CSCI 544: Applied Natural Language Processing

Deep Generative Models for Image Generation

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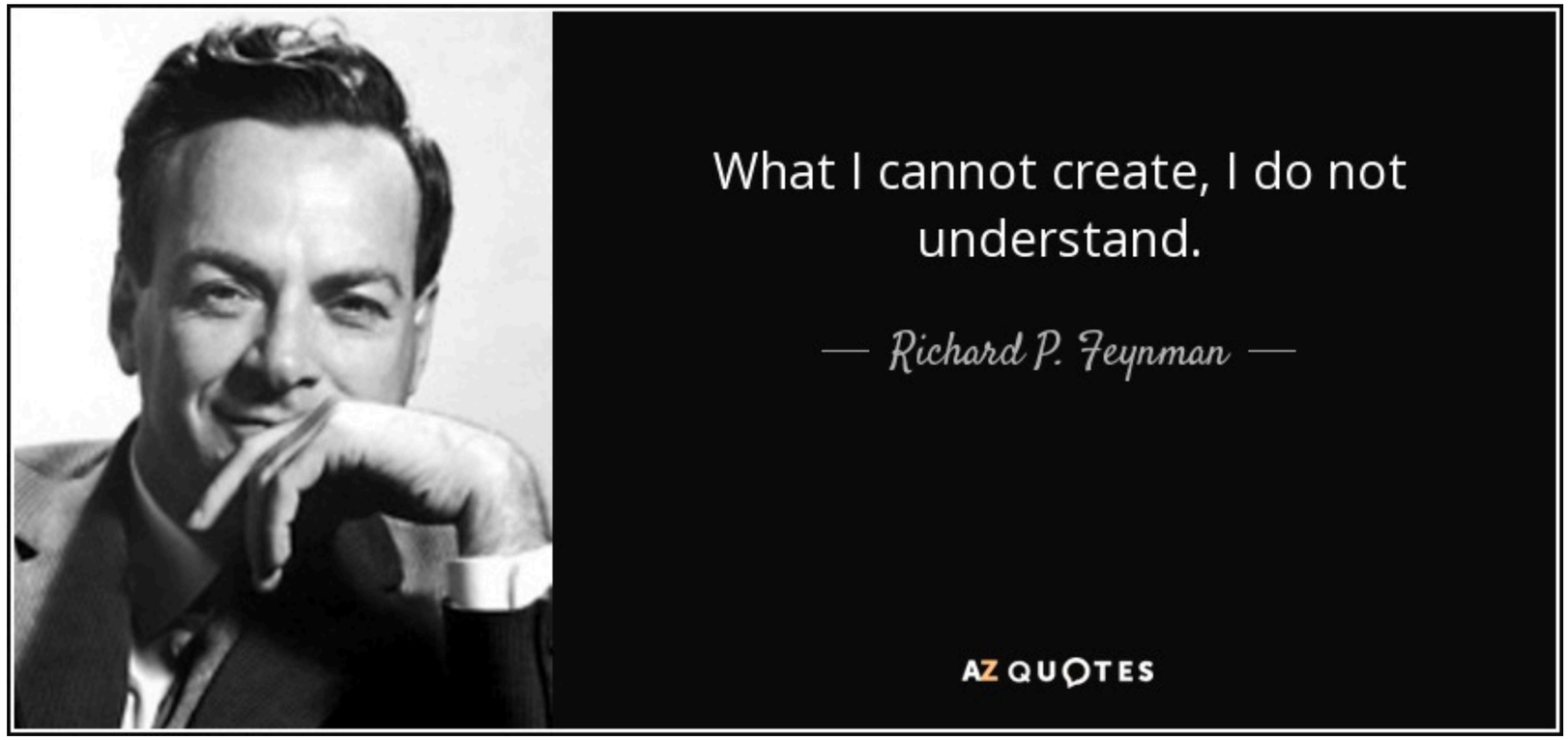
Generative Models

- **What are generative models**
  - Learning to generate new data from samples

Generative Models

- **Why generative models**
  - Requiring no labeled data
  - A good way to learn knowledge from data



Deep Generative Models

- **Distribution-based Generative Models**
  - Auto-regressive Models
  - Generative (Normalizing) Flows
  - Variational Auto-Encoders (VAEs)
  - Diffusion Models
- **Non-distribution Generative Models**
  - Generative Adversarial Networks (GANs)

Distribution-based Generative Models

- **Goal: learn to generate new data from samples**
  - How?
  - To model the data distribution $P(X)$
    - Closed-form analytic solution
    - Exact density estimation via “black-box” deep neural networks
    - Density/distribution approximation

Distribution-based Generative Models

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Closed-form Analytic Solution

- **Providing a closed-form analytic solution of $P(X)$**
  - Kernel-based approaches
  - Gaussian process
  - …
- **Pros**
  - Theoretically grounded
  - Analytic solution for future derivations
- **Cons**
  - Limited capacity
  - Unable to model complex data/distributions

Distribution-based Generative Models

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Deep Generative Models w. Exact Density Estimation

- **Exact density estimation via deep neural networks**
  - Autoregressive models
  - Generative (normalizing) flows

X

Deep Generative Models

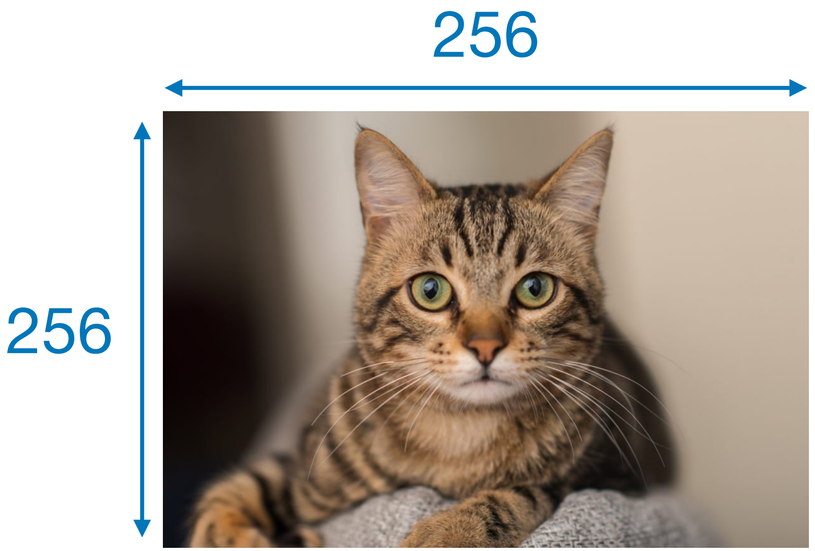
$P(X)$

Value only!

Autoregressive Models

- **Sequential data**
  - $X = \{x_1, x_2, \ldots, x_L\}$
  - Languages: sequences of words
  - Images: sequences of pixels
  - Audios: sequences of signals
- **Autoregressive Factorization**
  - $p_\theta(X) = \prod_{t=1}^{T} p_\theta(x_t \mid x_{<t})$
  - Autoregressive models
    - RNN, Transformer, …

Problems on Autoregressive Models for Image



256 x 256 x 3 = 131072 pixels

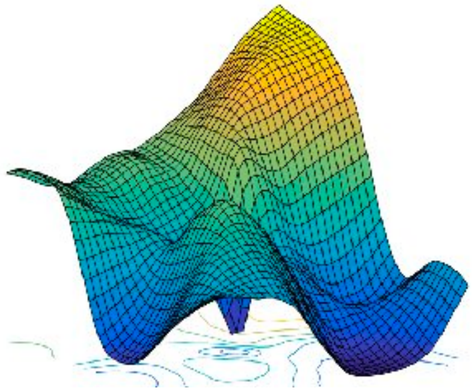
Problems:

- One pre-defined order
  - No clear order for data like images
- Error propagation
  - Limited context at beginning

Generative (Normalizing) Flows

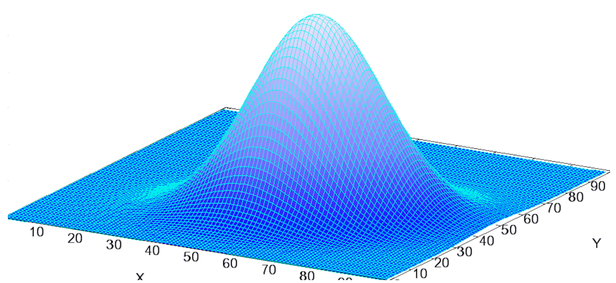
- **Modeling density via invertible mapping**
  - Directly modeling the joint distribution of all variates in X
  - Exact density estimation (no approximation)

Generative (Normalizing) Flows



$$\Gamma = f_\theta(X)$$

$$X = f_\theta^{-1}(\Gamma)$$



$X \sim p_\theta(X)$

$\Gamma \sim \text{Normal}(0, I)$

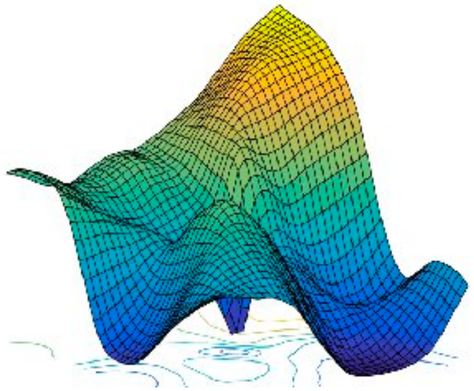
Change of Variable formula:

$$p_\theta(x) = \underline{p_\Gamma\left(f_\theta(x)\right)} \left| \det \underline{\left(\frac{\partial f_\theta(x)}{\partial x} \right)} \right|$$

Normal

Jacobian Matrix

Generative (Normalizing) Flows



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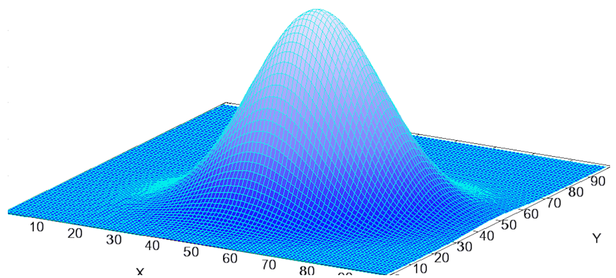

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Change of Variable formula:

$$p_\theta(x) = p_\Gamma\left(f_\theta(x)\right) \left| \det\left(\frac{\partial f_\theta(x)}{\partial x}\right) \right|$$

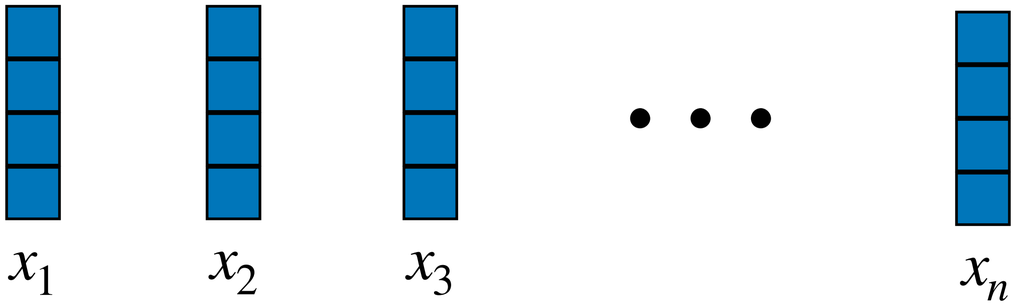
Generative Flow: A series of such f

$$X \underset{g_1}{\overset{f_1}{\longleftrightarrow}} H_1 \underset{g_2}{\overset{f_2}{\longleftrightarrow}} H2 \underset{g_3}{\overset{f_3}{\longleftrightarrow}} \cdots \underset{g_K}{\overset{f_K}{\longleftrightarrow}} \Gamma$$

Generative (Normalizing) Flows

- **ActNorm**

$$y_i = s \odot x_i + b$$



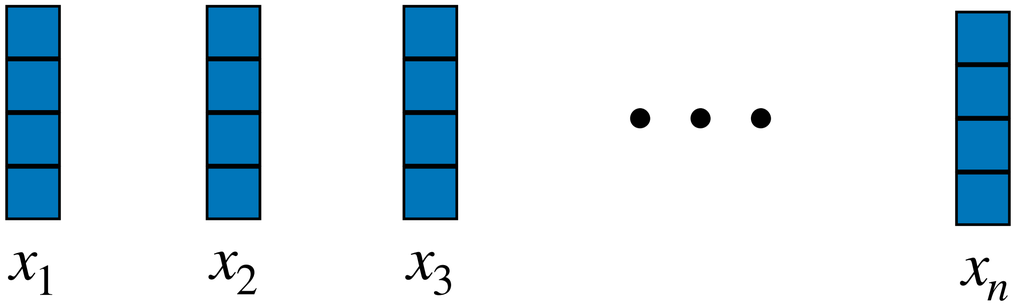
Generative (Normalizing) Flows

- **ActNorm**

$$y_i = s \odot x_i + b$$

- **Invertible Linear**

$$y_i = W x_i$$



Generative (Normalizing) Flows

- **ActNorm**

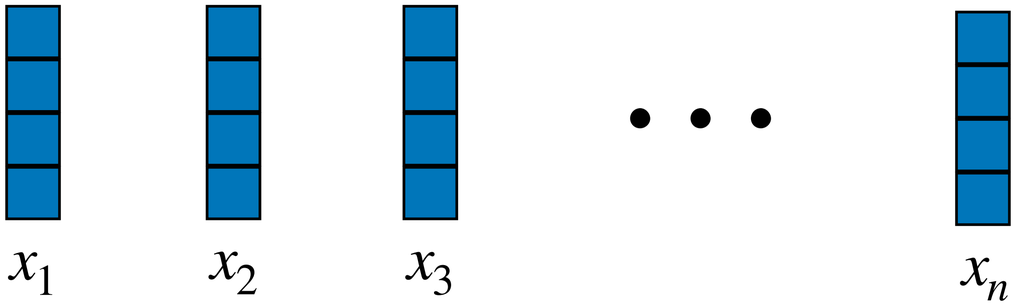
$$y_i = s \odot x_i + b$$

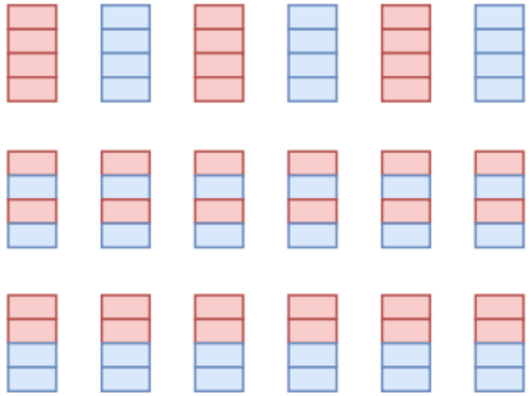
- **Invertible Linear**

$$y_i = W x_i$$

- **Affine Coupling**

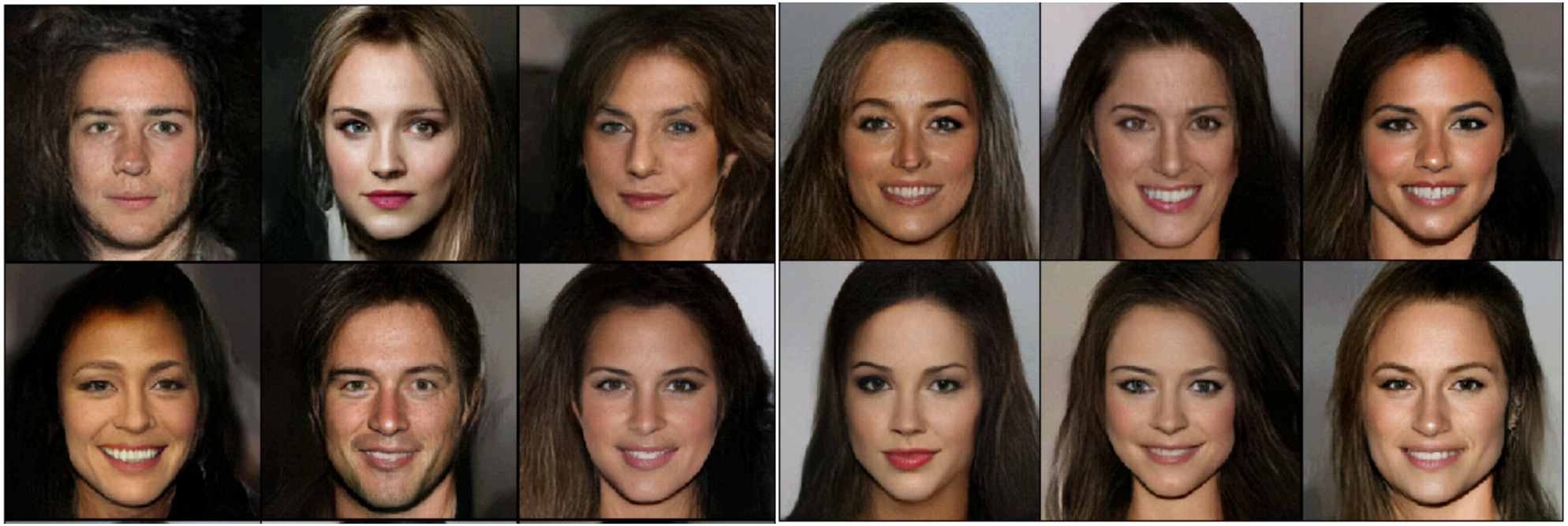
$$\begin{aligned} x_a, x_b &= \mathrm{split}(x) \\ y_a &= x_a \\ y_b &= \mathrm{s}(x_a) \odot x_b + \mathrm{b}(x_a) \\ y &= \mathrm{concat}(y_a, y_b), \end{aligned}$$





Generative (Normalizing) Flows: Pros and Cons

- Modeling the exact distribution $P(X)$
- No auto-regressive factorization
- A large number of layers: invertible function f_i is very weak
- Determinant calculation is expensive



Distribution-based Generative Models

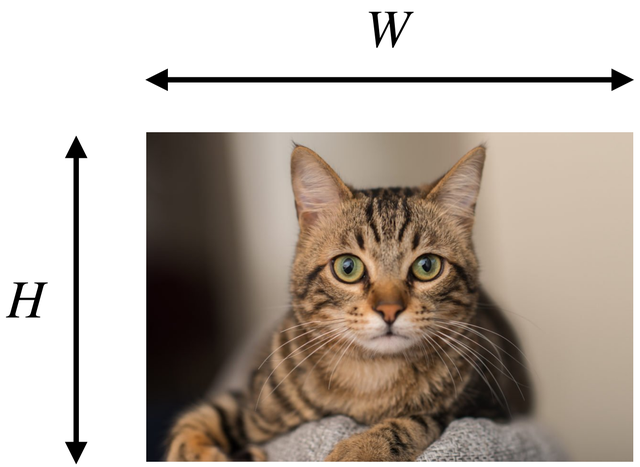
- **Goal: learn to generate new data from samples**
  - How?
  - To model the data distribution $P(X)$
    - Closed-form analytic solution
    - Exact density estimation via “black-box” deep neural networks
    - Density/distribution approximation

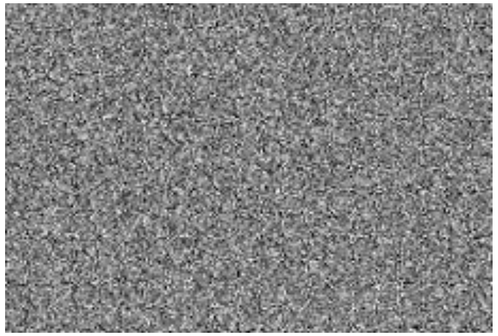
Problems of Exact Density Estimation

- **What are the problems of exact density estimation?**
  - The space of pixels is huge $|V| = 256^{H \times W \times 3}$
  - The manifold/sub-space of natural images is sparse w.r.t the whole space

$$|V'|/|V| \approx 0$$

  - Waste too much model capacity on garbage images/noises





Variational Auto-Encoders (VAEs)

- **Learning a (low-dimensional) latent representation**
  - The manifold/sub-space of natural images is sparse w.r.t the whole space

$$|V'|/|V| \approx 0$$

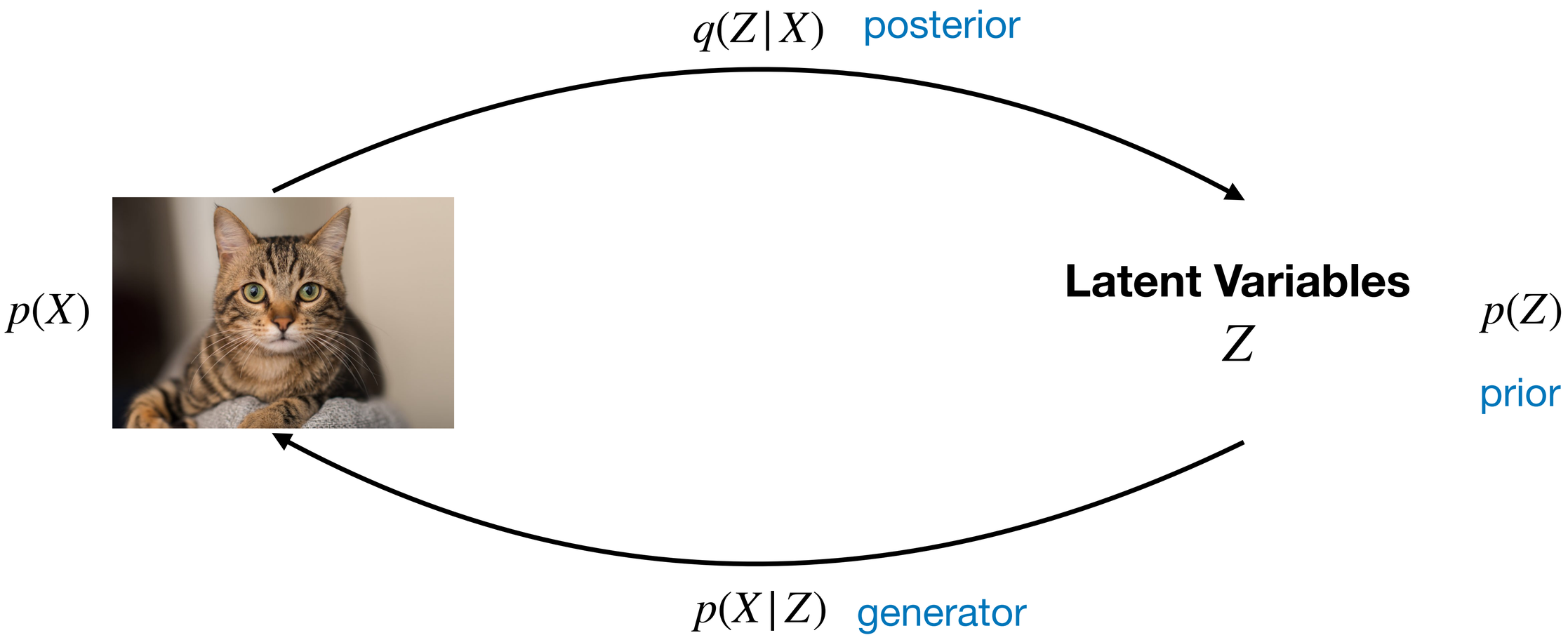
  - After down-project to low-dimension space of Z, natural images are less sparse

X

low-dimensional

Deep Generative Models w. Approx. Density Estimation

- Variational Auto-Encoders (VAEs)
- Diffusion Models



Variational Auto-Encoders

- **Low-dimensional latent variable $Z \in \mathbb{R}^d$**
- **Marginal distribution**

$$p(X) = \boxed{\int_Z p(X \mid Z) p(Z) dz,}$$

- How to compute/approximate the integral?
  - Variational Inference

Variational Inference

$$\underbrace{\log p(X)}_{\textbf{LL}} = \log \int_Z p(X|Z)p(Z)dz$$

Evidence Lower Bound (ELBO)

$$\geq \underbrace{\mathrm{E}_{\boxed{q(Z|X)}}[\log \boxed{p(X|Z)}] - \mathrm{KL}(q(Z|X)\,||\,\boxed{p(Z)})}_{\textbf{ELBO}}$$

Posterior **Generator** **Prior**

Variational Inference

$$\underbrace{\log p(X)}_{\textbf{LL}} = \log \int_Z p(X|Z)p(Z)dz$$

Evidence Lower Bound (ELBO)

$$\geq \underbrace{\mathrm{E}_{q(Z|X)}[\log p(X|Z)] - \mathrm{KL}(q(Z|X)||p(Z))}_{\textbf{ELBO}}$$

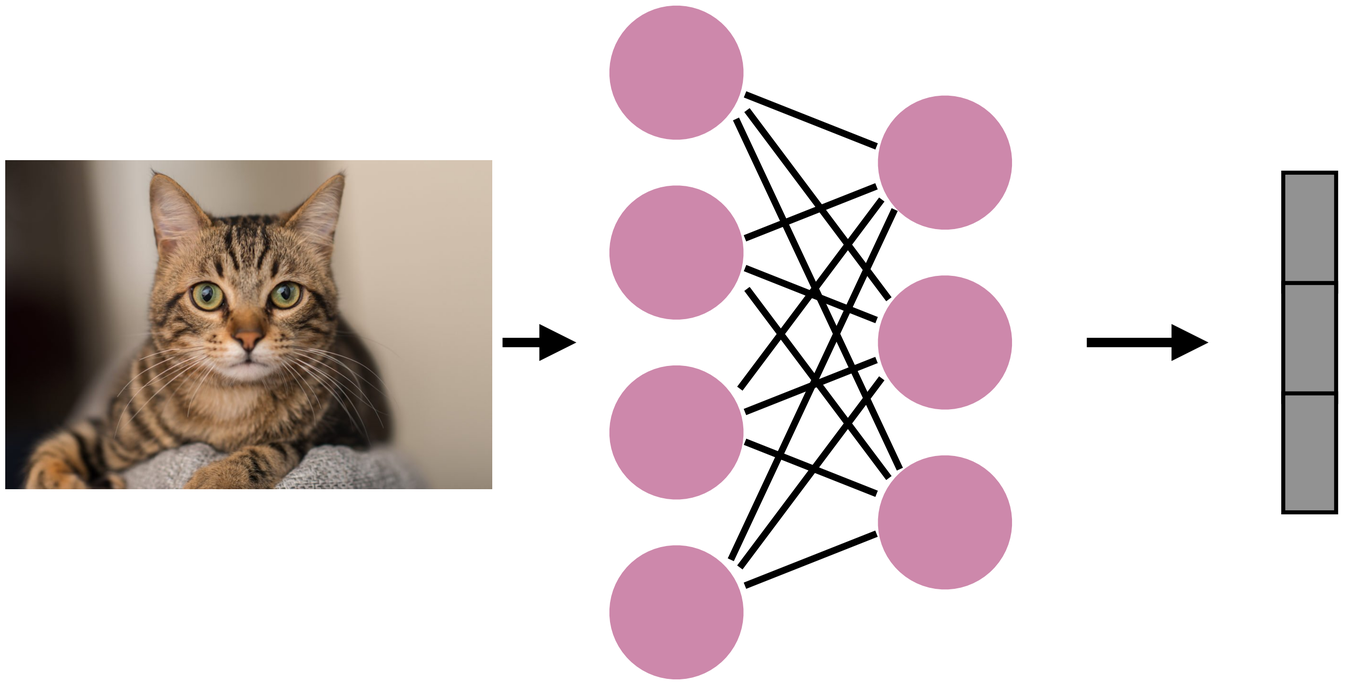
$$= \underbrace{\mathrm{E}_{q(Z|X)}[\log p(X|Z)]}_{\textbf{Reconstruction}} - \underbrace{\mathrm{KL}(q(Z|X)||p(Z))}_{\textbf{KL Regularizer}}$$

Variational Inference

Evidence Lower Bound (ELBO)

$$\underbrace{\log p_\theta(X)}_{\textbf{LL}} \geq \underbrace{\mathrm{E}_{\boxed{q_\phi(Z|X)}}[\log p_\theta(X|Z)] - \mathrm{KL}(q_\phi(Z|X)||p_\theta(Z))}_{\textbf{ELBO}}$$

Posterior



X $\quad$ $q_\phi(Z|X)$ $\quad$ Z

Variational Inference

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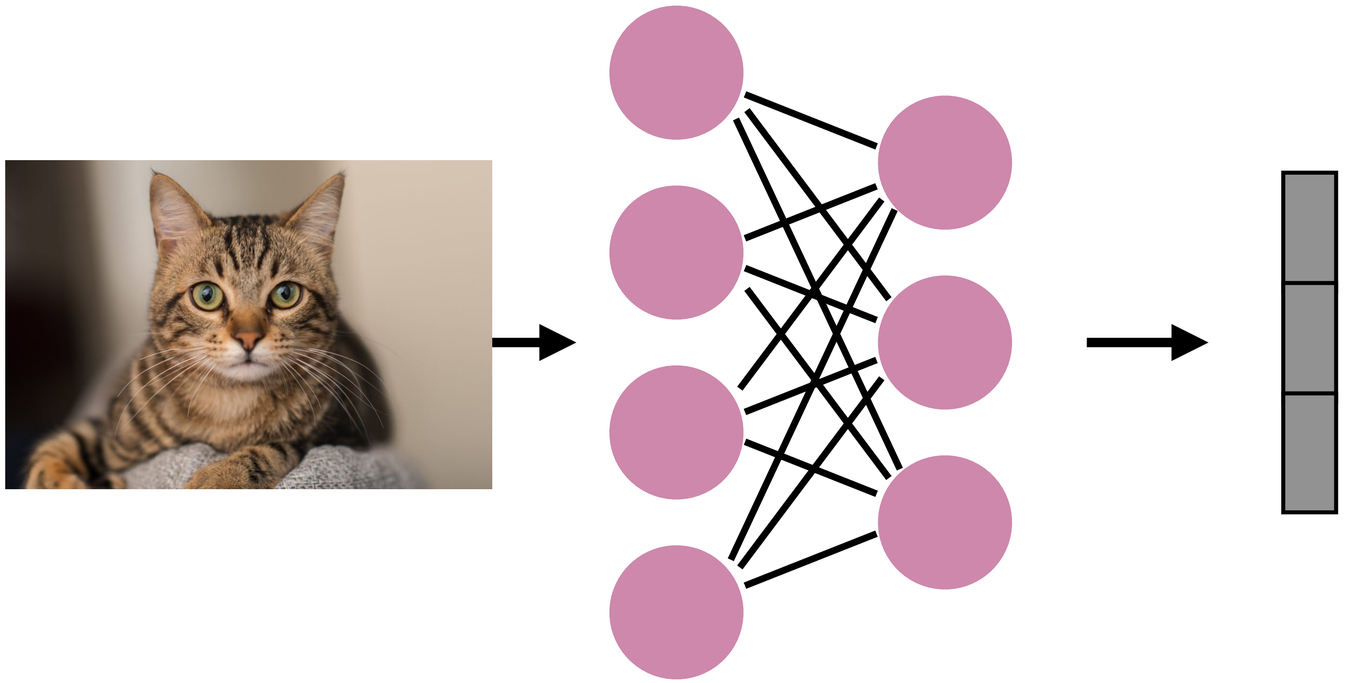
$$\underbrace{\log p_\theta(X)}_{\textbf{LL}} \geq \underbrace{\mathrm{E}_{q_\phi(Z|X)}[\log p_\theta(X|Z)] - \mathrm{KL}(q_\phi(Z|X)\,||\,\boxed{p_\theta(Z)})}_{\textbf{ELBO}}$$

Posterior

Prior



X

$q_\phi(Z|X)$

$Z \sim p_\theta(Z)$

Variational Inference

Evidence Lower Bound (ELBO)

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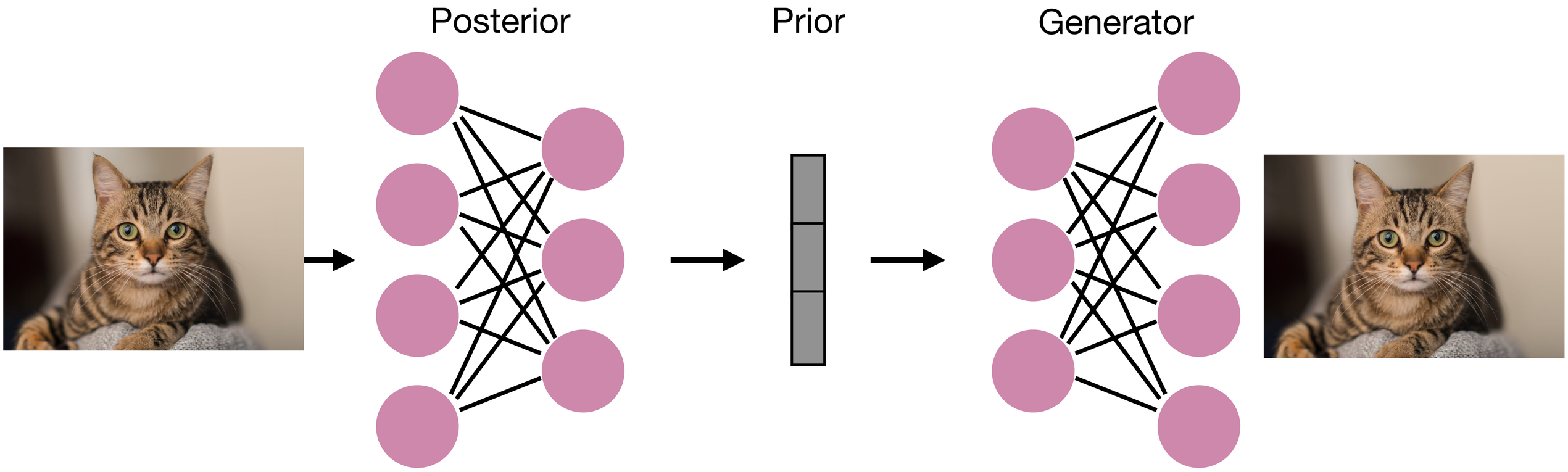


X $\quad$ $q_\phi(Z|X)$ $\quad$ $Z \sim p_\theta(Z)$ $\quad$ $p_\theta(X|Z)$

Variational Auto-Encoders

- **Prior**

$$P(Z)$$

- **Posterior**

$$q(Z|X)$$

Depends on tasks:

Gaussian

Auto-regressive model for sequences

Generative flows

...

- **Generater**

$$P(X|Z)$$

Variational Auto-Encoders

- **Prior**

$$P(Z) \sim \mathcal{N}(0,I)$$

Low-dimensional Gaussian

- **Posterior**

$$q(Z|X) \sim \mathcal{N}(\underline{\mu(X)}, \underline{\sigma^2(X)})$$

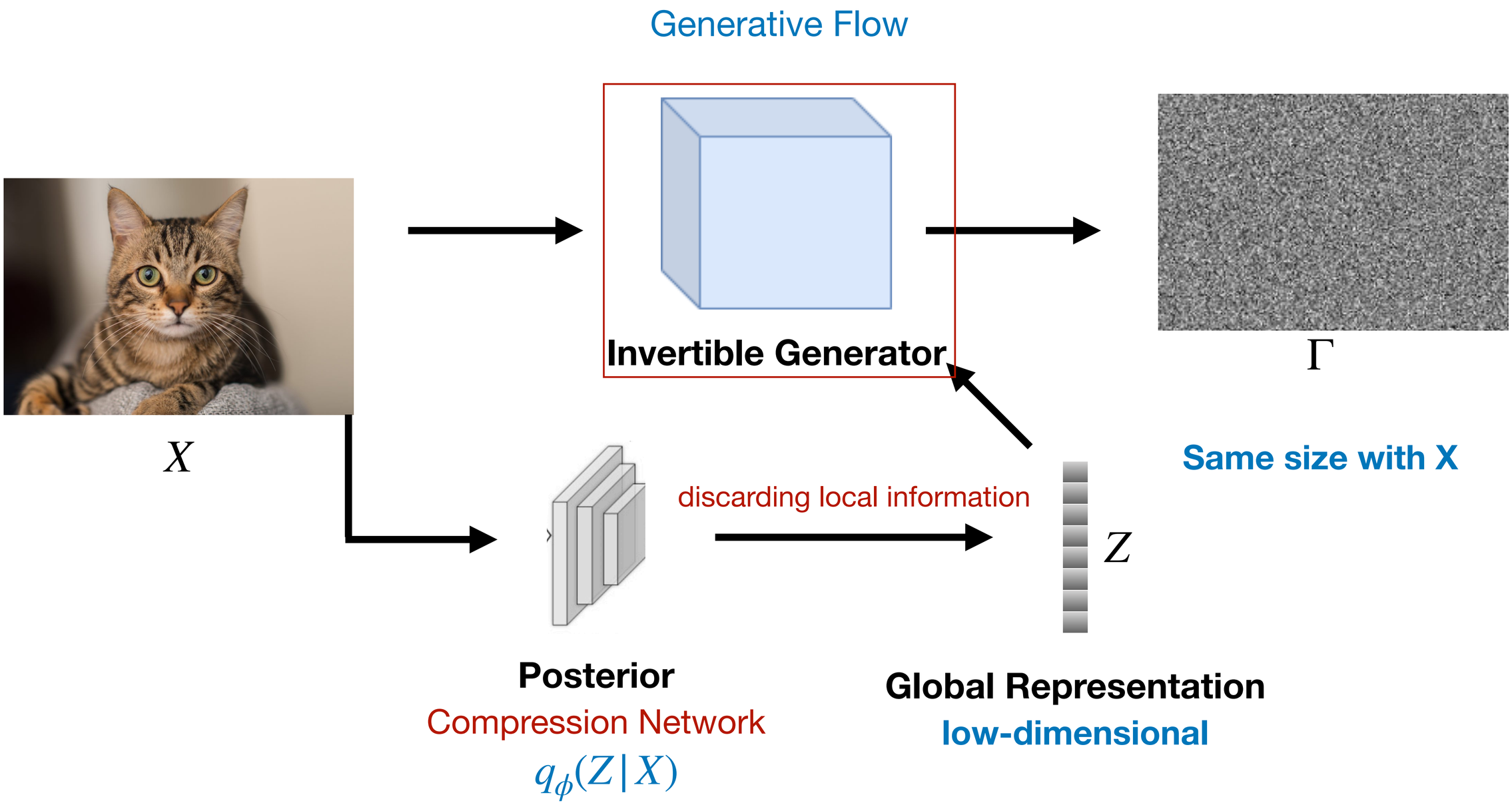
Low-dimensional Gaussian

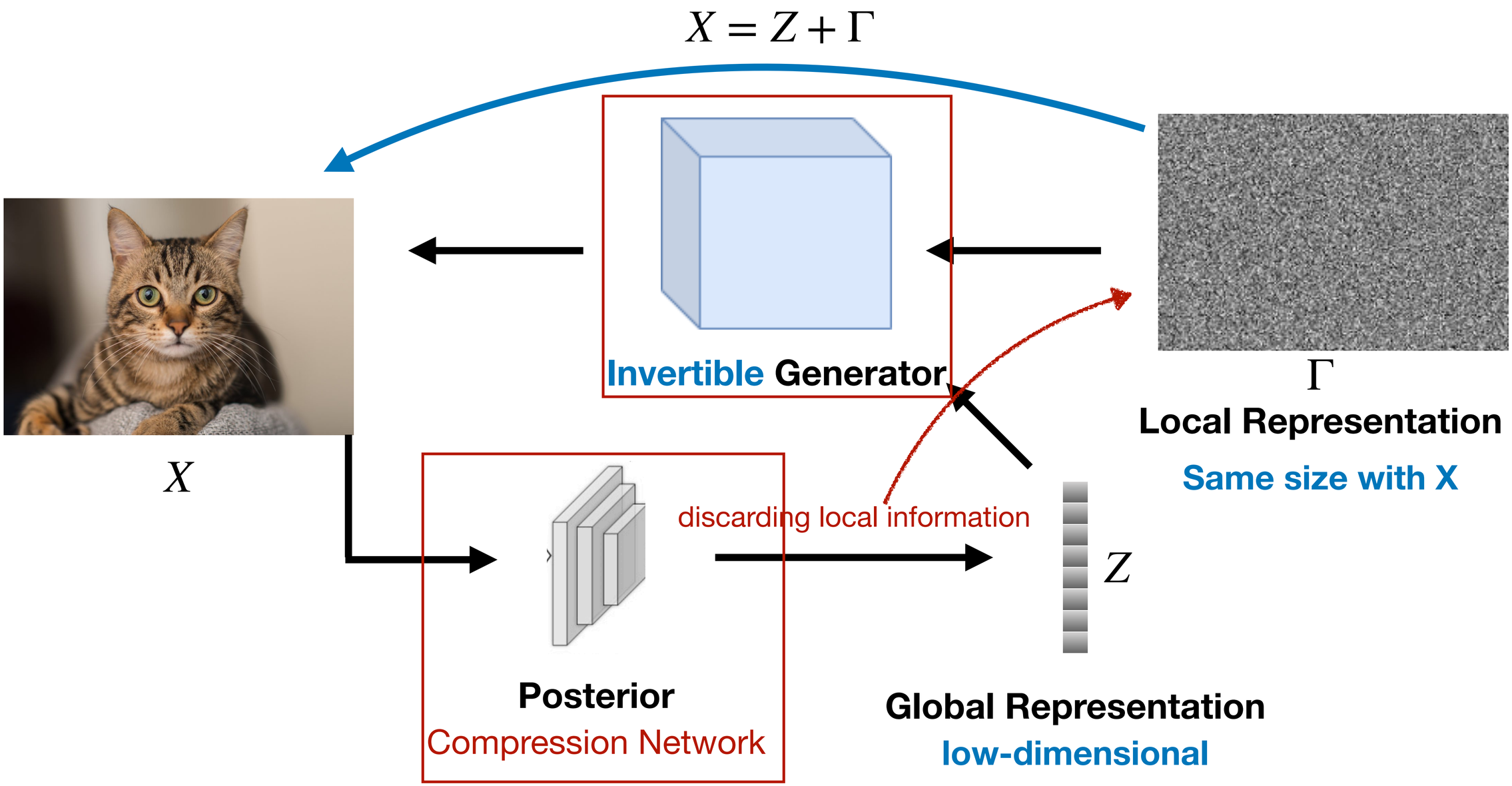
Neural Network

- **Generater**

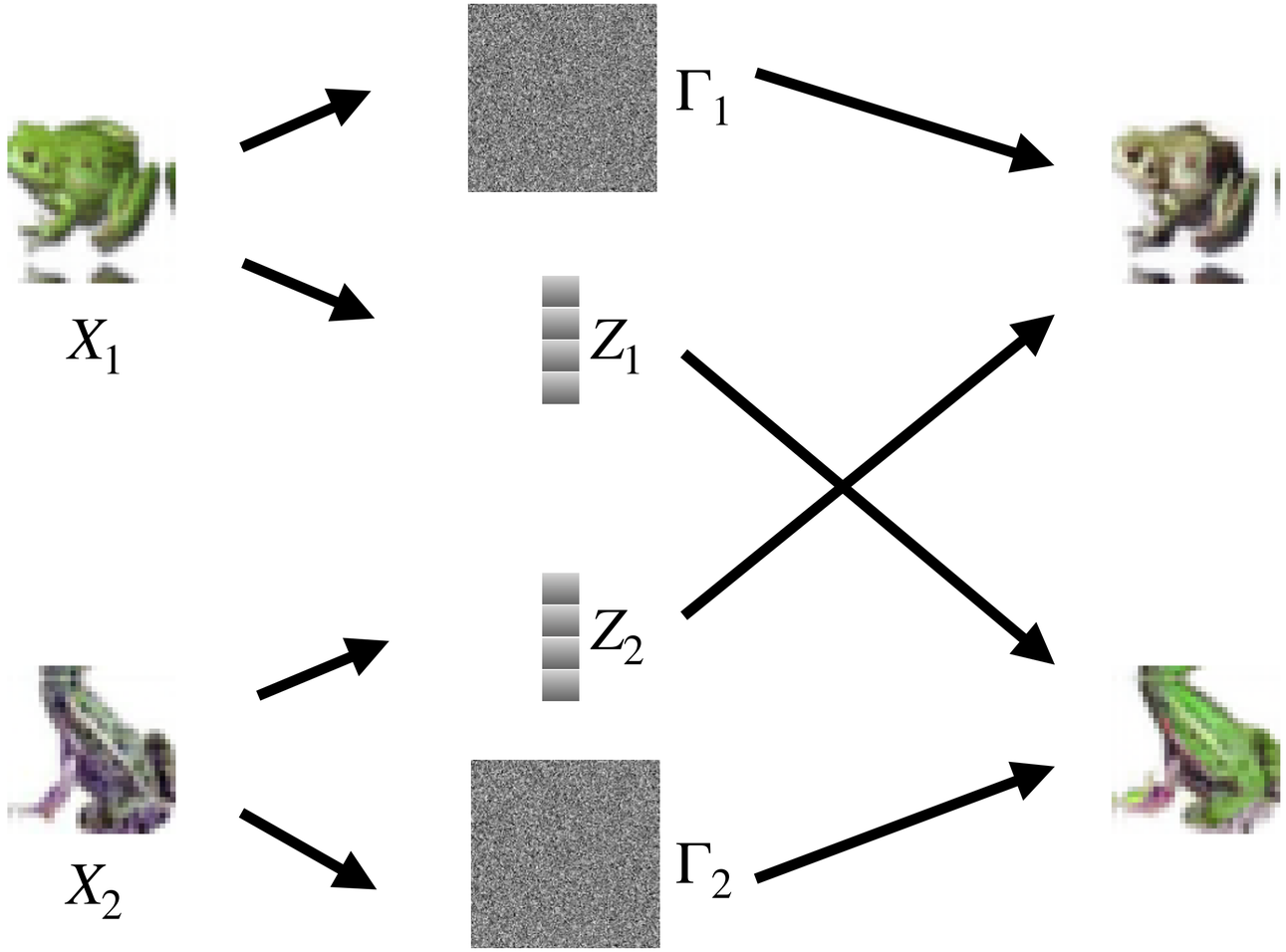
$$P(X|Z)$$

Generative Flow

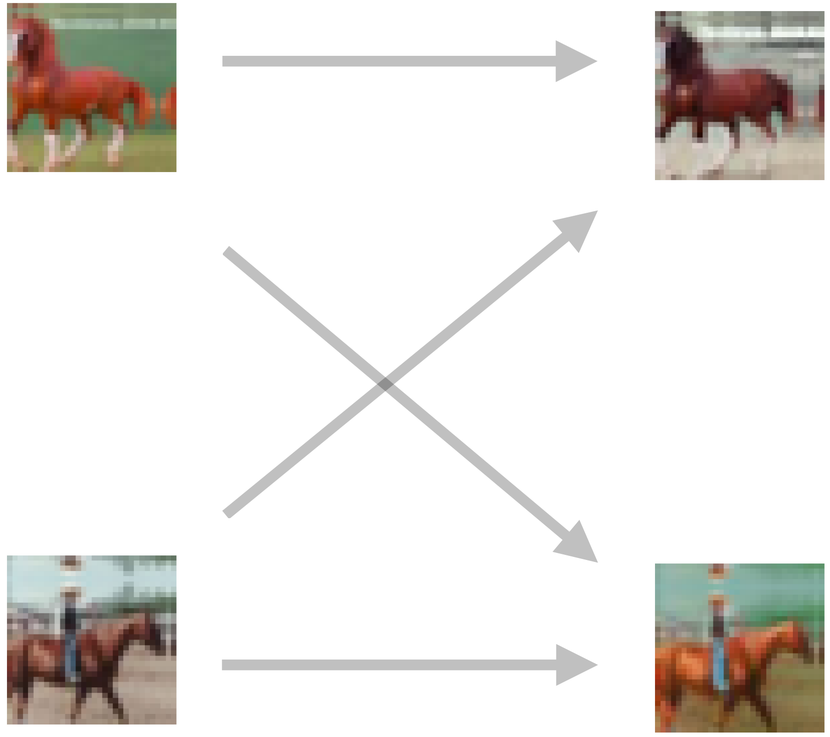

Generative Flow
Invertible Generator
Γ
X
Same size with X
discarding local information
Z
Posterior
Compression Network
$q_\phi(Z|X)$
Global Representation
low-dimensional


$X = Z + \Gamma$
Invertible Generator
X
Γ
Local Representation
Same size with X
discarding local information
Z
Posterior
Compression Network
Global Representation
low-dimensional

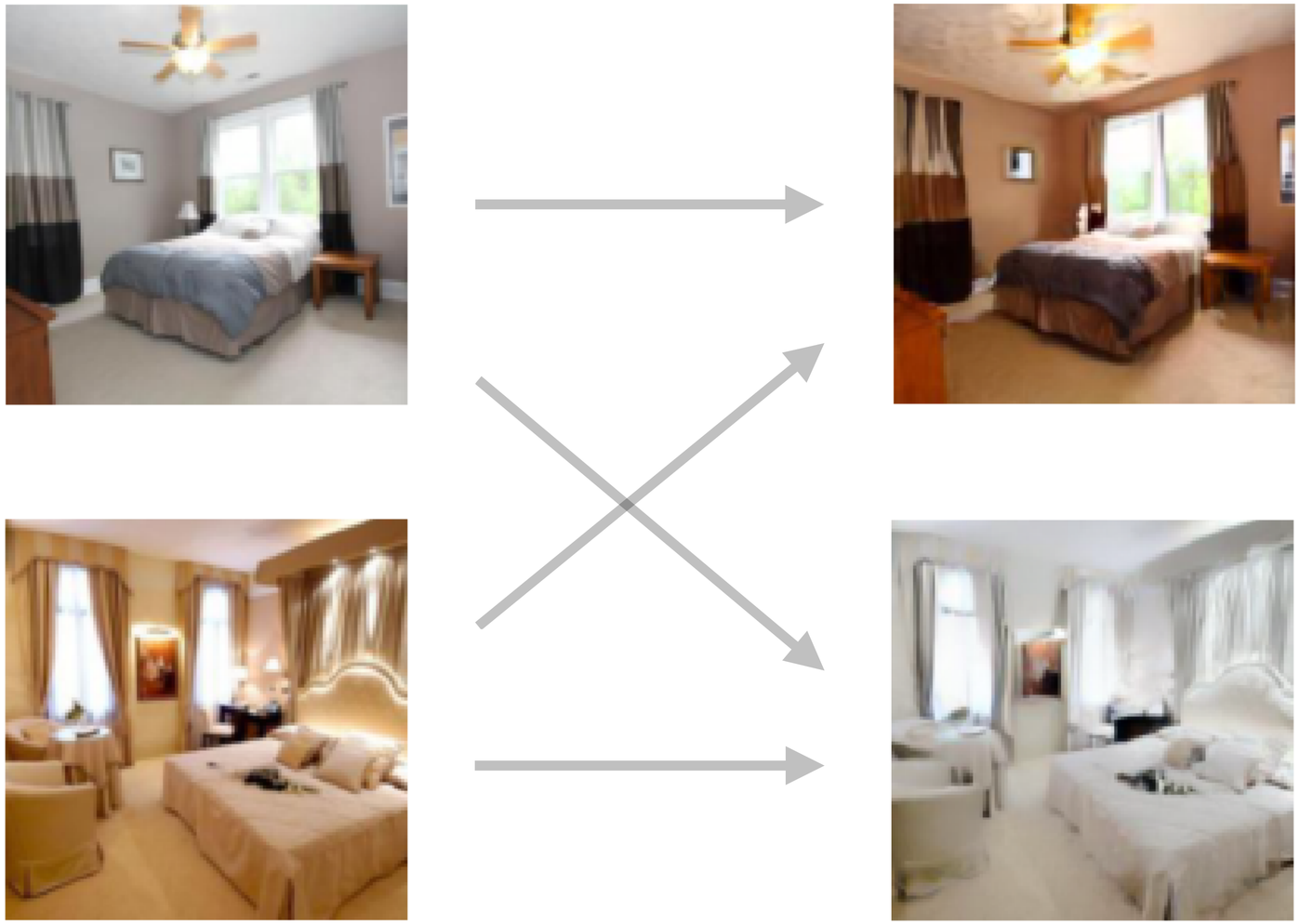
Switch Operation Demo: CIFAR-10



Switch Operation Demo: CIFAR-10



Switch Operation Demo: LSUN-Bedroom



Switch Operation Demo: CelebA-HQ

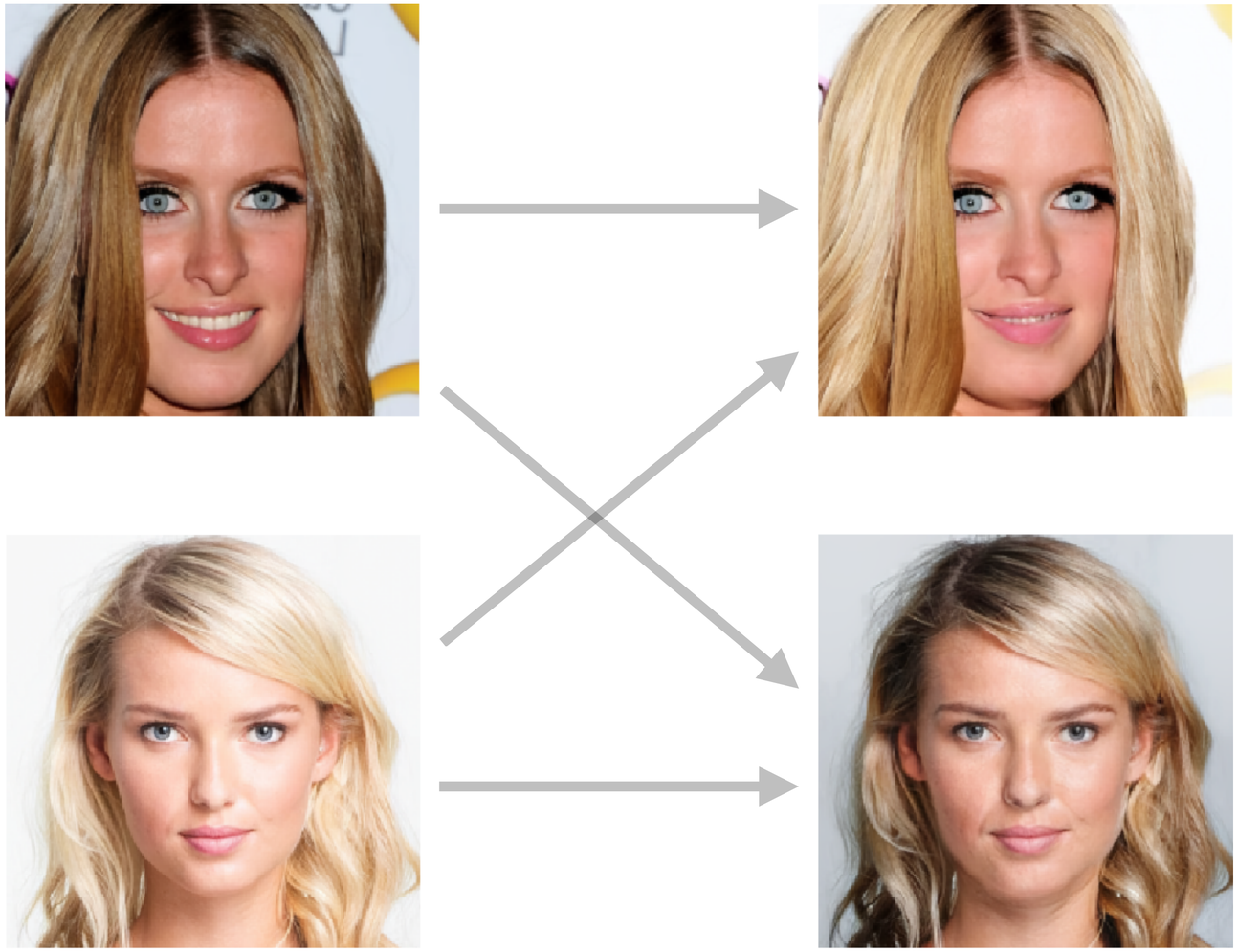
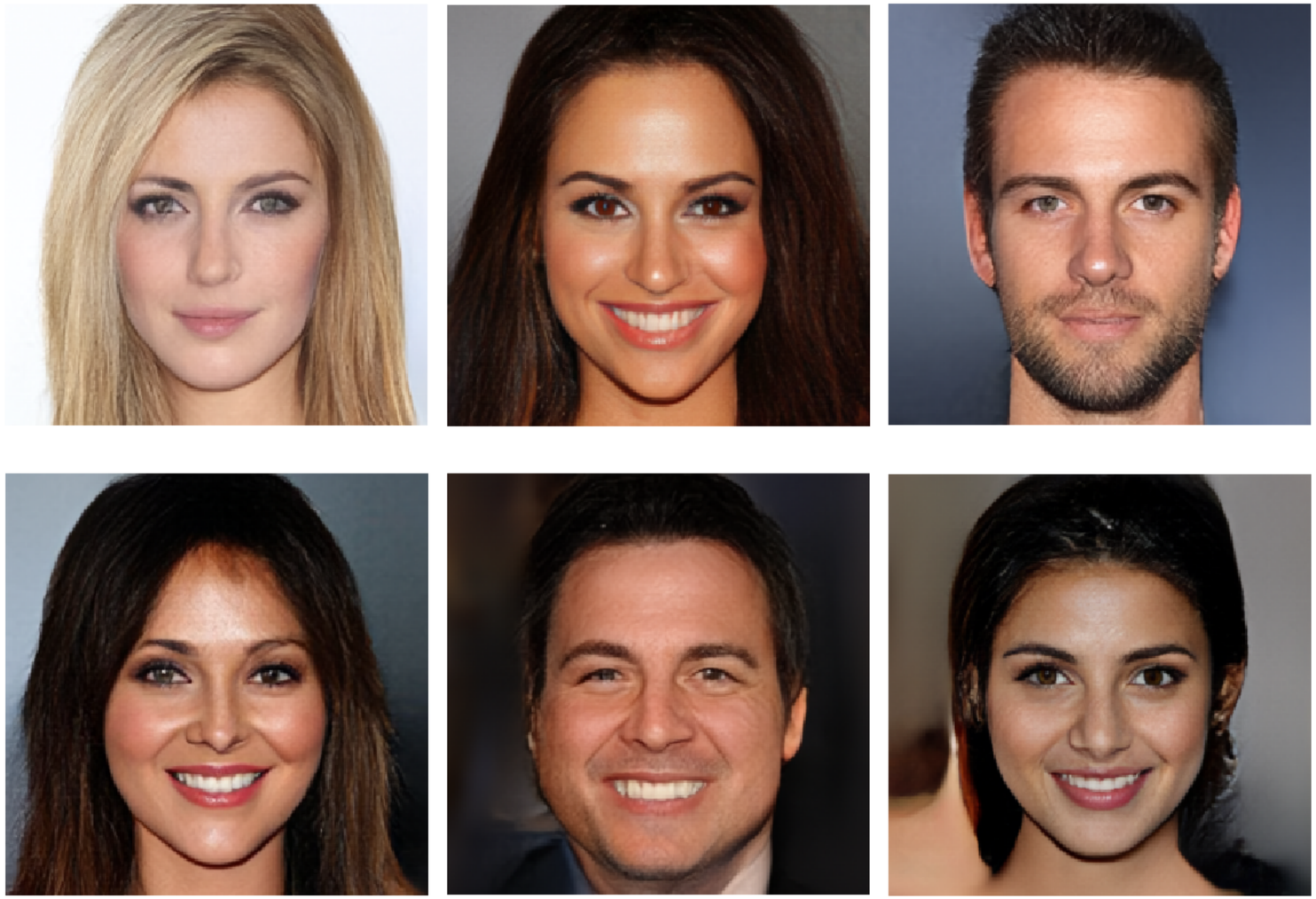


Image Generation

Random Samples



Variational Auto-Encoders

- **Prior**

$$P(Z) \sim \mathcal{N}(0,I)$$

Generative Flow

- **Posterior**

$$q(Z|X) \sim \mathcal{N}(\mu(X), \sigma^2(X))$$

High-dimensional Gaussian

Neural Network

- **Generater**

$$P(X|Z)$$

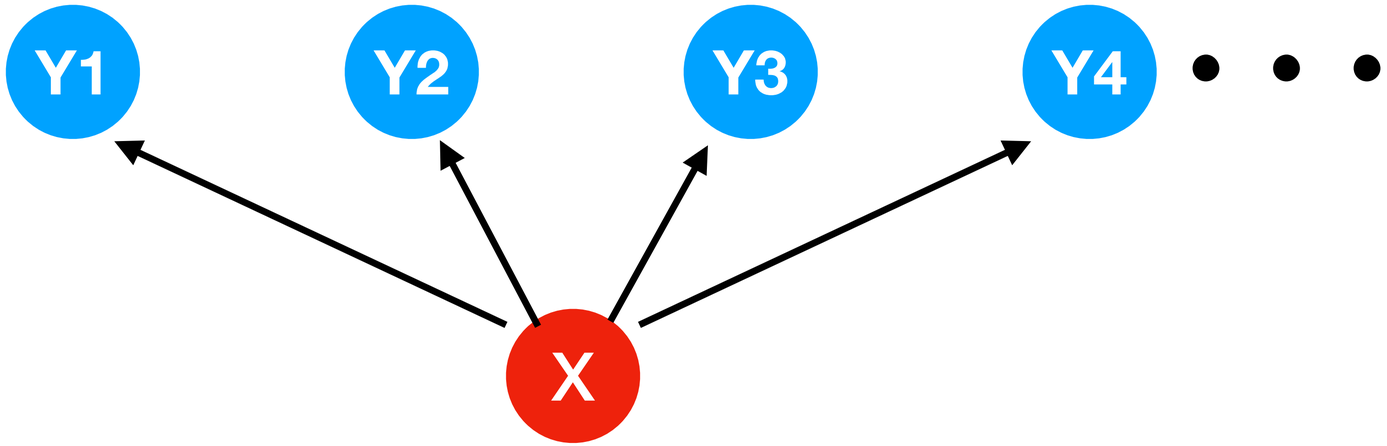
Non-autoregressive model

Non-Autoregressive MT

Non-Autoregressive MT?

- A naïve solution:

$$p_\theta(Y|X) = \prod_{t=1}^{T} p_\theta(y_t|X)$$



Too Strong Independent Assumption!

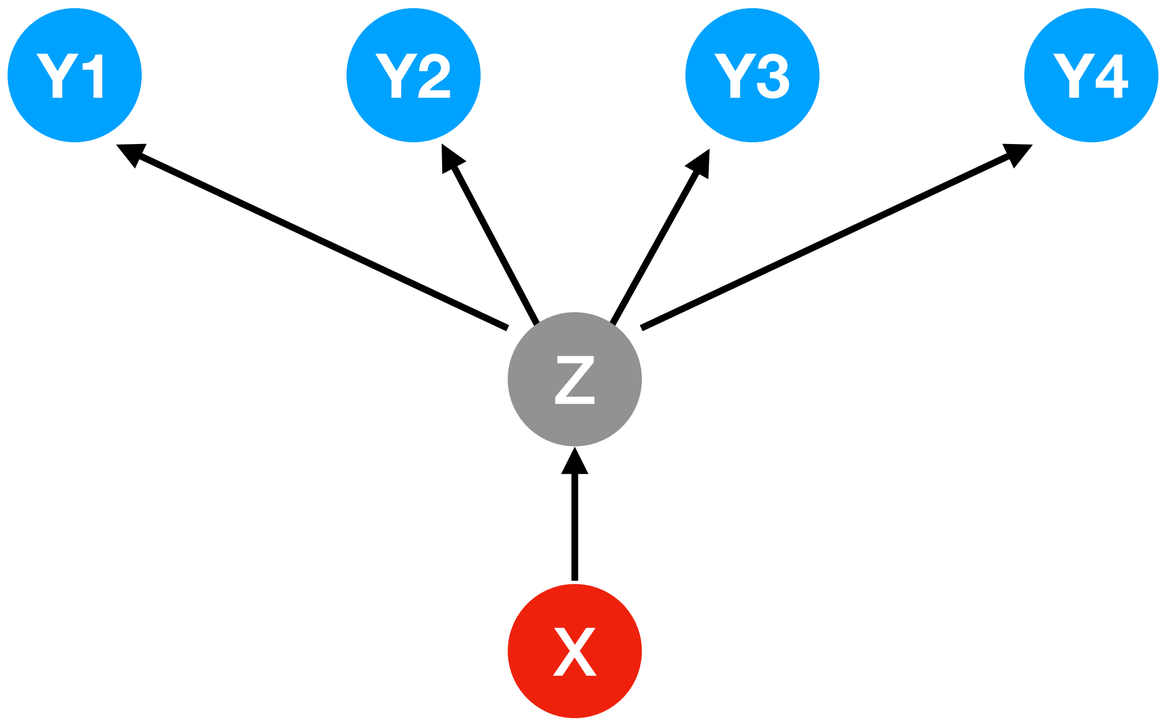
Latent Variable Models

Latent Variable Z

$$p_\theta(Y|X) = \int_Z p_\theta(Y|Z,X)p_\theta(Z|X)dz,$$

Non-Autoregressive

$$p_\theta(Y|Z,X) = \prod_{t=1}^{T} p_\theta(y_t|Z,X)$$



Latent Variable Models

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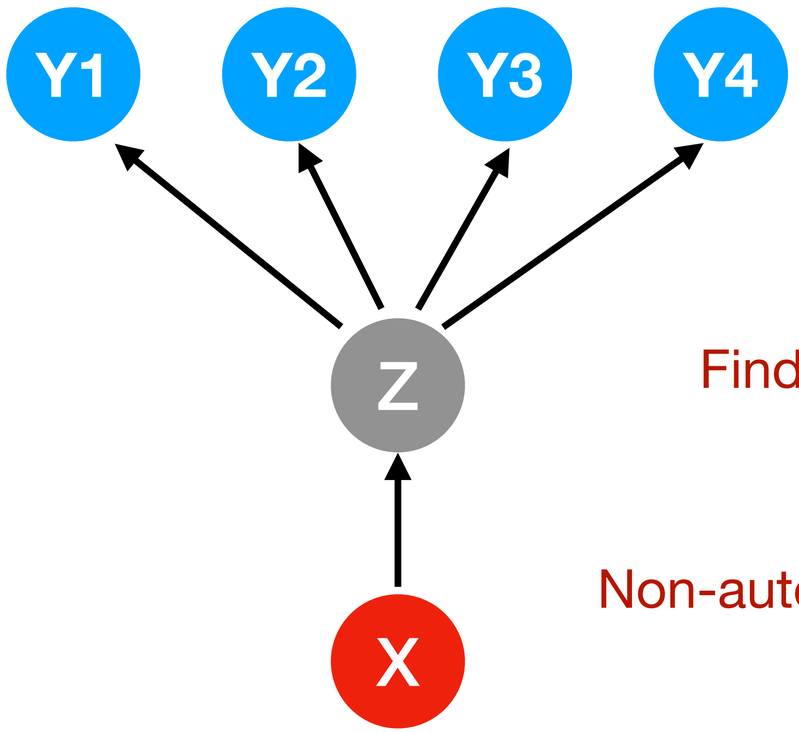

Advantages:

- No direct independent assumptions between X and Y
- Efficient Decoding:

Find optimal Z

$$z^* = \text{argmax}_{z \in \mathcal{Z}} p_\theta(z|x)$$

Non-autoregressive $\Longleftrightarrow$

$$y^* = \text{argmax}_{y \in \mathcal{Y}} p_\theta(y|z^*,x)$$

$$y_t^* = \text{argmax}_{y_t \in V} p_\theta(y_t|z^*,x), \forall t$$

Latent Variable Models

Latent Variable Z

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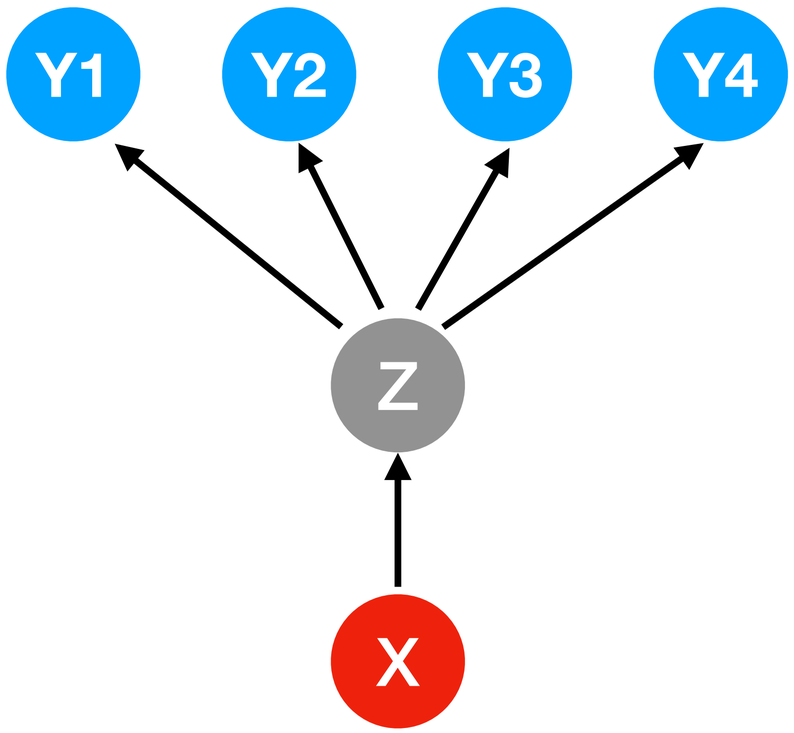
Non-Autoregressive

$$p_\theta(Y|Z,X) = \boxed{\prod_{t=1}^{T} p_\theta(y_t|Z,X)}$$



Problems:

- How to compute the integral of $p_\theta(Y|X)$?
  - Variational Inference
- Z needs to encode all the structured dependencies of Y
  - High-dimensional Z
  - How to model $p_\theta(Z|X)$? Generative Flow

Encoding Structured Dependencies into Z

High-dimensional Latent Variables $Z = \{z_1, z_2, \ldots, z_T\} \in \mathrm{R}^{d \times T}$

Posterior: mapping *X*, *Y* to *Z* $q_\phi(z_t \mid Y, X) = \mathrm{Normal}(\mu_t(Y, X), \sigma_t^2(Y, X))$

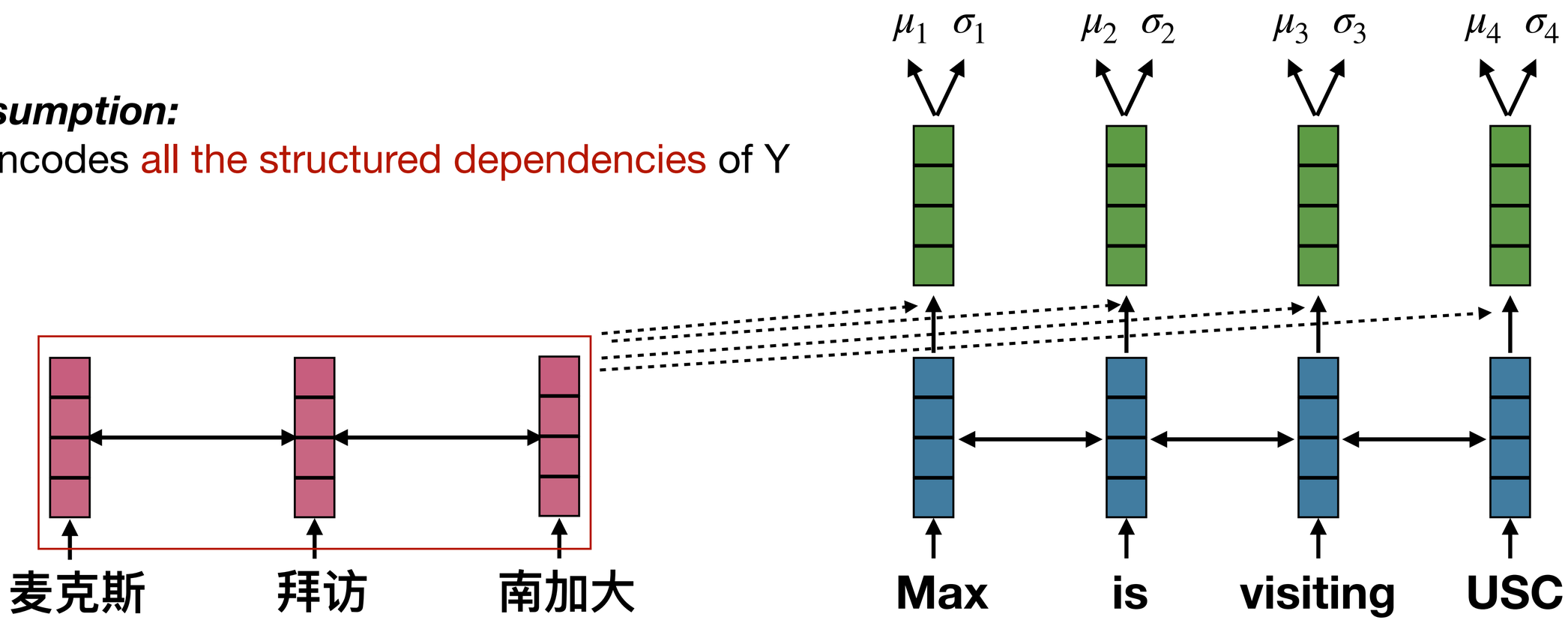
Neural Network

Encoding Structured Dependencies into Z

High-dimensional Latent Variables $Z = \{z_1, z_2, \ldots, z_T\} \in \mathrm{R}^{d \times T}$

Posterior: mapping *X*, *Y* to *Z* $q_\phi(z_t \mid Y, X) = \mathrm{Normal}(\mu_t(Y, X), \sigma_t^2(Y, X))$

Assumption:
Z encodes all the structured dependencies of Y



Latent Variable Models

Latent Variable Z

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Non-Autoregressive

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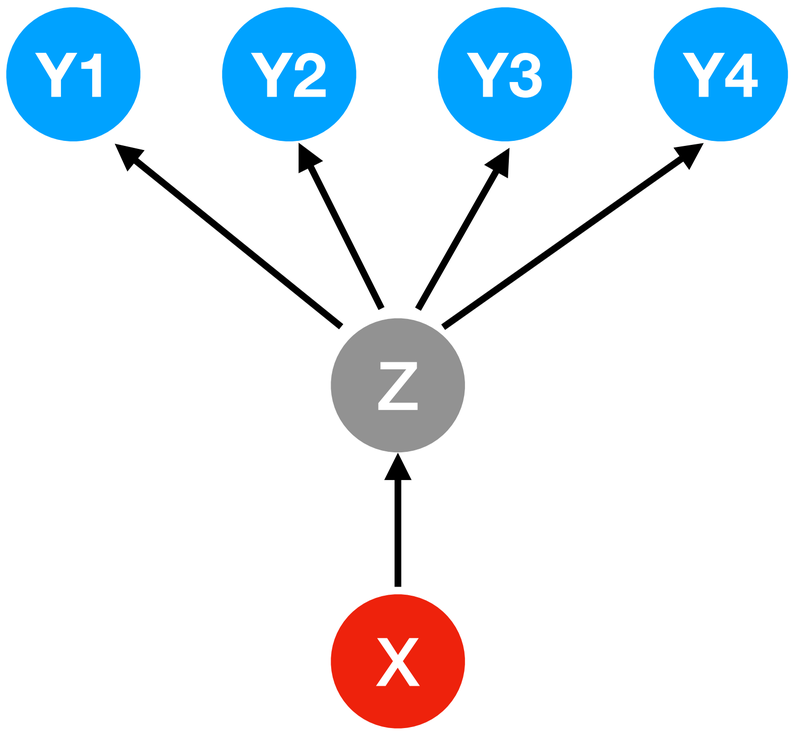

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  - How to model $p_\theta(Z|X)$? Generative Flow

Generative Flow for Prior $p_\theta(Z|X)$

- **Prior** $p_\theta(Z|X)$

$$Z = \{z_1, z_2, \ldots, z_T\} \in \mathrm{R}^{d \times T}$$

Generative Flow

$$\Gamma = f_\theta(Z; X)$$

$$\longrightarrow$$

$$\longleftarrow$$

$$\boxed{Z = f_\theta^{-1}(\Gamma; X)}$$

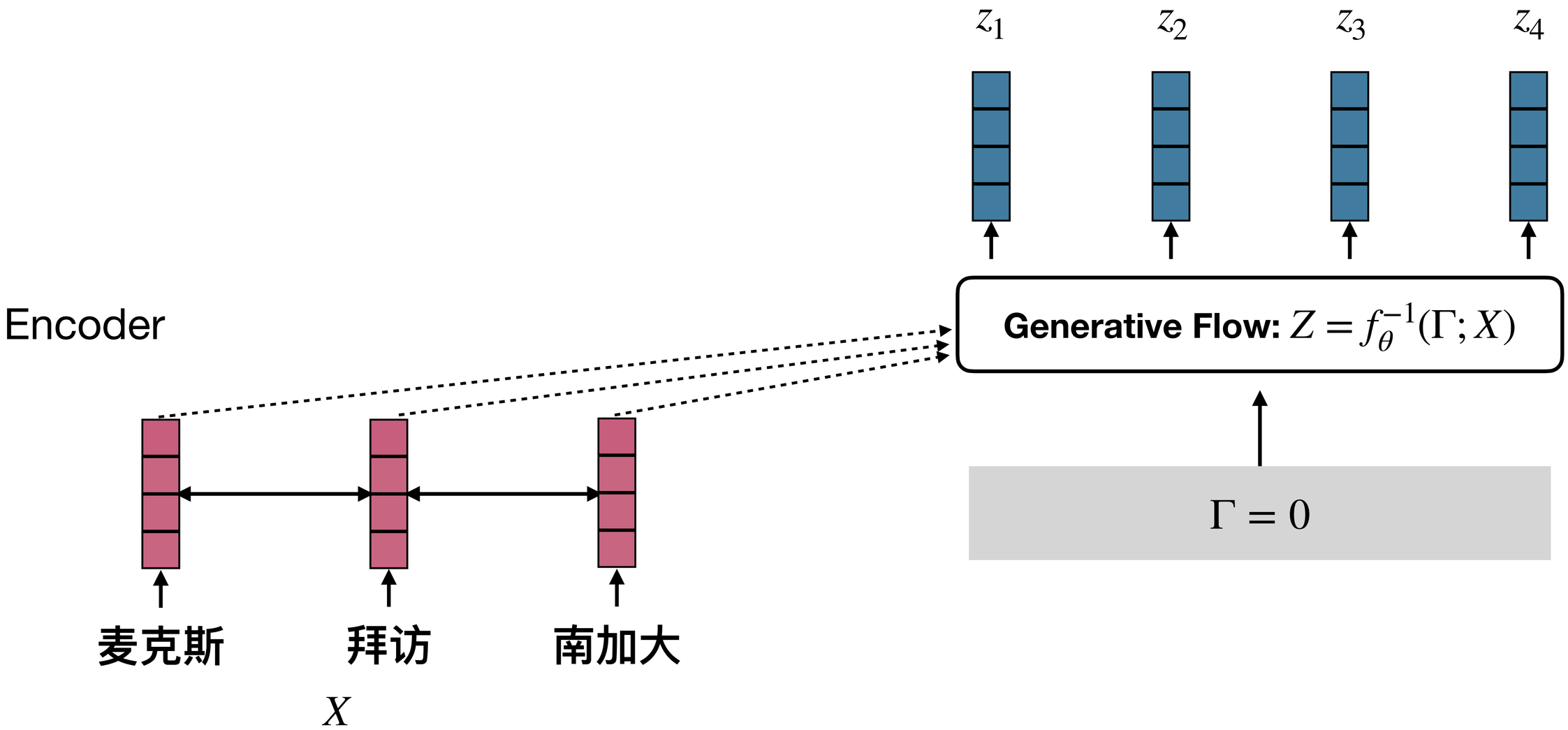
$$\Gamma = \{\gamma_1, \gamma_2, \ldots, \gamma_T\} \in \mathrm{R}^{d \times T}$$

$$\boxed{\gamma_t \sim \mathrm{Normal}(0, I), \forall t}$$

- **Efficient Decoding** $z^* = \mathrm{argmax}_{z \in \mathcal{Z}} p_\theta(z|x)$

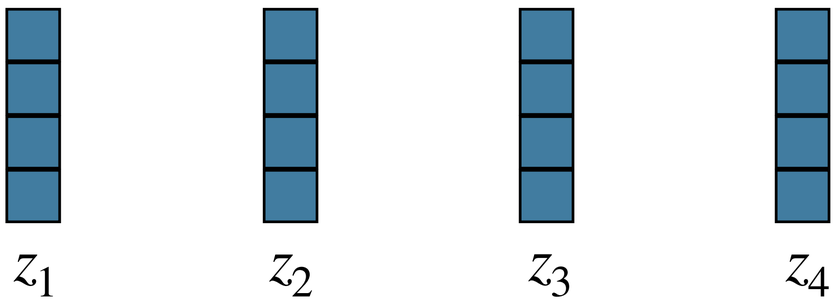
$$z^* \approx f_\theta^{-1}(\Gamma = 0; x)$$

Decoding in FlowSeq

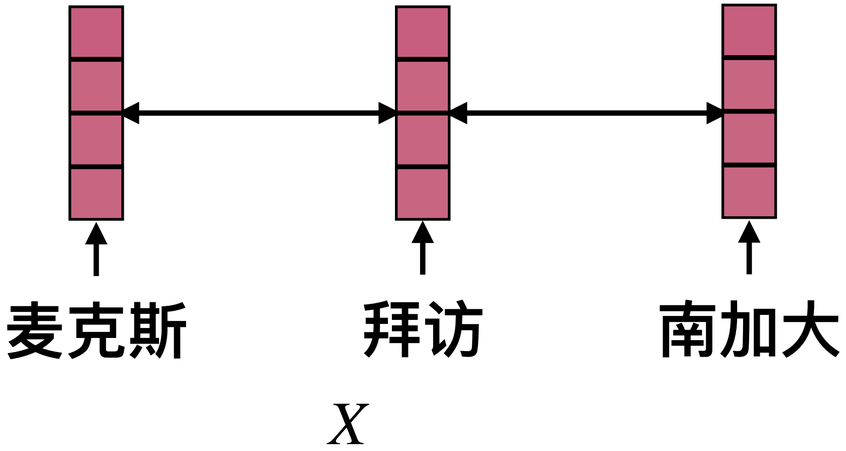


Decoding in FlowSeq

Decoding: $y_t^* = \text{argmax}_{y_t \in V} p_\theta(y_i \mid z, x), \forall t$



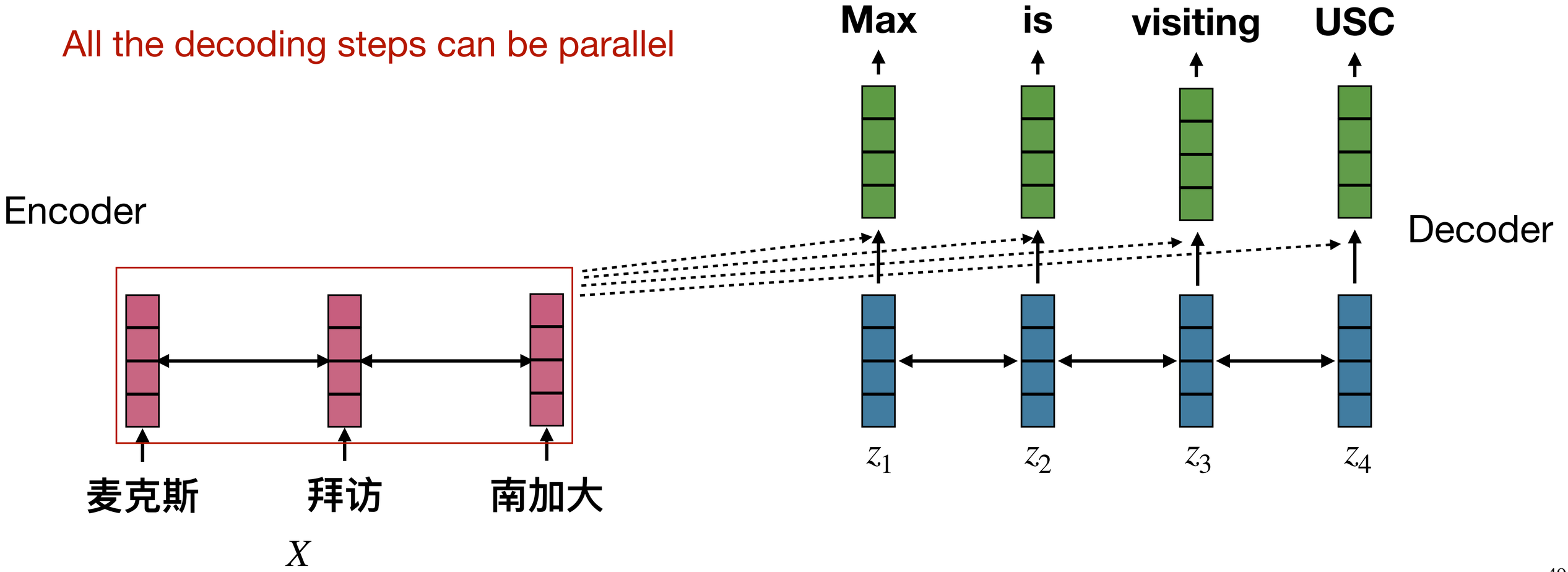
Encoder



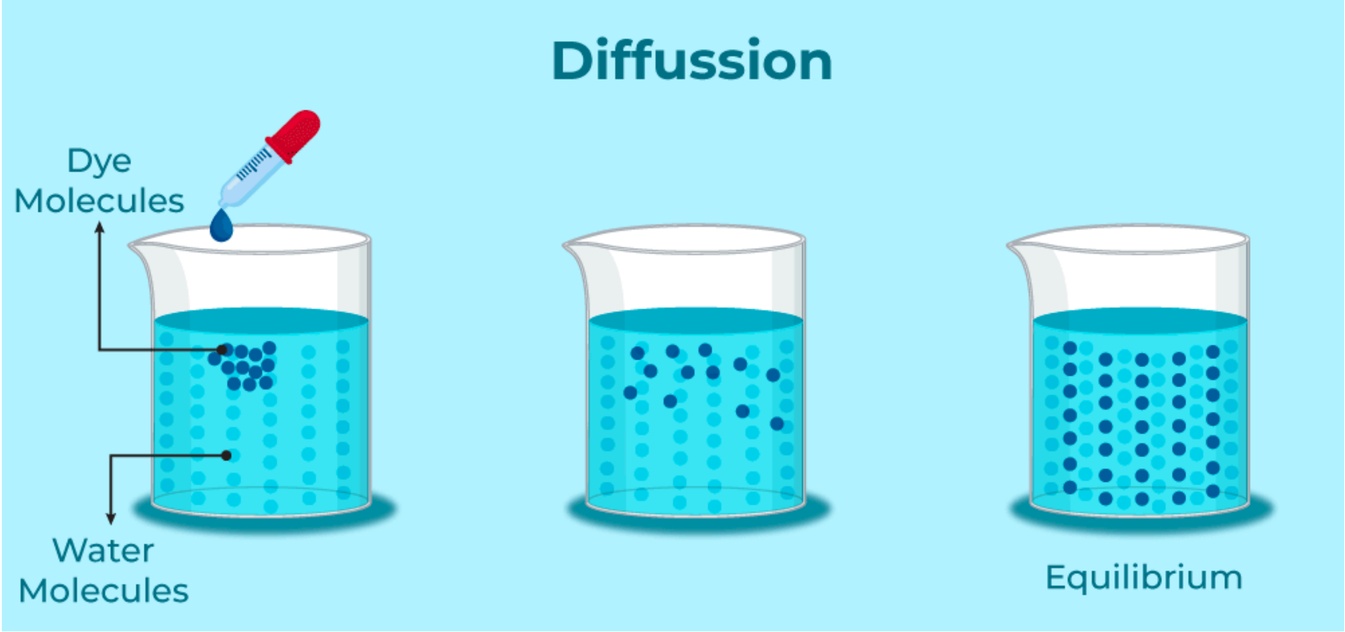
Decoding in FlowSeq

Decoding: $y_t^* = \text{argmax}_{y_t \in V} p_\theta(y_i \mid z, x), \forall t$

All the decoding steps can be parallel



Diffusion Models



Variational Auto-Encoders

- **Why VAEs generate better images than exact density models?**
  - Low-dimension Z
  - Simple prior and posterior distributions

$q(Z|X)$ posterior

$p(X)$

Latent Variables

Z

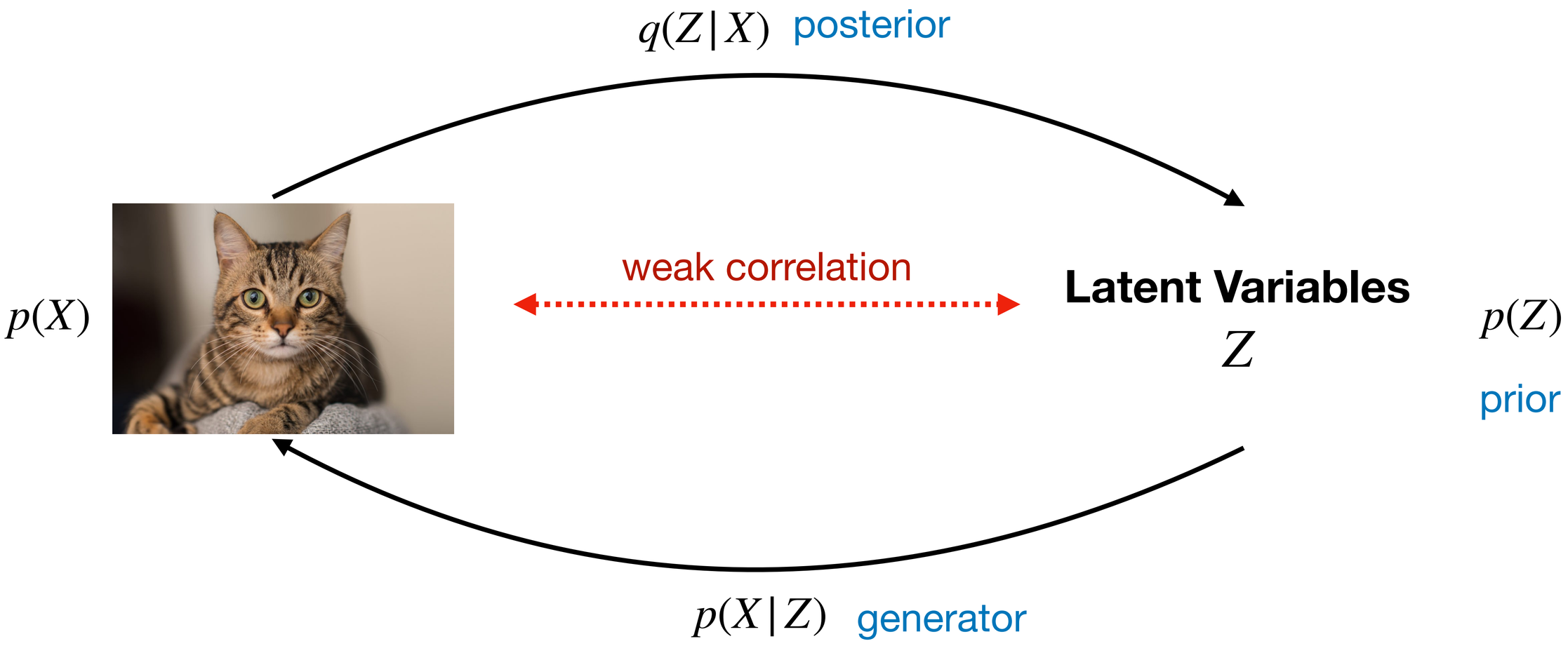
$p(Z)$

prior

$p(X|Z)$ generator

Variational Auto-Encoders

- **Problems?**
  - Connection between X and Z is sometimes weak



Diffusion Models

- **Multi-step hierarchical VAEs**
- **A chain of latent variables**
  - $Z_1, Z_2, \ldots, Z_T$, where each Z_t has the same dimension of X

Prior: $P(Z_T) \sim \mathcal{N}(0, I)$

Posterior: $q(Z_1, Z_2, \ldots, Z_T | X) = \prod_{t=1}^{T} q(Z_t | Z_{t-1}), \quad Z_0 := X$

Forward process

$q(Z_t | Z_{t-1}) \sim \mathcal{N}(\sqrt{1-\beta_t} \cdot Z_{t-1}, \beta_t I)$

Generator: $p(X, Z_1, \ldots, Z_T) = p(Z_T) \prod_{t=1}^{T} p(Z_{t-1} | Z_t)$

Reserve process

$p(Z_{t-1} | Z_t) \sim \mathcal{N}(\mu(Z_t), \Sigma(Z_t))$

Diffusion Models

- **Training Objective**
  - ELBO (the same as VAEs)
- **Sampling**
  - Reverse process
  - $Z_T \rightarrow Z_{T-1} \rightarrow \ldots \rightarrow Z_1 \rightarrow X$

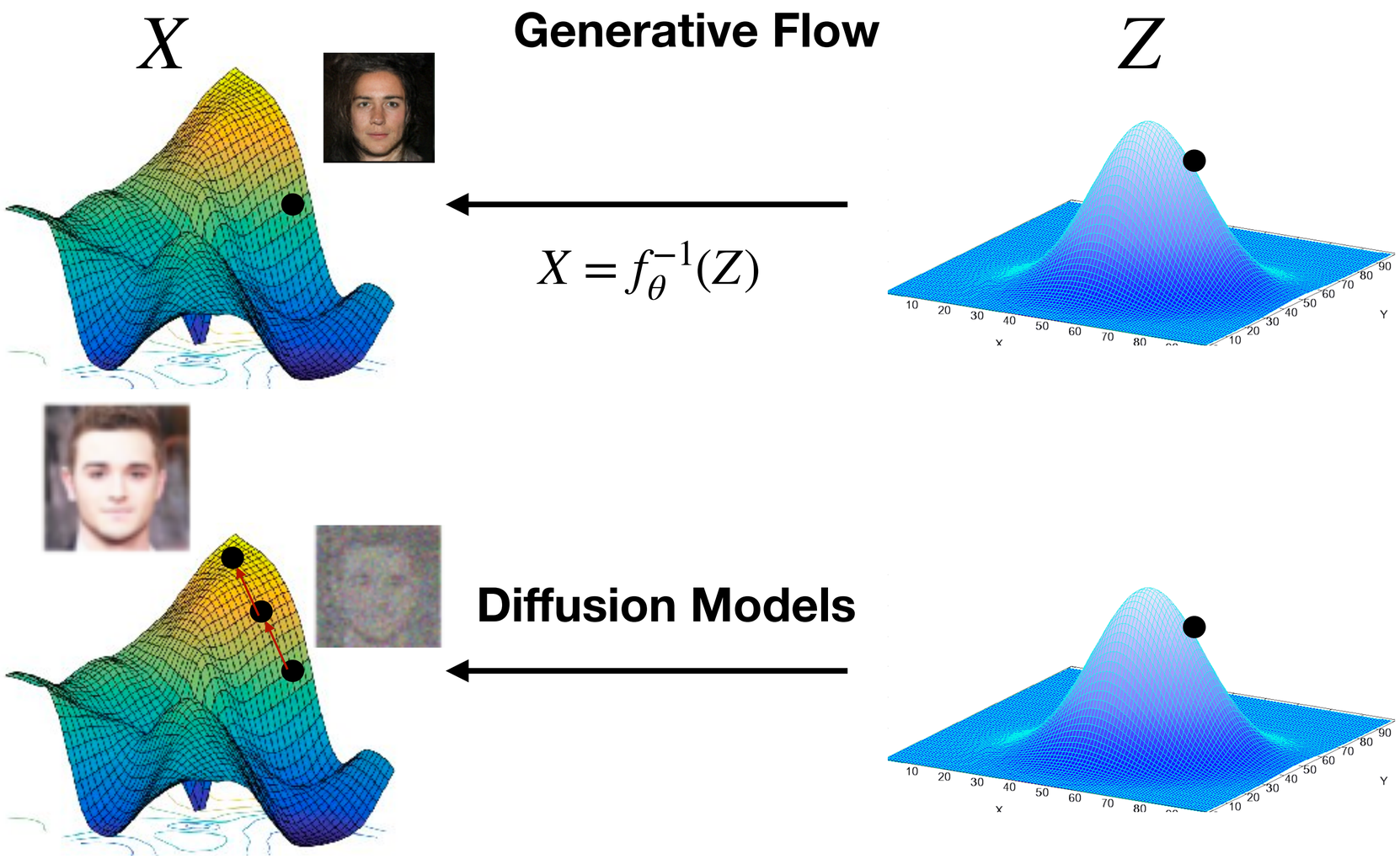
Diffusion Models

- Diffusion models are good at generating high-quality images, but optimized for approximating density
- Why?

Theoretical Explanation of Diffusion Models

- **Stochastic Gradient Langevin Dynamics**
  - $X_t = X_{t-1} + \frac{\delta}{2} \nabla_X \log q(X_{t-1}) + \sqrt{\delta}\epsilon_t$, where $\epsilon_t \sim \mathcal{N}(0,I)$
- **Connection with diffusion models**
  - The reverse process in diffusion models is equivalent to the Stochastic Gradient Langevin Dynamics

Diffusion Models



Reading Materials

- **Relavant Papers**
  - Non-Autoregressive NMT
  - Decoupled Representations
  - Efficient Attention Mechanims