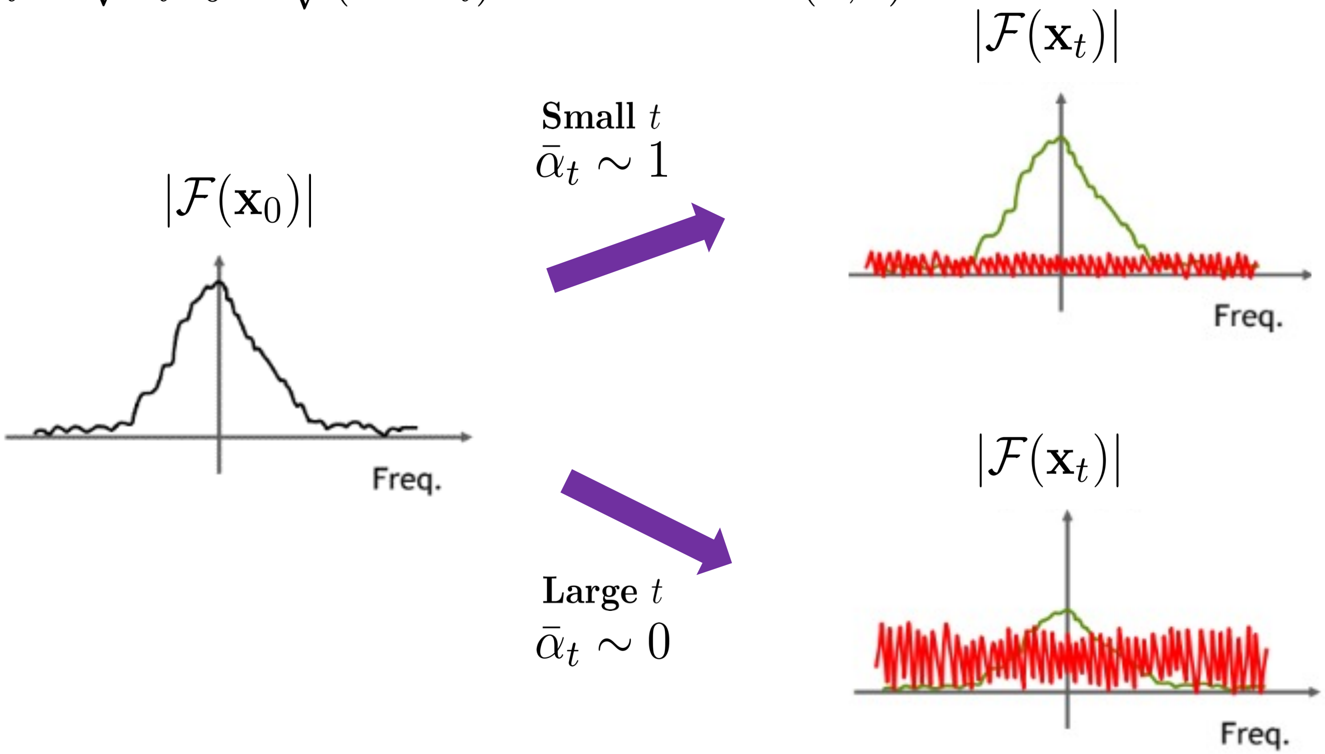
What happens to an image in the forward diffusion process?

Recall that sampling from $q(\mathbf{x}_t|\mathbf{x}_0)$ is done using $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{a}_t)}\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon$$

Fourier Transform

$$\mathcal{F}(\mathbf{x}_t) = \sqrt{\bar{\alpha}_t}\mathcal{F}(\mathbf{x}_0) + \sqrt{(1-\bar{\alpha}_t)}\mathcal{F}(\epsilon)$$



In the forward diffusion, the high frequency content is perturbed faster.

Content-Detail Tradeoff

Reverse denoising process (generative) →

Data

Noise

$\mathbf{x}_0$ $\mathbf{x}_1$ $\mathbf{x}_2$ $\mathbf{x}_3$ $\mathbf{x}_4$ $\ldots$ $\mathbf{x}_T$

The denoising model is specialized for generating the high-frequency content (i.e., low-level details)

The denoising model is specialized for generating the low-frequency content (i.e., coarse content)

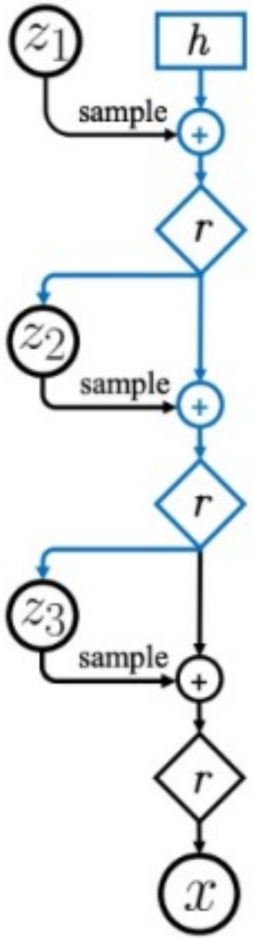
The weighting of the training objective for different timesteps is important!

Connection to VAEs

Diffusion models can be considered as a special form of hierarchical VAEs.

However, in diffusion models:

- The endocder is fixed
- The latent variables have the same dimension as the data
- The denoising model is shared across different timestep
- The model is trained with some reweighting of the variational bound



https://arxiv.org/abs/2007.03898
https://arxiv.org/abs/1602.02282

Summary

Denoising Diffusion Probabilistic Models

The model is trained by sampling from the forward diffusion process and training a denoising model to predict the noise.

We discussed how the forward process perturbs the data distribution or data samples.

The devil is in the details:

- Network architectures
- Objective weighting
- Diffusion parameters (i.e., noise schedule)

See "Elucidating the Design Space of Diffusion-Based Generative Models" by Karras et al. for important design decision.

https://arxiv.org/abs/2206.00364

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