Introduction to Deep Generative Modeling

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BLOG ABOUT DEEP GENERATIVE MODELING

If you are interested in going deeper into deep generative modeling, please take a look at my blog: **[Blog]**

- **Intro**: **[Link]**
- **ARMs**: **[Link]**
- **Flows**: **[Link]**, **[Link]**
- **VAEs**: **[Link]**
- **Hybrid modeling**: TBD

DEEP GENERATIVE MODELING: IS LEARNING CLASSIFIERS ENOUGH?

Let’s assume we have a perfectly trained neural net.

What happens if we add noise to an image?

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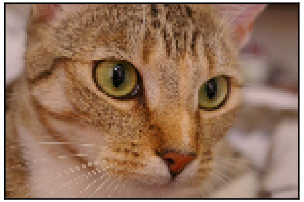
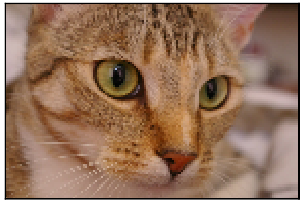


$p(y = cat|\mathbf{x}) = 0.90$
$p(y = dog|\mathbf{x}) = 0.05$
$p(y = horse|\mathbf{x}) = 0.05$

+

noise

=



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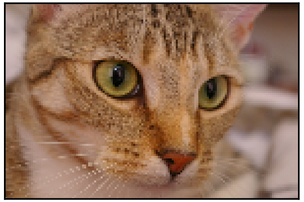

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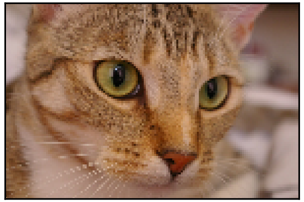

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It may fail completely…

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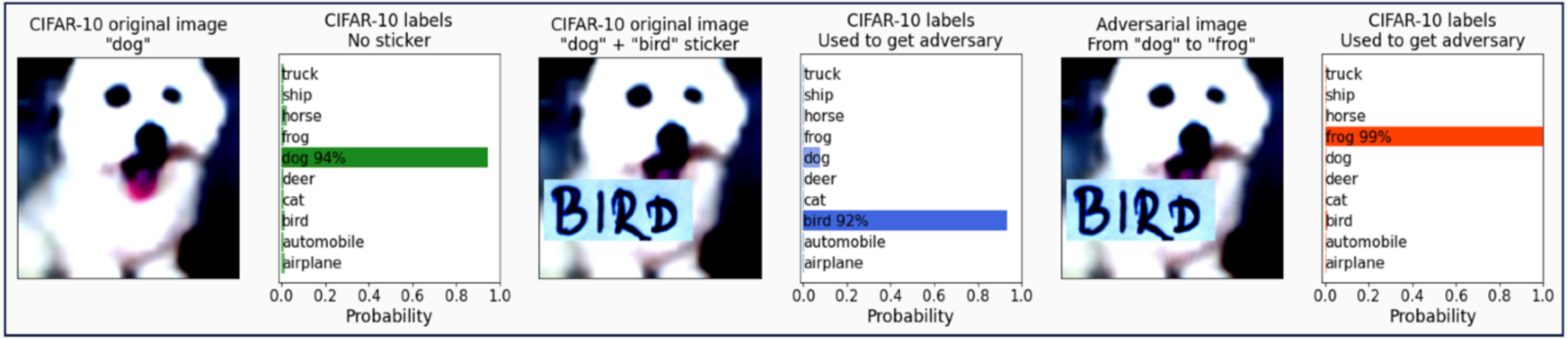

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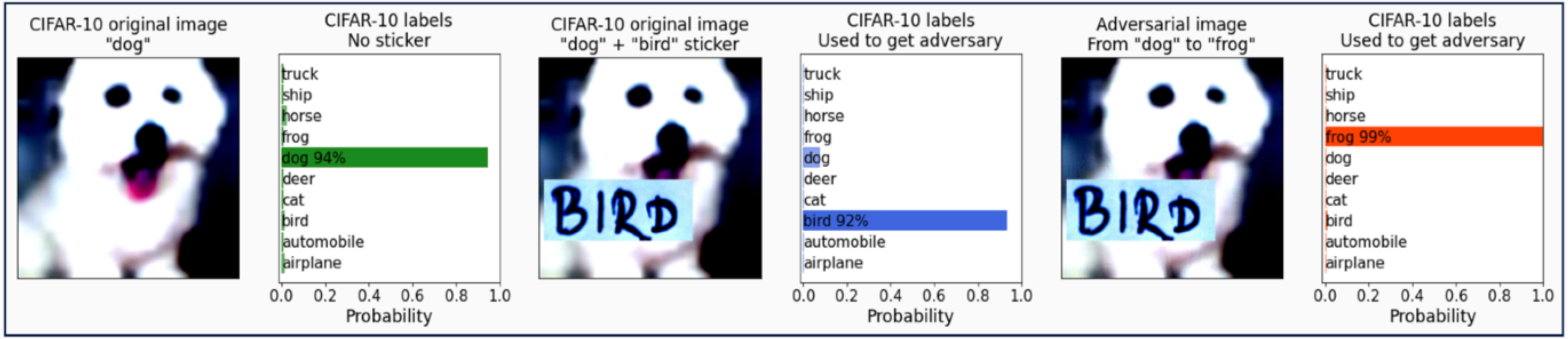

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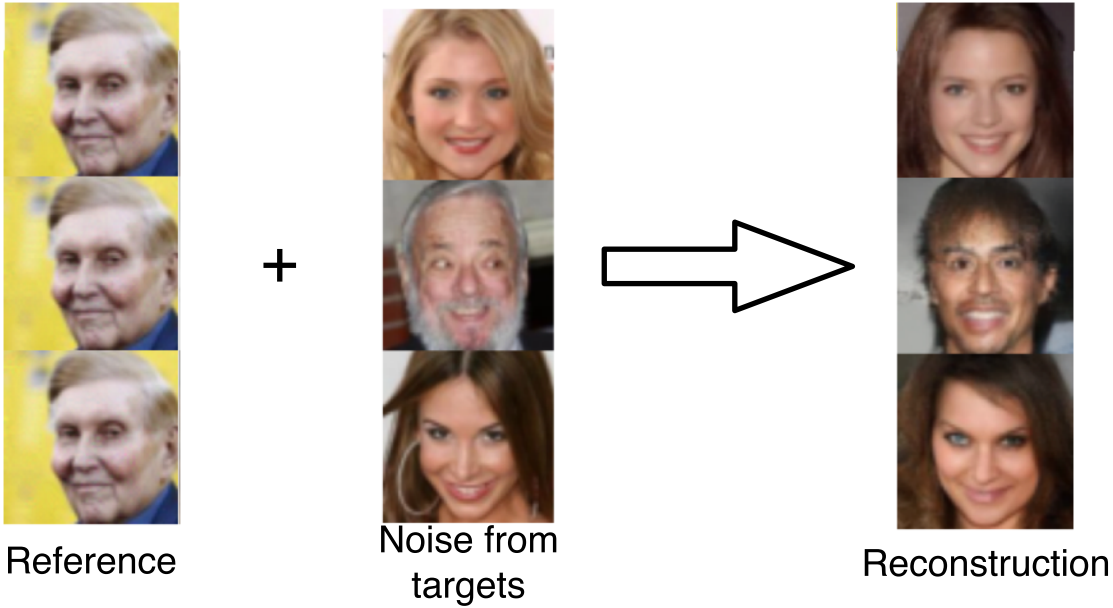

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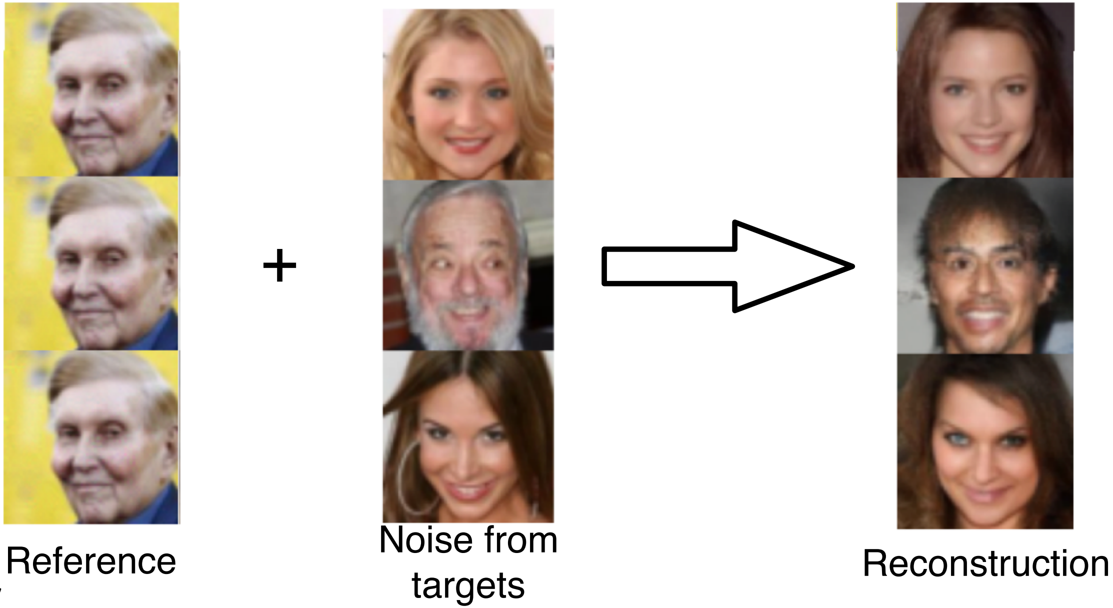

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DEEP GENERATIVE MODELING: IS LEARNING CLASSIFIERS ENOUGH?

We clearly see that training a neural network (i.e., a conditional distribution):

$$p(y\,|\,\mathbf{x}) = \mathrm{softmax}\left(NN(\mathbf{x})\right)$$

is **not enough**!

Granny Smith	0.1%
iPod	99.7%
library	0.0%
pizza	0.0%
toaster	0.0%
dough	0.0%

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What can we do then?

Or, how to modify the **wrong certainty**?

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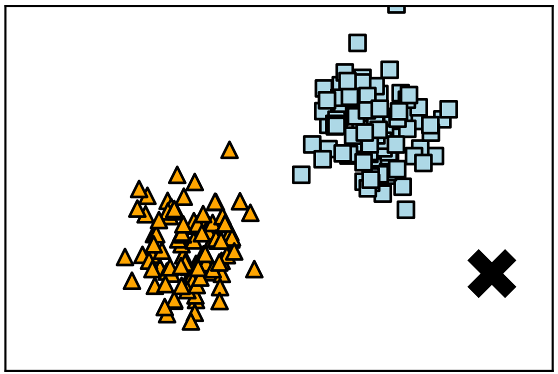
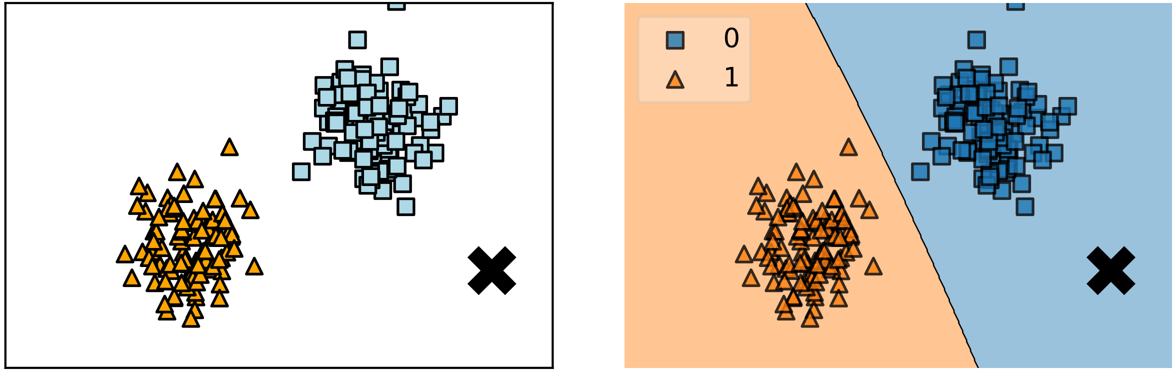
DEEP GENERATIVE MODELING: WHY DO WE NEED THE JOINT DISTRIBUTION?



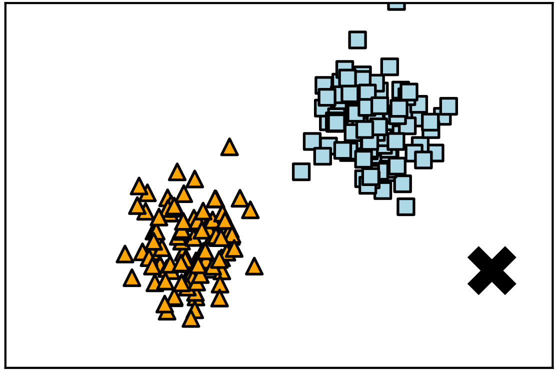
Data

DEEP GENERATIVE MODELING: WHY DO WE NEED THE JOINT DISTRIBUTION?



Data $\qquad$ $p(y|\mathbf{x})$

$p(blue|\mathbf{x})$ is high
= certain decision!



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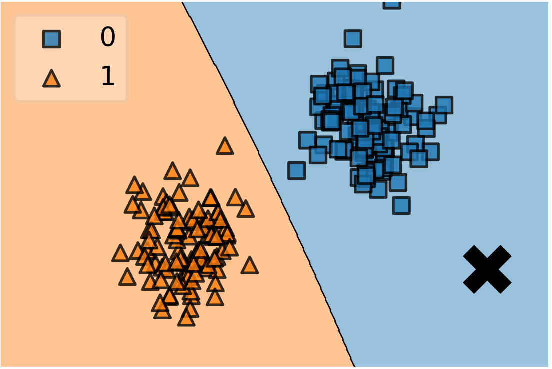

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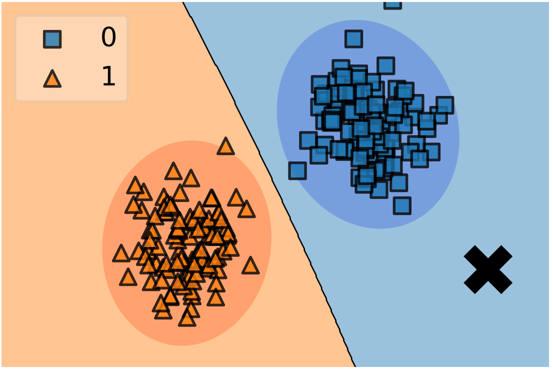

$p(\mathbf{x}, y) = p(y|\mathbf{x})\ p(\mathbf{x})$

$p(blue|\mathbf{x})$ is high
and $p(\mathbf{x})$ is low
= uncertain decision!

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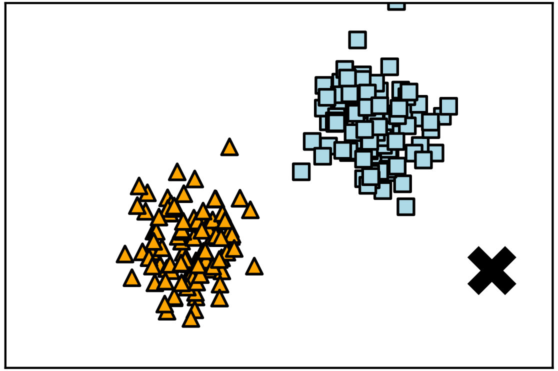

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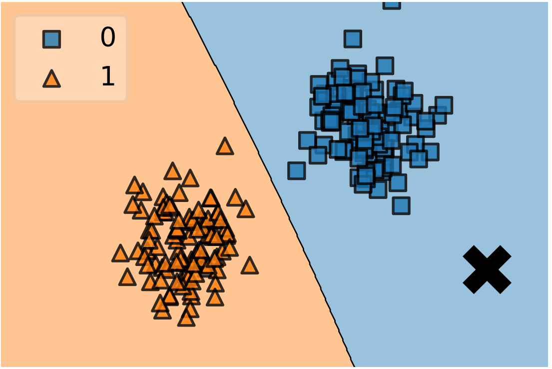

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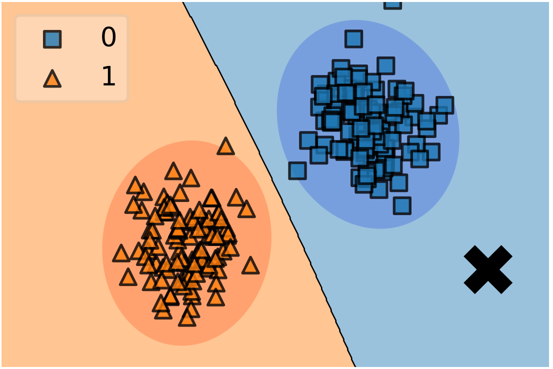

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Thus, learning the conditional is a part of the story!
How can we learn p(x)?

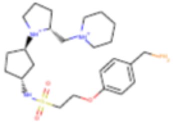
DEEP GENERATIVE MODELING: WHERE CAN WE USE IT?

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .

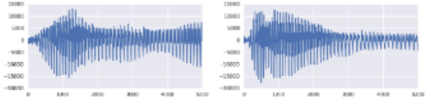
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Text analysis

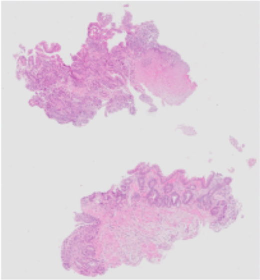
Image analysis



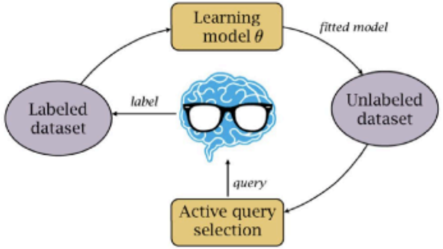
Graph analysis



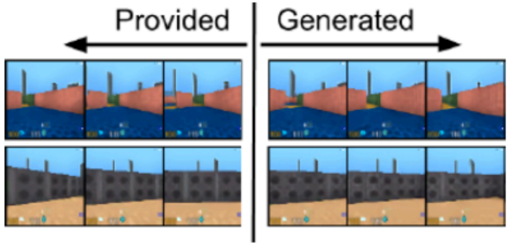
Audio analysis



Medical data



Active Learning



Reinforcement Learning

and more...

DEEP GENERATIVE MODELING: HOW WE CAN FORMULATE IT?

- **Deep Generative Models**
  - **Autoregressive models** (e.g., PixelCNN)
  - **Flow-based models** (e.g., RealNVP)
  - **Latent variable models**
    - **Implicit models** (e.g., GANs)
    - **Prescribed models** (e.g., VAEs)

DEEP GENERATIVE MODELING: HOW WE CAN FORMULATE IT?

Deep Generative Models

+ Energy-based models

- **Autoregressive models** (e.g., PixelCNN)
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+ Diffusion models

DEEP GENERATIVE MODELING: HOW WE CAN FORMULATE IT?

Generative models	Training	Likelihood	Sampling	Lossy compression	Lossless compression
Autoregressive models	stable	exact	slow	no	yes
Flow-based models	stable	exact	fast/slow	no	yes
Implicit models	unstable	no	fast	no	no
Prescribed model	stable	approximate	fast	yes	no

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AUTOREGRESSIVE MODELS (ARMS)

We are interested in modeling

$$p(\mathbf{x})$$

where $\mathbf{x} \in \{0,1,\ldots,255\}^{D\times 3}$ is an RGB image (for instance).

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$$p(\mathbf{x}) = p(x_1)\prod_{d=2}^{D} p(x_d | \mathbf{x}_{<d})$$

where $\mathbf{x}_{<d} = [x_1, x_2, \ldots, x_{d-1}]^\top$

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Example:

$$p(\mathbf{x}) = p(x_1)p(x_2 | x_1)p(x_3 | x_1, x_2)$$

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Training objective:

$$\ln p(\mathbf{x}) = \ln p(x_1) + \sum_{d=2}^{D} \ln p(x_d | \mathbf{x}_{<d})$$

Question: How we can model the conditionals $p(x_d | \mathbf{x}_{<d})$ **efficiently**?

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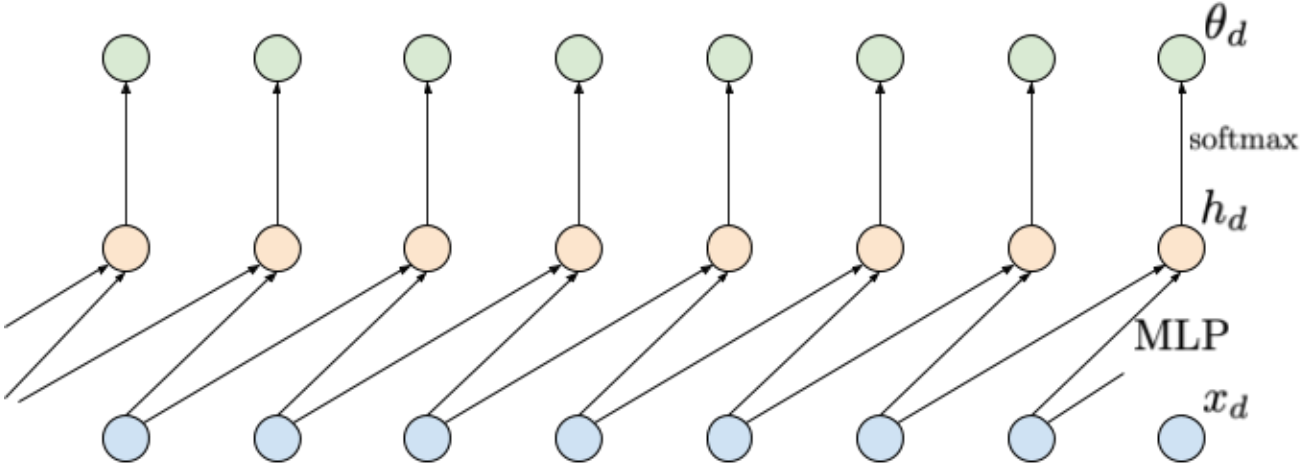
Approach 1: **Finite memory**



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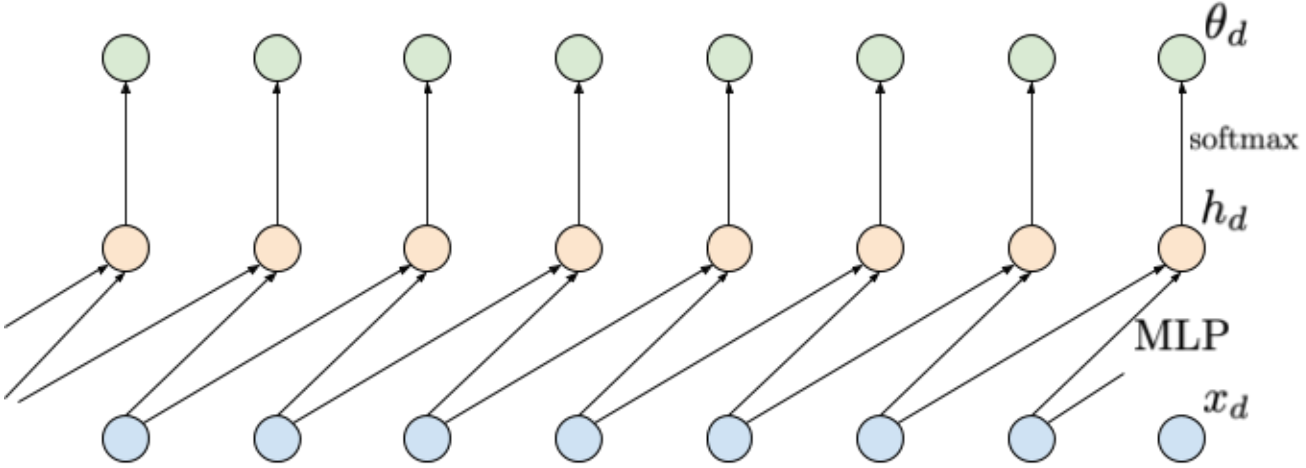
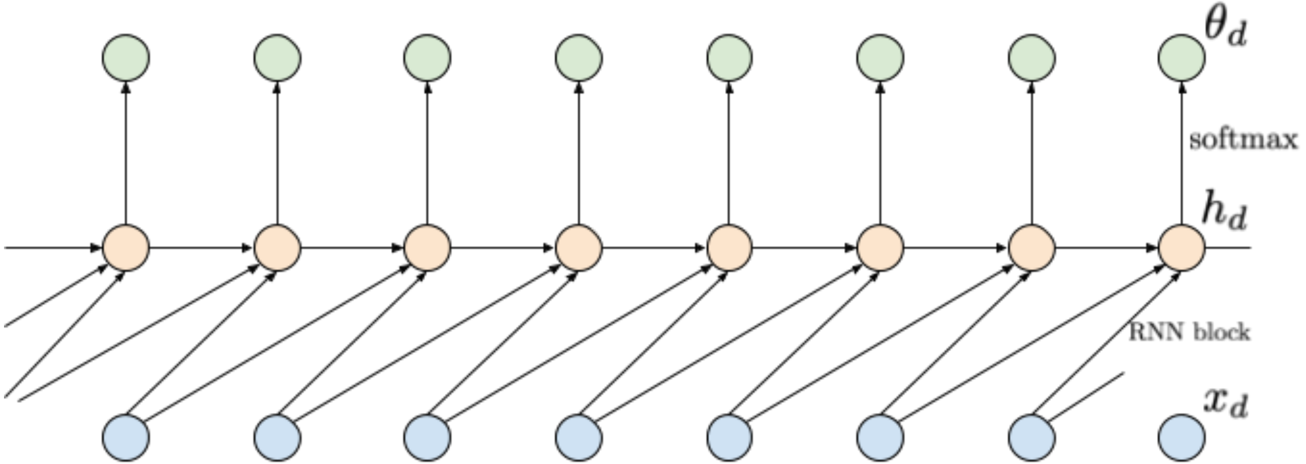


Easy!

Limited dependencies!
How many we should take?

Question: How we can model the conditionals $p(x_d | \mathbf{x}_{<d})$ **efficiently**?

Approach 2: **Long-range memory with RNNs**



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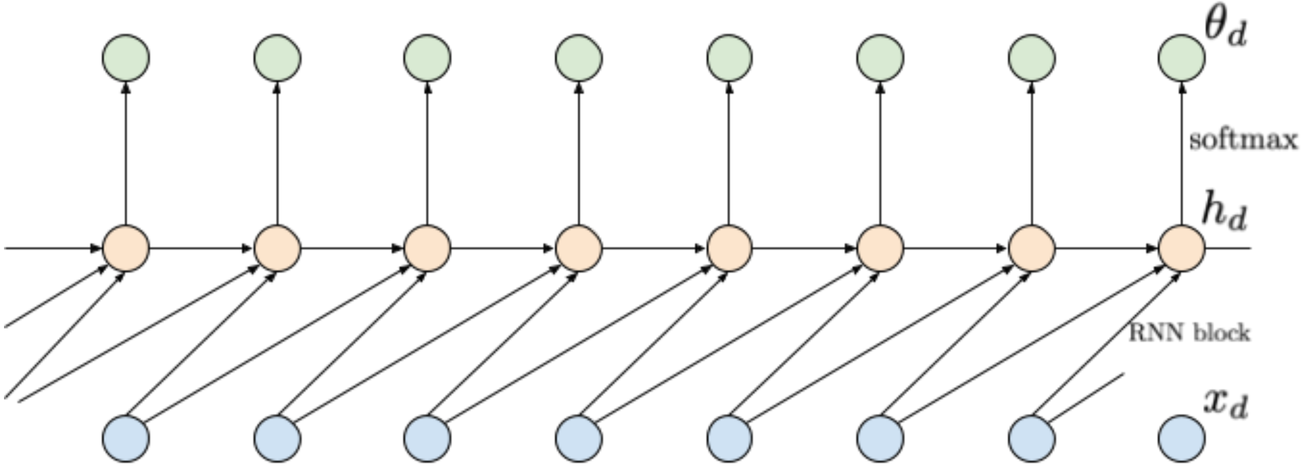
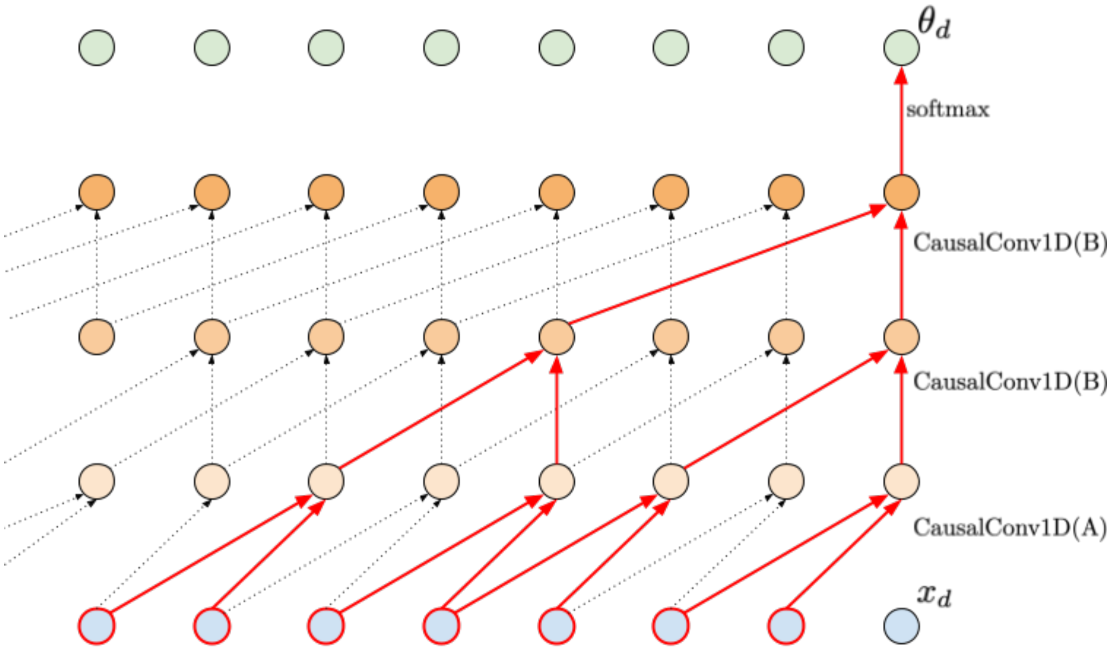


Easy!
Long-range dependencies!

Sequential -> slow
Vanishing gradient problem

Question: How we can model the conditionals $p(x_d \mid \mathbf{x}_{<d})$ **efficiently**?

Approach 3: **Long-range memory with CNNs**



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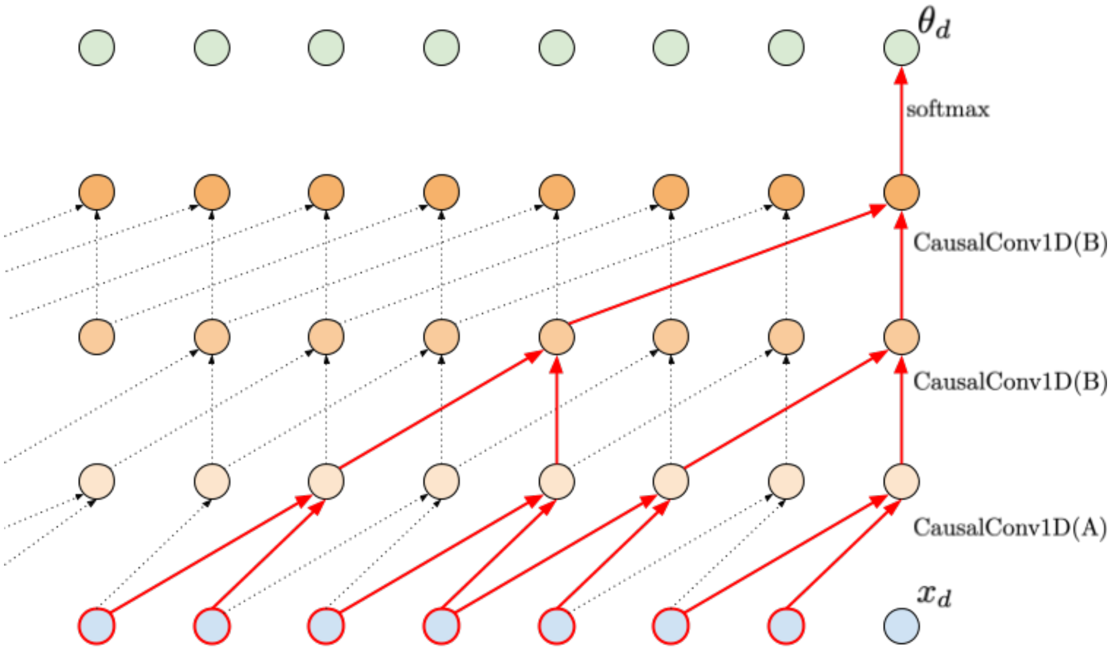
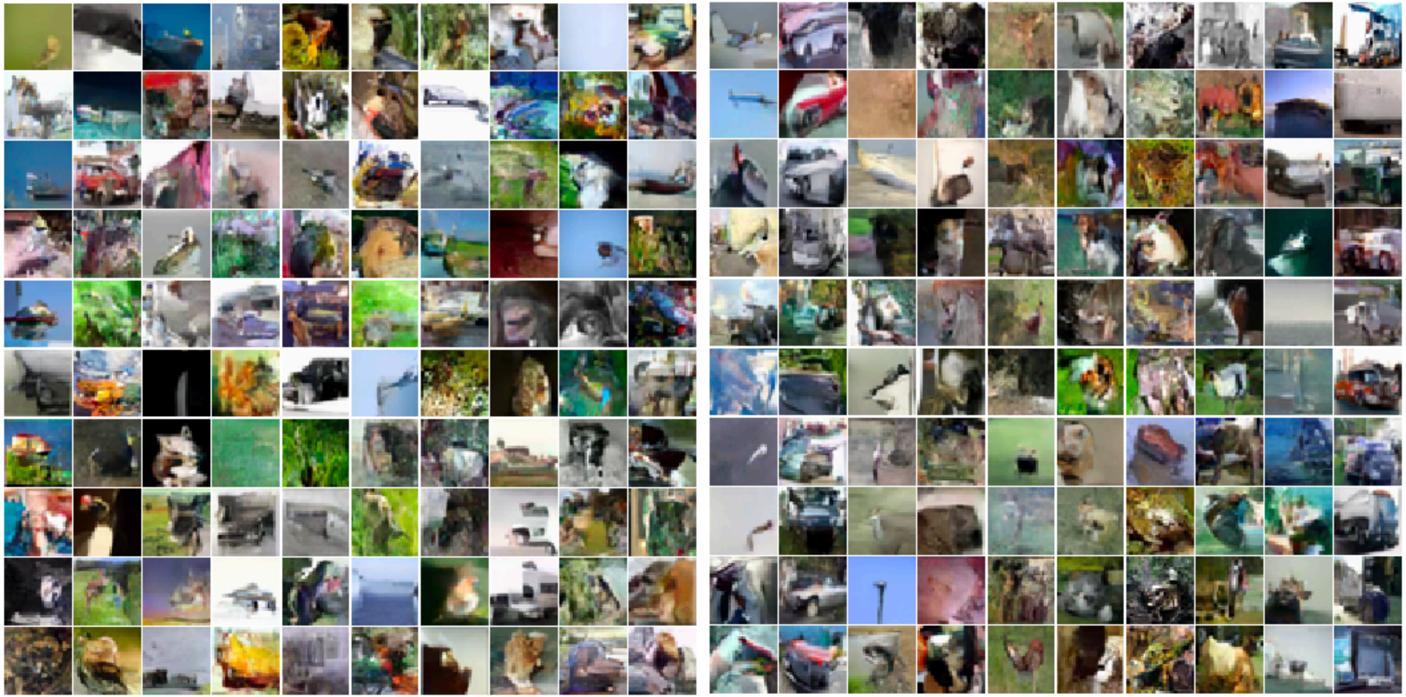


Easy!
Long-range dependencies!
No training issues!

Slow generation

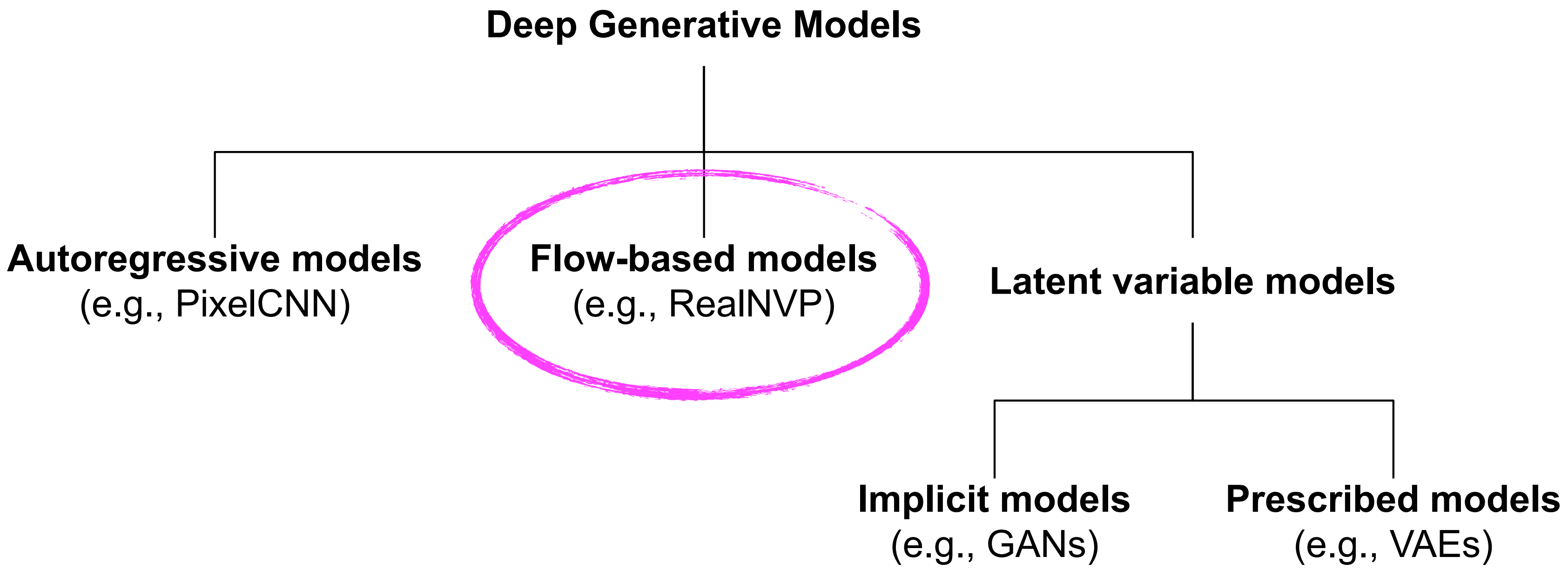
AUTOREGRESSIVE MODELS (ARMS)



Samples from a PixelCNN

 Chen, Xi, et al. "Pixelsnail: An improved autoregressive generative model." *ICML 2018*

DEEP GENERATIVE MODELING: HOW WE CAN FORMULATE IT?



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FLOWS (FLOW-BASED MODELS)

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What is the answer? $\mathcal{N}(x \,|\, 1,0.75)$!

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What is the answer? $\mathcal{N}(x|1,0.75)$!

How can we calculate that? Through the **change of variables formula**:

$$p(x) = \pi\left(z = f^{-1}(x)\right)\left|\frac{\partial f^{-1}(x)}{\partial x}\right|$$

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Change of volume (Jacobian)

Invertible function

FLOWS (FLOW-BASED MODELS)

We change a random variable **x** to another random variable **z** using **invertible** transformations, $\mathbf{x}, \mathbf{z} \in \mathbb{R}^D$:

$$p(\mathbf{x}) = \pi\left(\mathbf{z}_0 = f^{-1}(\mathbf{x})\right) \prod_{i=1}^{K} \left| \mathbf{J}_{f_i}(z_{i-1}) \right|^{-1}$$

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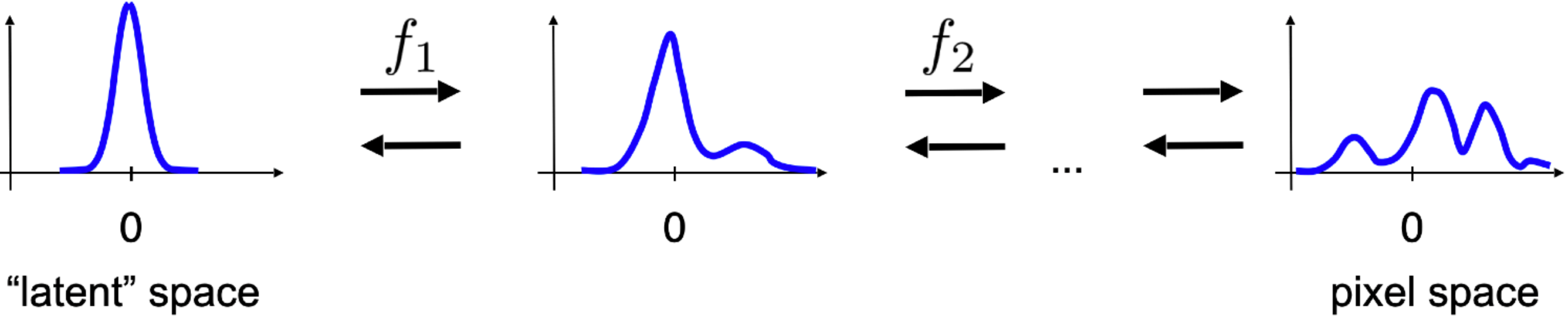

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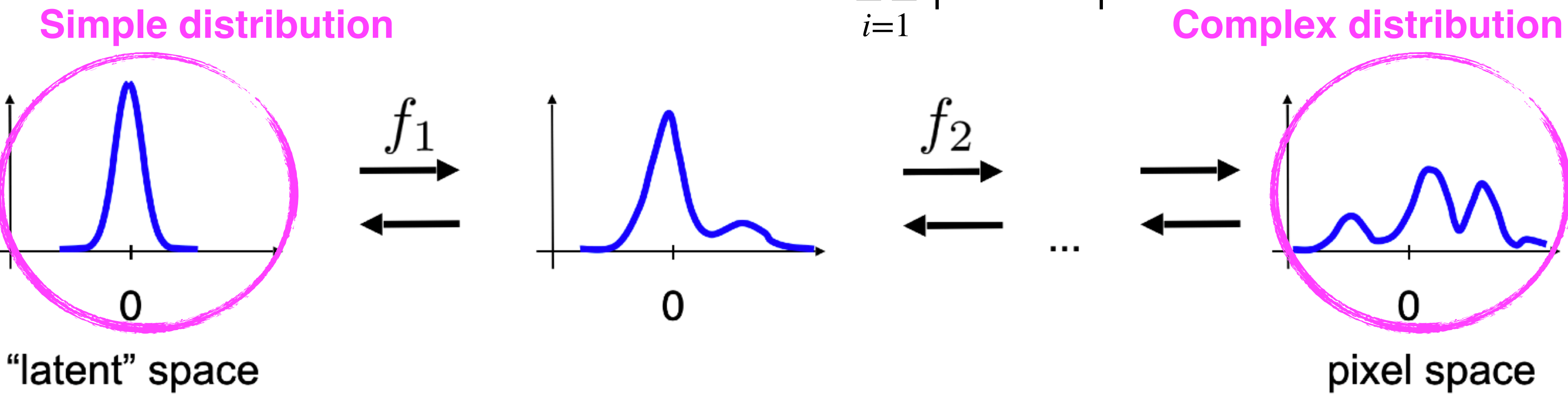

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Known, e.g., Gaussian

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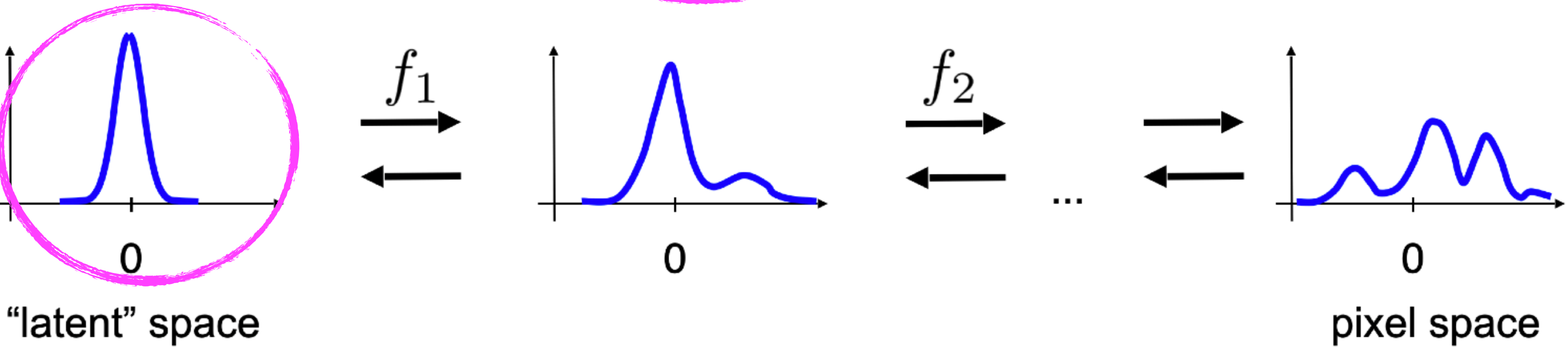

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Jacobian must be tractable

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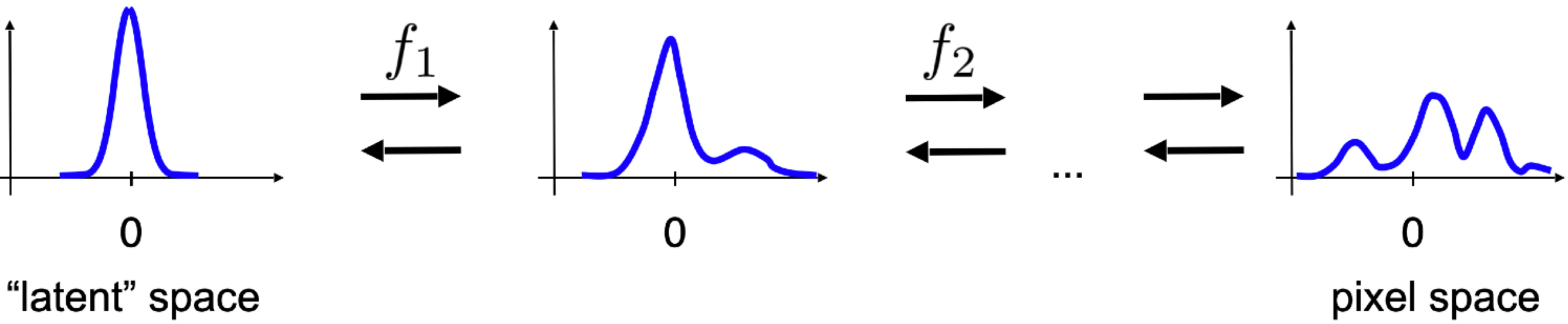

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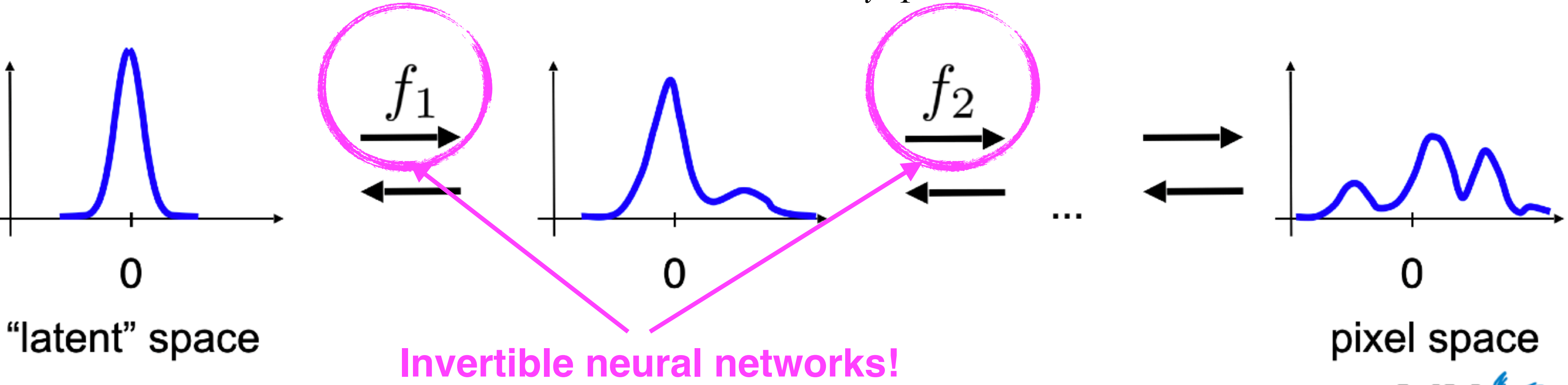

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Training objective:

$$\ln p(\mathbf{x}) = \ln \pi\left(\mathbf{z}_0 = f^{-1}(\mathbf{x})\right) - \sum_{i=1}^{K} \ln \left| \mathbf{J}_{f_i}(z_{i-1}) \right|$$

Two main components

1) **Coupling layer**:

$$\mathbf{y}_a = \mathbf{x}_a$$
$$\mathbf{y}_b = \exp\left(s\left(\mathbf{x}_a\right)\right) \odot \mathbf{x}_b + t\left(\mathbf{x}_a\right)$$

is invertible by design:

$$\mathbf{x}_b = \left(\mathbf{y}_b - t(\mathbf{y}_a)\right) \odot \exp\left(-s(\mathbf{y}_a)\right)$$
$$\mathbf{x}_a = \mathbf{y}_a$$

2) **Permutation layer**

Two main components

1) **Coupling layer**:

$$\mathbf{y}_a = \mathbf{x}_a$$
$$\mathbf{y}_b = \exp\left(s\left(\mathbf{x}_a\right)\right) \odot \mathbf{x}_b + t\left(\mathbf{x}_a\right)$$

Jacobian is tractable!

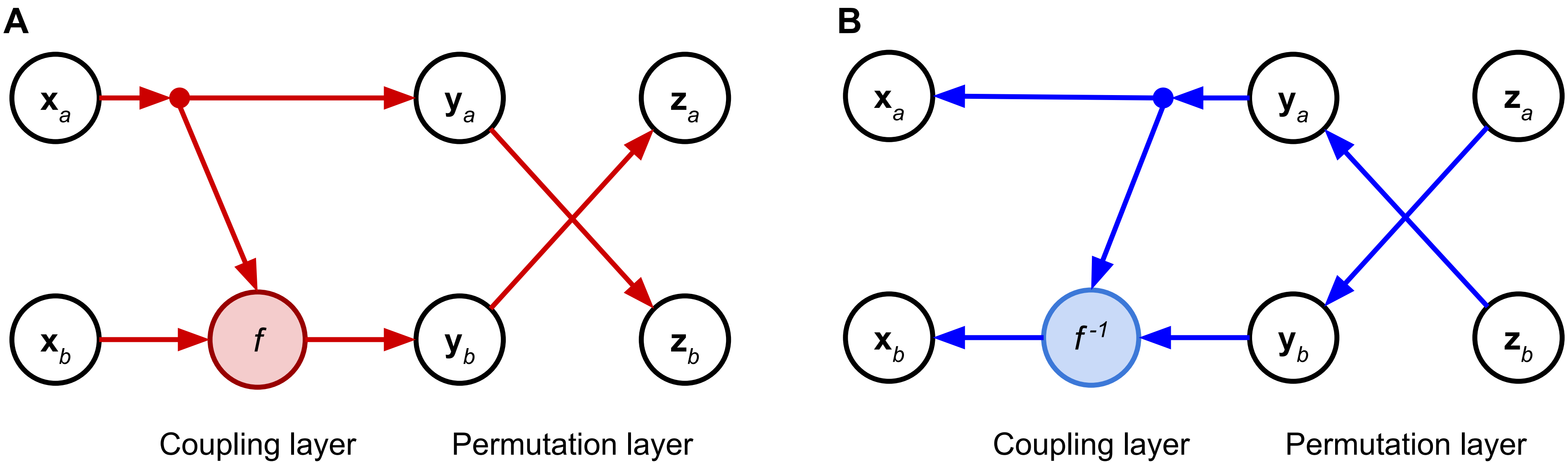
$$\det(\mathbf{J}) = \prod_{j=1}^{D-d} \exp\left(s\left(\mathbf{x}_a\right)\right)_j = \exp\left(\sum_{j=1}^{D-d} s\left(\mathbf{x}_a\right)_j\right)$$

is invertible by design:

$$\mathbf{x}_b = \left(\mathbf{y}_b - t(\mathbf{y}_a)\right) \odot \exp\left(-s(\mathbf{y}_a)\right)$$
$$\mathbf{x}_a = \mathbf{y}_a$$

2) **Permutation layer** $\det(\mathbf{J}) = 1$

FLOWS (FLOW-BASED MODELS): INVERTIBLE LAYERS



A: Forward pass. **B**: Inverse pass.

FLOWS (FLOW-BASED MODELS)

 Kingma, D.P., and Prafulla D. "Glow: Generative flow with invertible 1x1 convolutions." *NeurIPSx 2018*

DEEP GENERATIVE MODELING: HOW WE CAN FORMULATE IT?

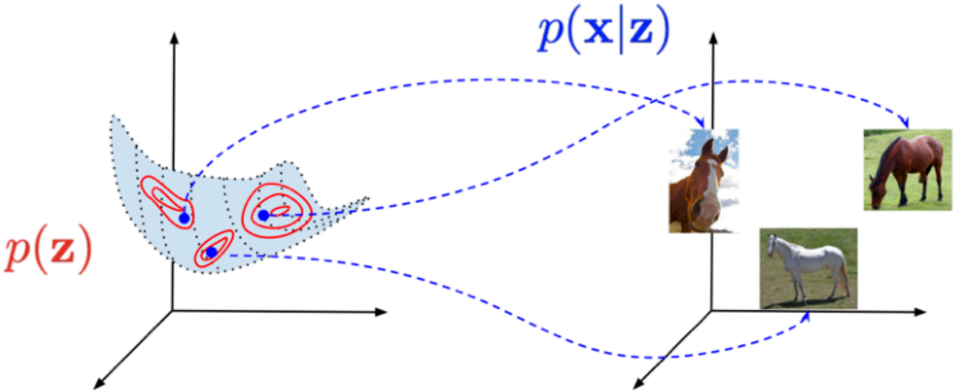
Deep Generative Models

- **Autoregressive models** (e.g., PixelCNN)
- **Flow-based models** (e.g., RealNVP)
- **Latent variable models**
  - **Implicit models** (e.g., GANs)
  - **Prescribed models** (e.g., VAEs)

Let's consider a **latent variable model** where we distinguish:

- **latent variables** $\mathbf{z} \in \mathcal{Z}^M$
- **observable variables** $\mathbf{x} \in \mathcal{X}^D$

Latent variables lie on a **low-dimensional manifold**.



Generative process:

1. $\mathbf{z} \sim p(\mathbf{z})$
2. $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$

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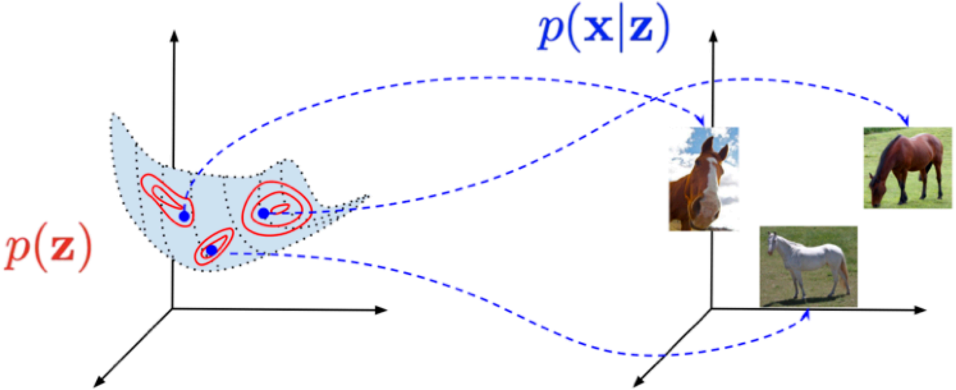

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The objective function:

$$\ln p(\mathbf{x}) = \ln \int p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) \, \mathrm{d}\mathbf{z}$$

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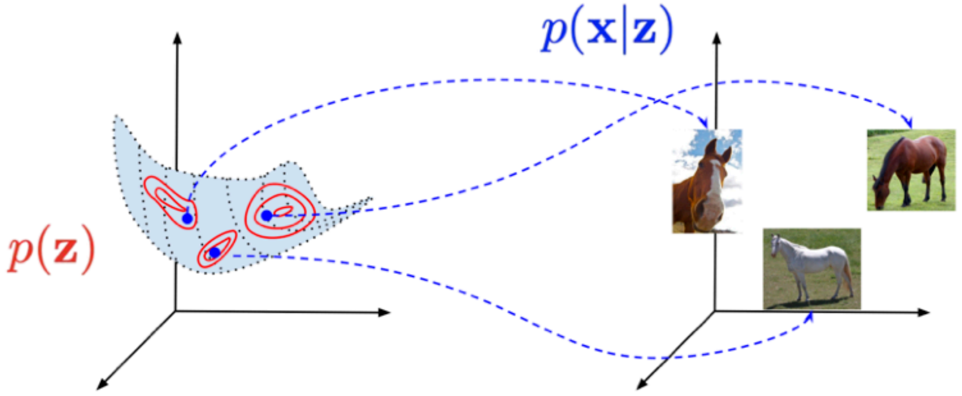

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The integral is intractable…

$$\ln p(\mathbf{x}) = \ln \int p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z}) \; \mathrm{d}\mathbf{z}$$

$$= \ln \int \frac{q_\phi(\mathbf{z})}{q_\phi(\mathbf{z})} p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z}) \; \mathrm{d}\mathbf{z}$$

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Variational posteriors

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$$
\begin{aligned}
\ln p(\mathbf{x}) &= \ln \int p(\mathbf{x}\,|\,\mathbf{z})p(\mathbf{z})\ \mathrm{d}\mathbf{z} \\
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Reconstruction error **"Regularization" term**

$$= \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z})}\left[\ln p(\mathbf{x}\,|\,\mathbf{z}) + \ln p(\mathbf{z}) - \ln q_\phi(\mathbf{z})\right]$$

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ELBO: Evidence Lower Bound

 Kingma, D.P., and Welling, M.. "Auto-encoding variational bayes." *ICLR 2014*

VARIATIONAL AUTO-ENCODERS

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In other words, a single parameterization for each new input **x**.

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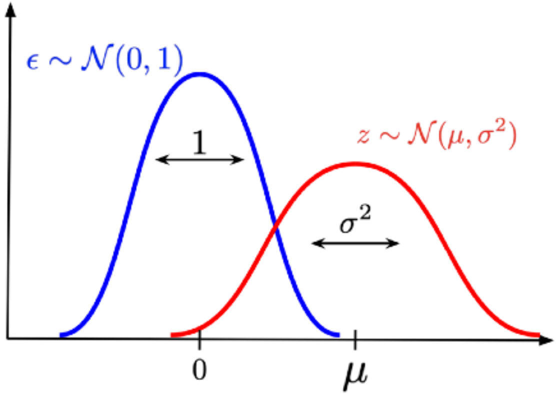
Moreover, we use **reparameterization trick**:

Every Gaussian variable could be defined as:

$z = \mu + \sigma \cdot \varepsilon$

where $\varepsilon \sim \mathcal{N}(0,1)$



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We consider **amortized inference**: $q_\phi(\mathbf{z}\,|\,\mathbf{x})$

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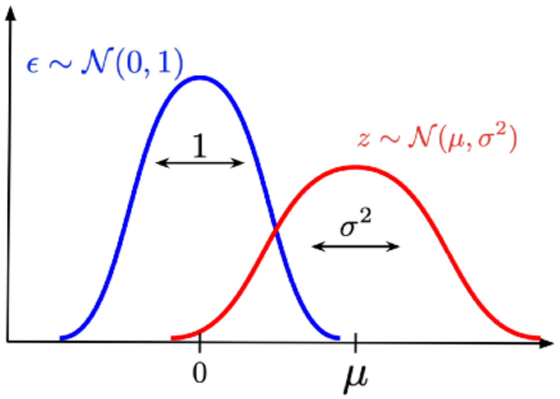
Moreover, we use **reparameterization trick**:

It reduces the variance of the gradients.

It allows to get randomness outside **z**.

$$z = \mu + \sigma \cdot \varepsilon$$



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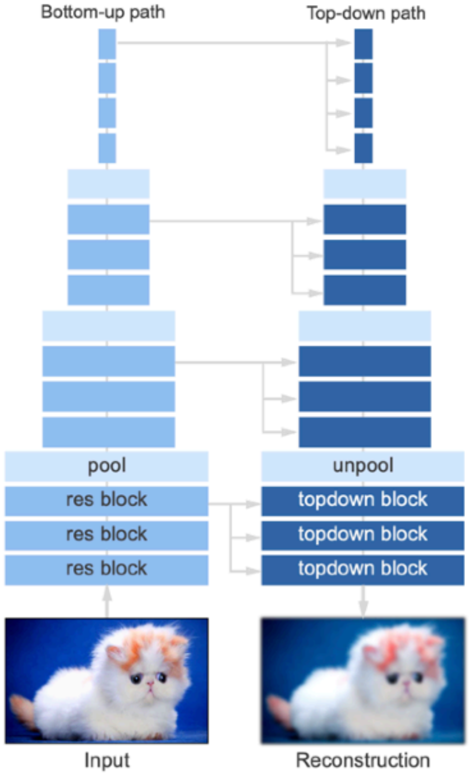
VARIATIONAL AUTO-ENCODERS

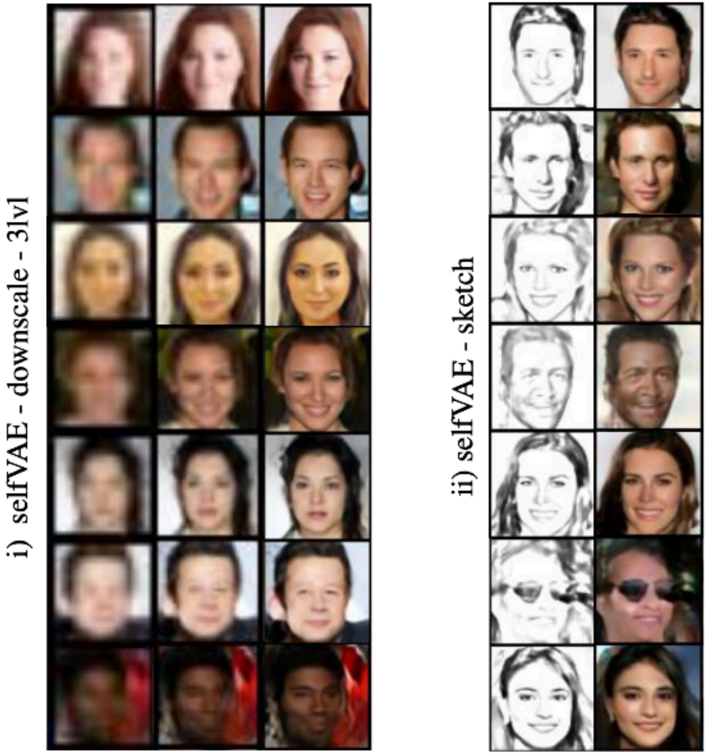
Generations



Very Deep VAE

67 Child, R. "Very Deep VAEs Generalize Autoregressive Models and Can Outperform Them on Images." *ICLR 2021*

VARIATIONAL AUTO-ENCODERS



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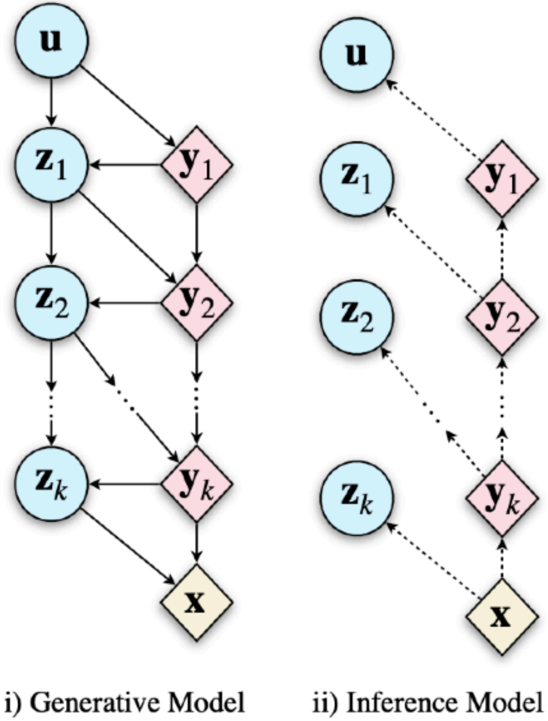

Hierarchical VAE

Gatopoulos, I., and Tomczak, J.M., "Self-Supervised Variational Auto-Encoders." *arXiv preprint arXiv:2010.02014* (2020).

CONCLUSION

- Here: **the likelihood-based generative models**.

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$$p(\mathbf{x}, y) = p(y \mid \mathbf{x})\, p(\mathbf{x})$$

CONCLUSION

- Here: **the likelihood-based generative models**.
- We **skipped** Generative Adversarial Nets & others.
- Why generative modeling?

$$p(\mathbf{x}, y) = p(y \,|\, \mathbf{x})\, p(\mathbf{x})$$

- Important directions:

➡ Better uncertainty quantification

➡ New parameterization (new neural networks)

➡ Out-of-Distribution

➡ Continual learning

THANK YOU FOR YOUR ATTENTION

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