Why AI needs Deep Generative Modeling?

Jakub M. Tomczak

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What is **intelligence**?

What is **intelligence**?

…

What is **intelligence**?

…

What is **artificial intelligence**?

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…

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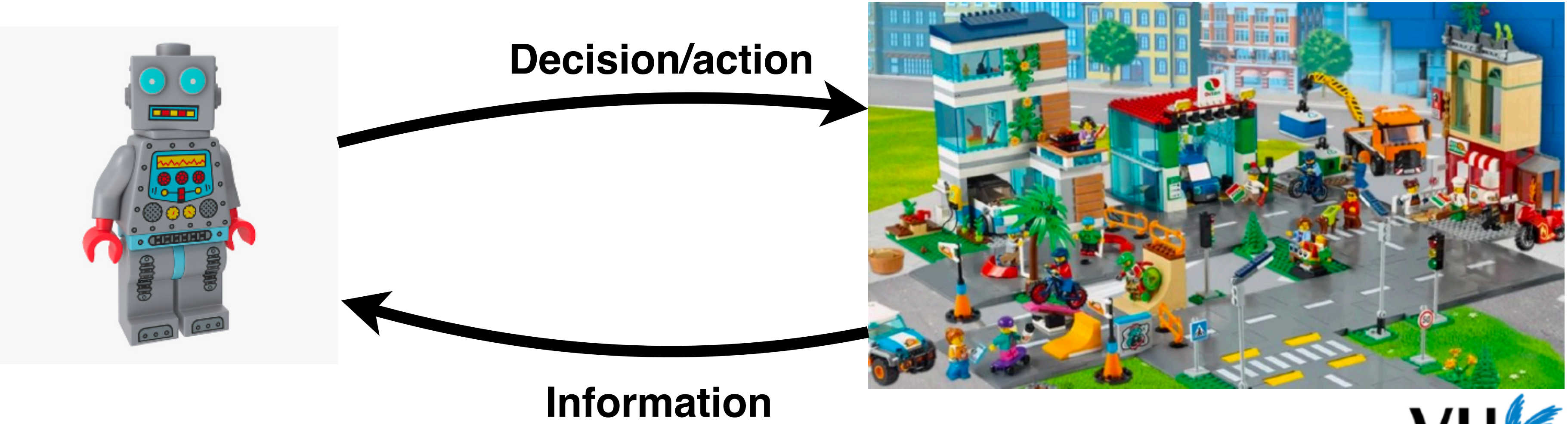

What is **intelligence**?

…

What is **artificial intelligence**?

Decision/action

Information

0001101010011…

What is **artificial intelligence**?

- **Information** processing
- **Information** storing
- **Information** transmission

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Learning

Knowledge representation

Models…

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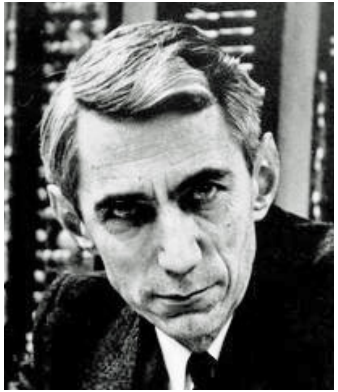
Learning

Knowledge representation

Models…

The question is how to formalize the problem of AI?

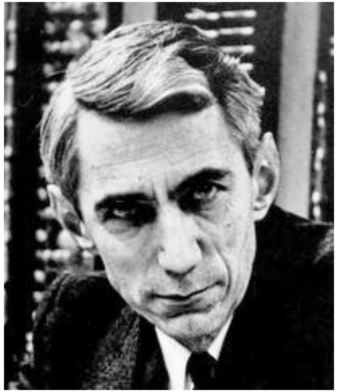
Information (a quick recap)



Claude Shannon

Information (a quick recap)

We have a random source of data x.



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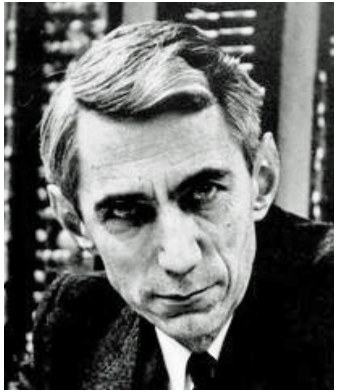
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We have a random source of data x.

We can quantify the **uncertainty** of this source by calculating **the entropy**:

$$\mathbb{H}[x] = -\sum_{x} p(x) \log p(x)$$

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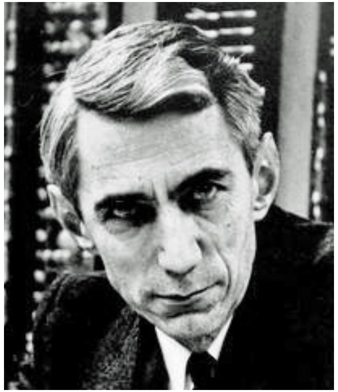

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$$\mathbb{H}[x] = -\sum_{x} p(x) \log p(x)$$

Entropy is max if all x's are equiprobable.

Entropy is min if the probability of one value is 1.

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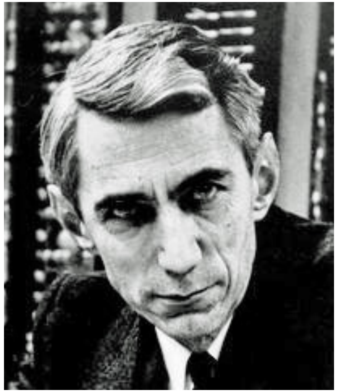

Claude Shannon

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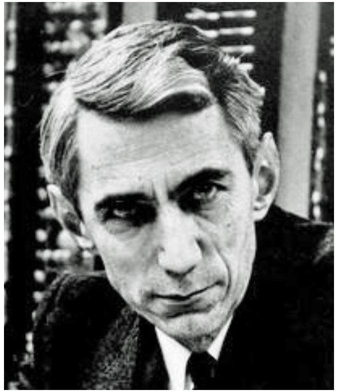
Optimal message length ≈ the entropy.



Claude Shannon

Information (a quick recap)

We have two random sources: x and y.

We can quantify the **uncertainty** of them by calculating **the joint entropy**:

$$\mathbb{H}[x, y] = -\sum_{x,y} p(x, y) \log p(x, y)$$

or **the conditional entropy**:

$$\mathbb{H}[y \,|\, x] = -\sum_{x,y} p(x, y) \log p(y \,|\, x)$$

Mutual Information (a quick recap)

We have two random sources: x and y.

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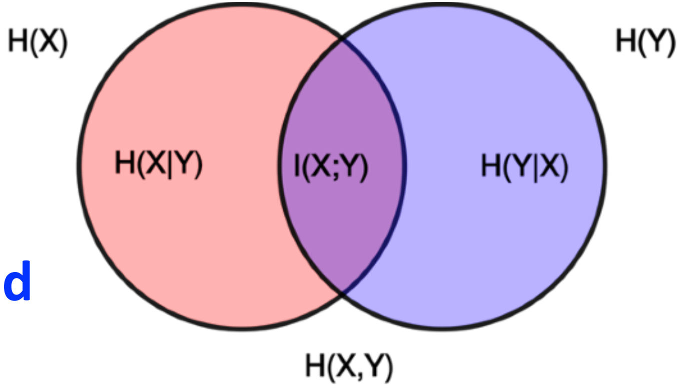

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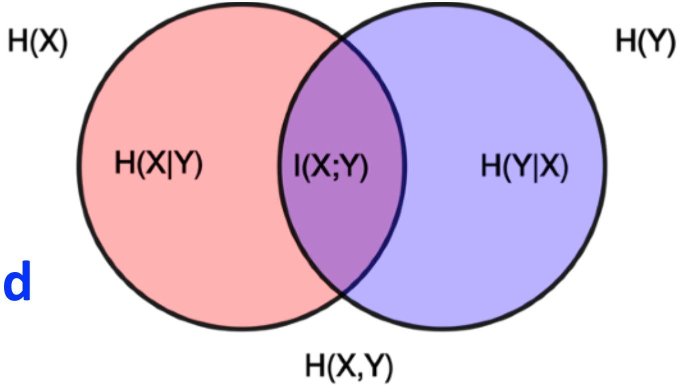
We can quantify how much **information is shared by the two sources:**

$$\mathbb{I}[x; y] = \mathbb{H}[y] - \mathbb{H}[y \,|\, x]$$

Mutual Information (a quick recap)



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or **how much knowing one source reduces uncertainty about the other.**

We have two random sources: x (e.g., images) and y (e.g., decisions).

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We have also a **model** m (a representation of a world).

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The **goal** of AI is to **maximize** the **mutual information** between (x, y) and m:

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Entropy of the world (model has no influence on that)

That's the "real" goal!

The **goal** of AI is to **maximize** the **mutual information** between (x, y) and m

(or minimize $\mathbb{H}[x, y \mid m]$, i.e., minimize uncertainty of the world):

$$\mathbb{H}[x, y \mid m] = \sum_{x,y,m} p(x, y, m)\left[\log p(y \mid x, m) + \log p(x \mid m)\right]$$

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A model for decision making

A model for understanding the world.

The **goal** of AI is to **maximize** the **mutual information** between (x, y) and m (or minimize $\mathbb{H}[x, y \,|\, m]$, i.e., minimize uncertainty of the world).

In order to achieve that, AI should focus on learning **two models**:

- **A model for decision making:** $p(y \,|\, x, m)$
- **A model for understanding the world:** $p(x \,|\, m)$

WHAT HAPPENS IF WE LEARN ONLY DECISION MAKING

The bulk of AI is focused on the decision making part **only**!

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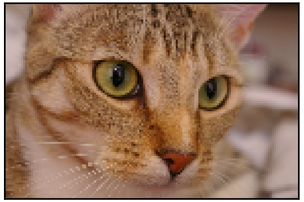
Example: Let’s say we have a model that is well trained.



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

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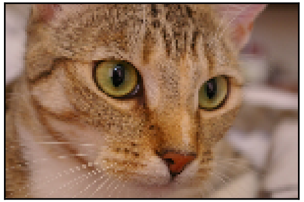

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$p(y = dog|\mathbf{x}) = 0.05$
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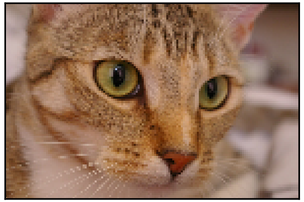
+

noise

=

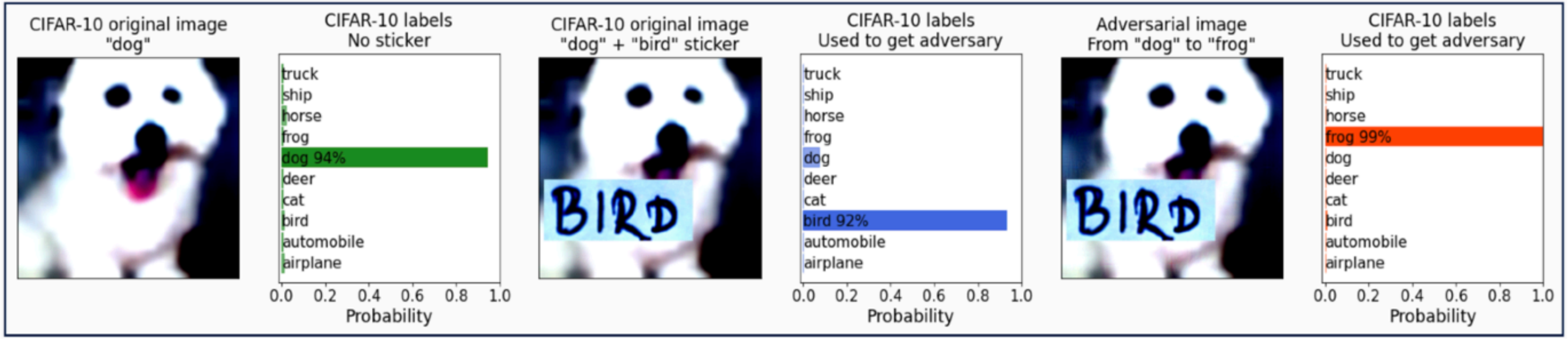


$p(y = cat|\mathbf{x}) = 0.05$
$p(y = dog|\mathbf{x}) = 0.05$
$p(y = horse|\mathbf{x}) = 0.90$

But after adding a little noise it could fail completely…

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

What happens if we add (adversarial) noise to an image?



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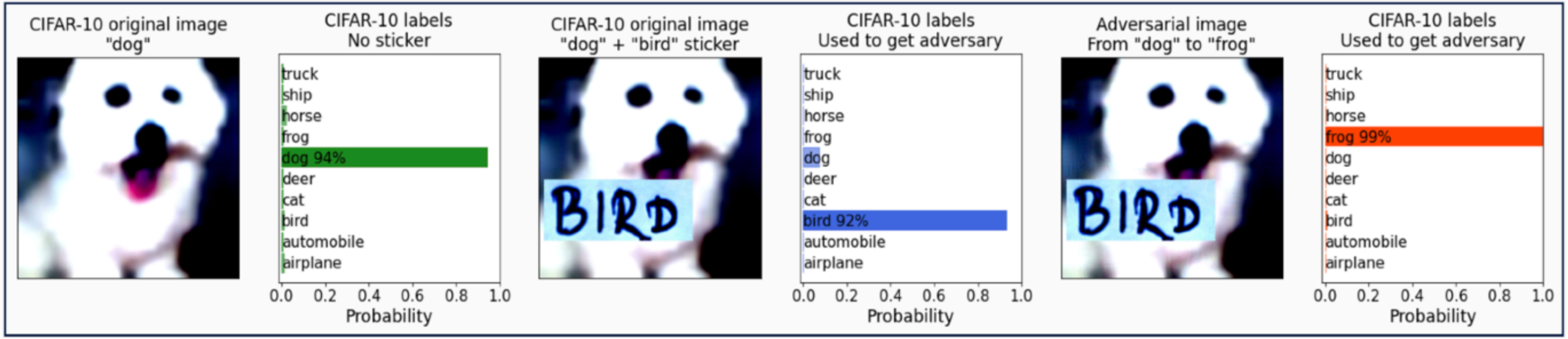

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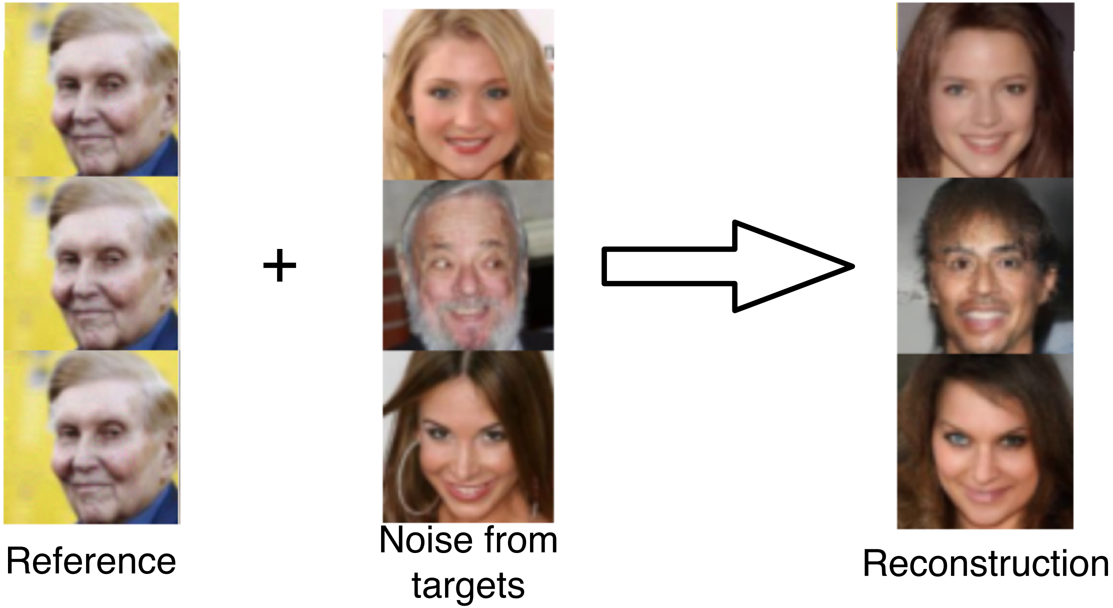

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Reference

Noise from targets

Reconstruction

It fails completely…

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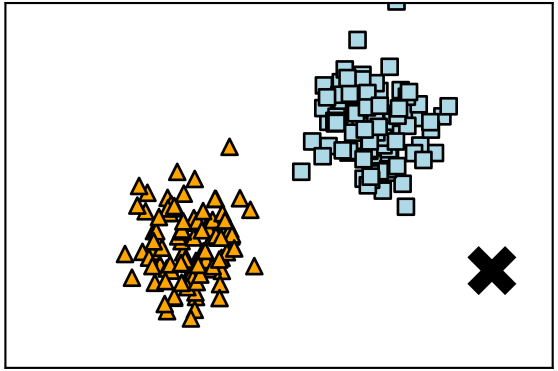
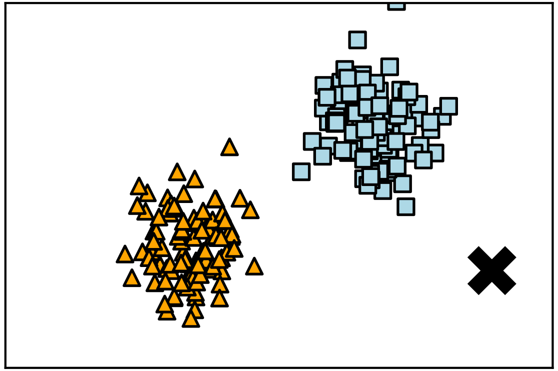
DEEP GENERATIVE MODELING: WHY DO WE NEED THEM?

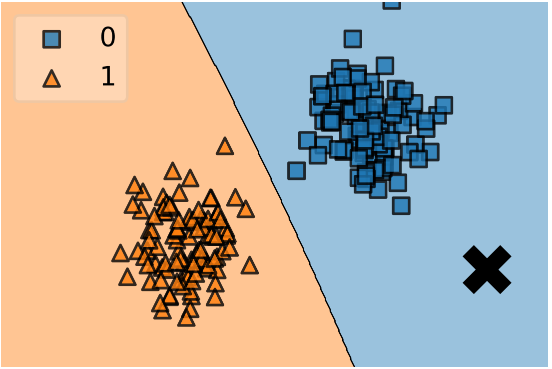


Data

DEEP GENERATIVE MODELING: WHY DO WE NEED THEM?



Data



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

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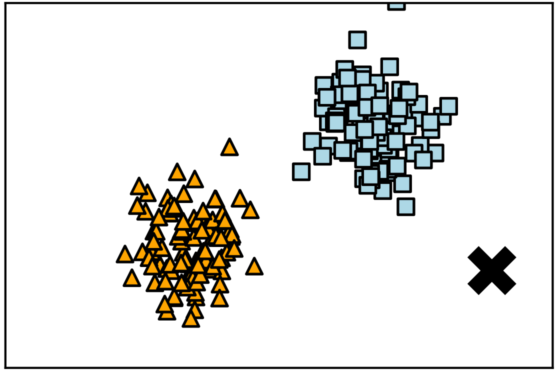

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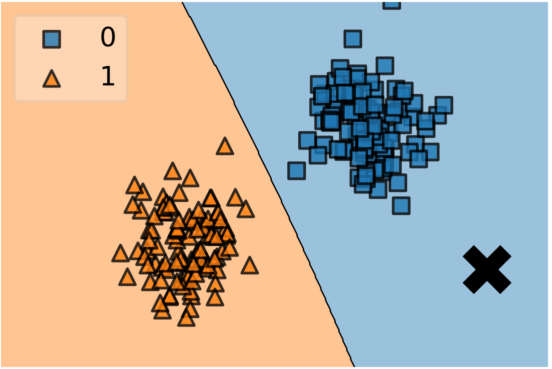

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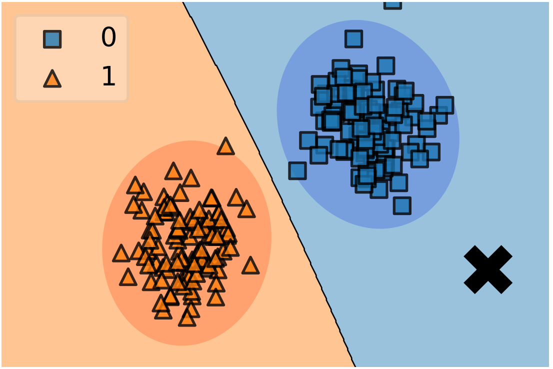

$p(\mathbf{x}, y) = p(y|\mathbf{x})\ p(\mathbf{x})$

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and $p(\mathbf{x})$ is low
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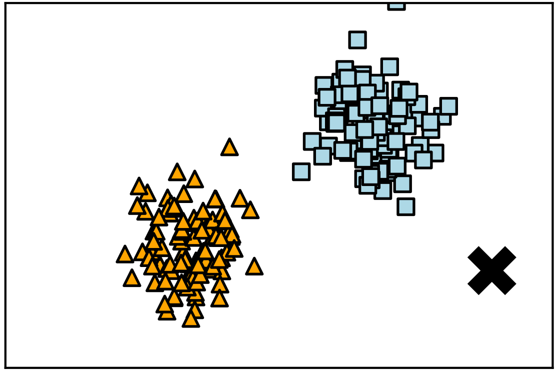

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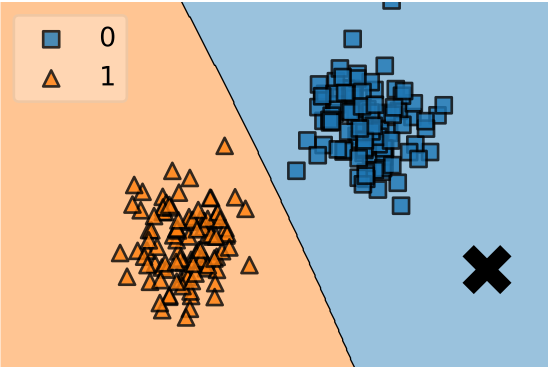

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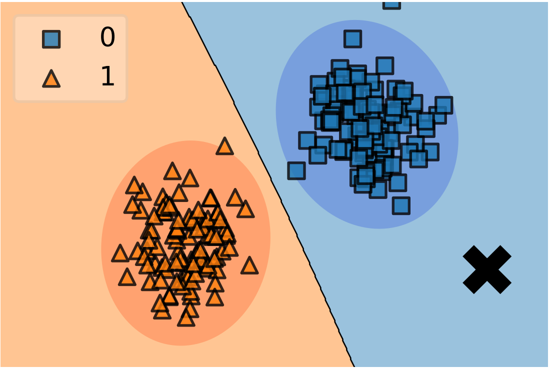

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Thus, learning the conditional is only a part of the story!
How can we learn p(x)?

DEEP GENERATIVE MODELING: WHY DO WE NEED THEM?

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

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

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: 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)

Flow-based models
(e.g., RealNVP)

Latent variable models

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(e.g., GANs)

Prescribed models
(e.g., VAEs)

+ 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

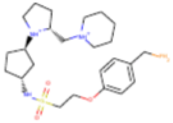
DEEP GENERATIVE MODELING: WHERE CAN WE USE IT?

“ 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 .

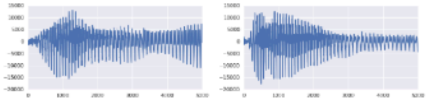
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Text analysis

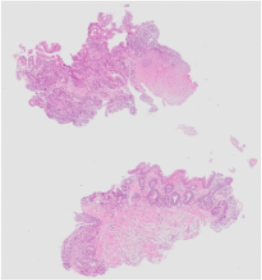
Image analysis



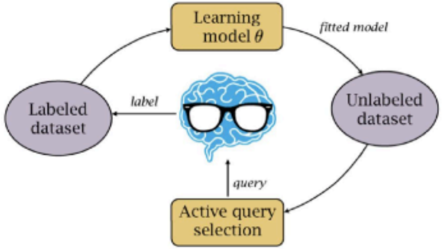
Graph analysis



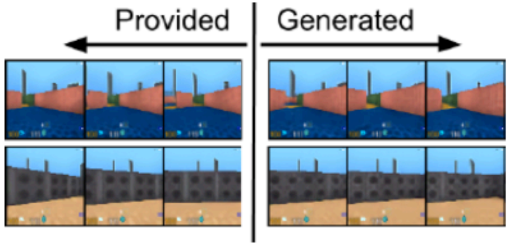
Audio analysis



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

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Prescribed models
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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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We can use the **product rule**:

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

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

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Example:

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

AUTOREGRESSIVE MODELS (ARMS)

We are interested in modeling

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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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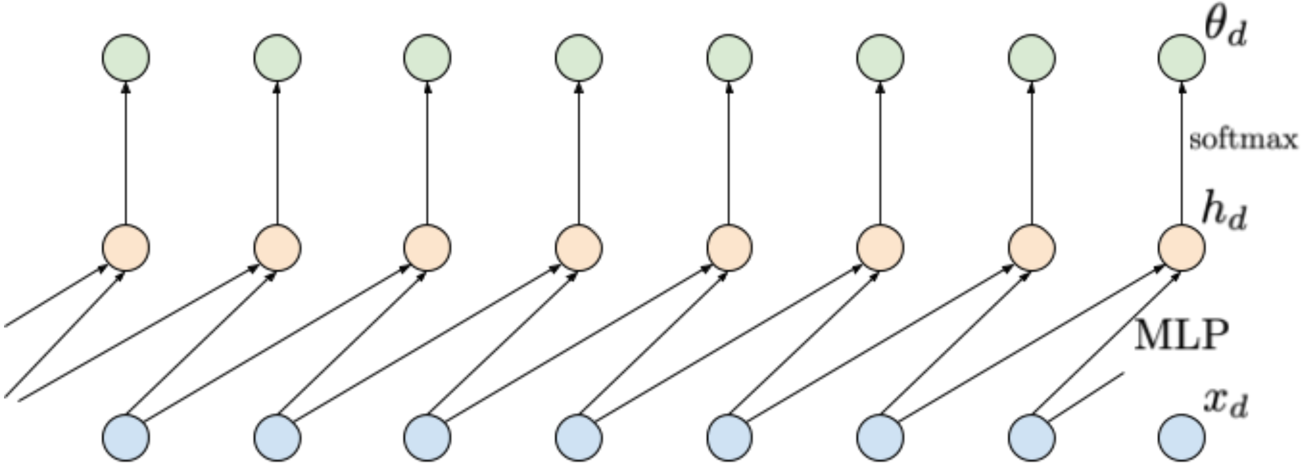
Approach 1: Finite memory



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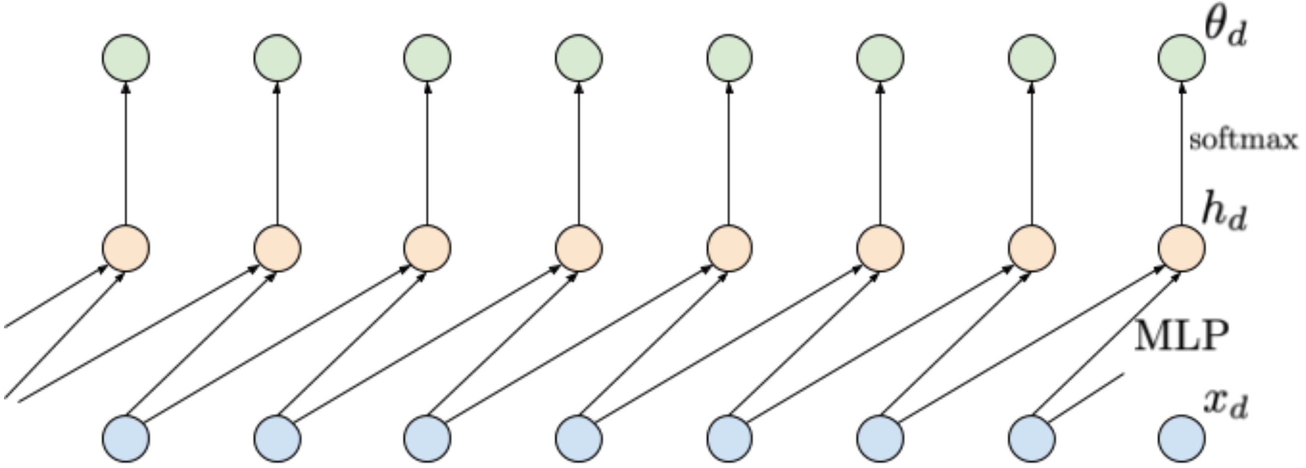
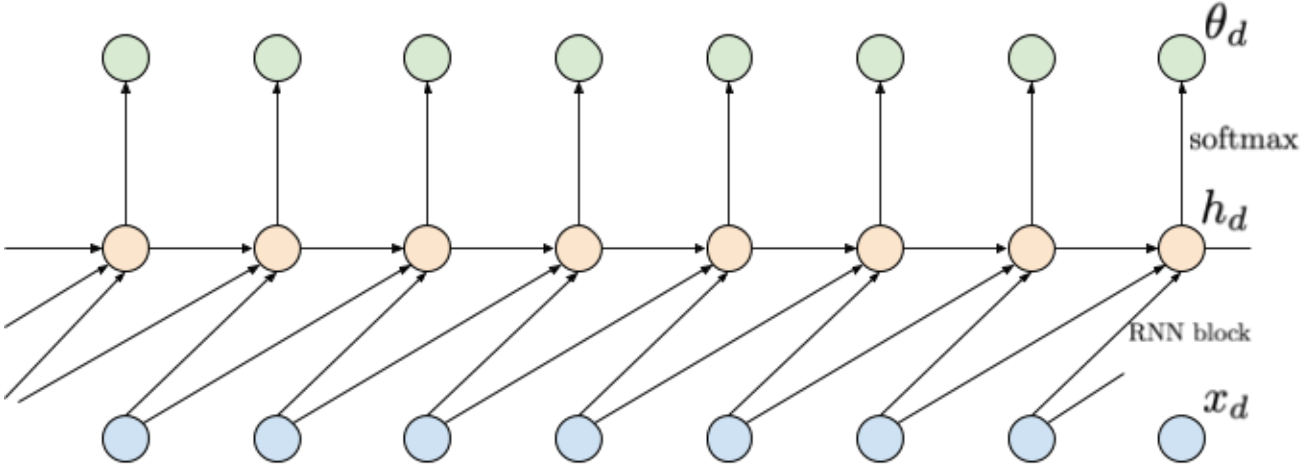


Easy!

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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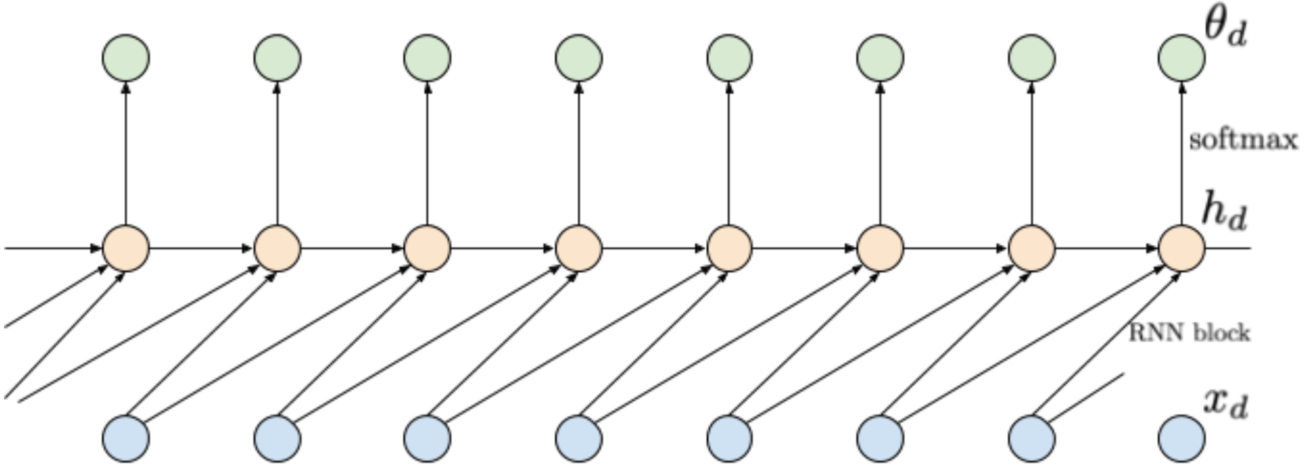
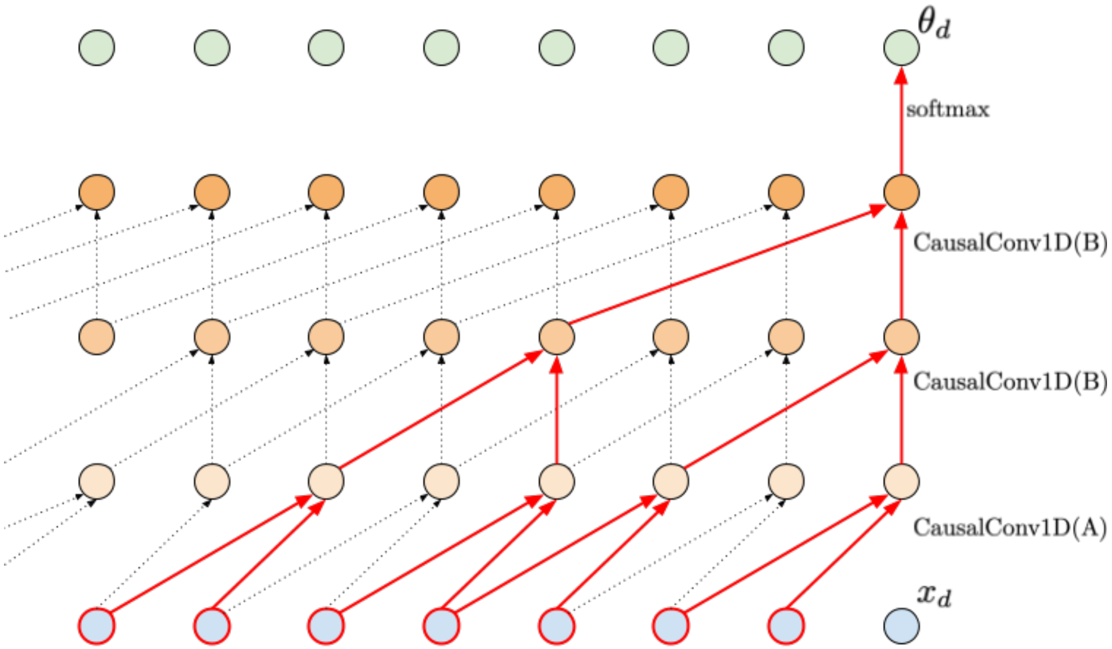


Easy!
Long-range dependencies!

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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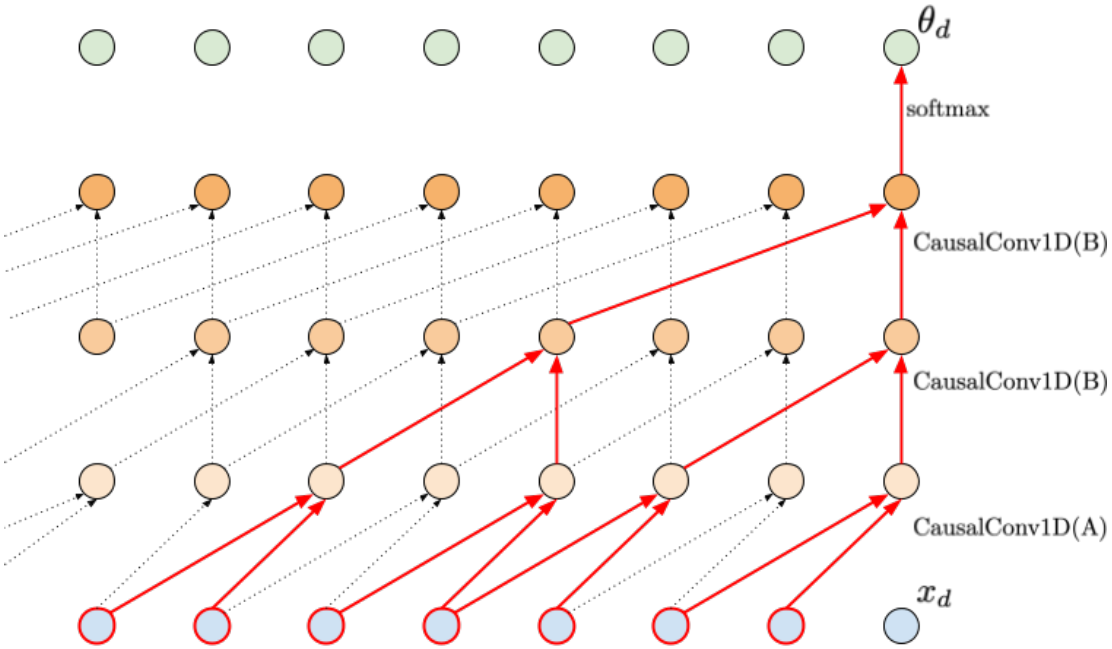
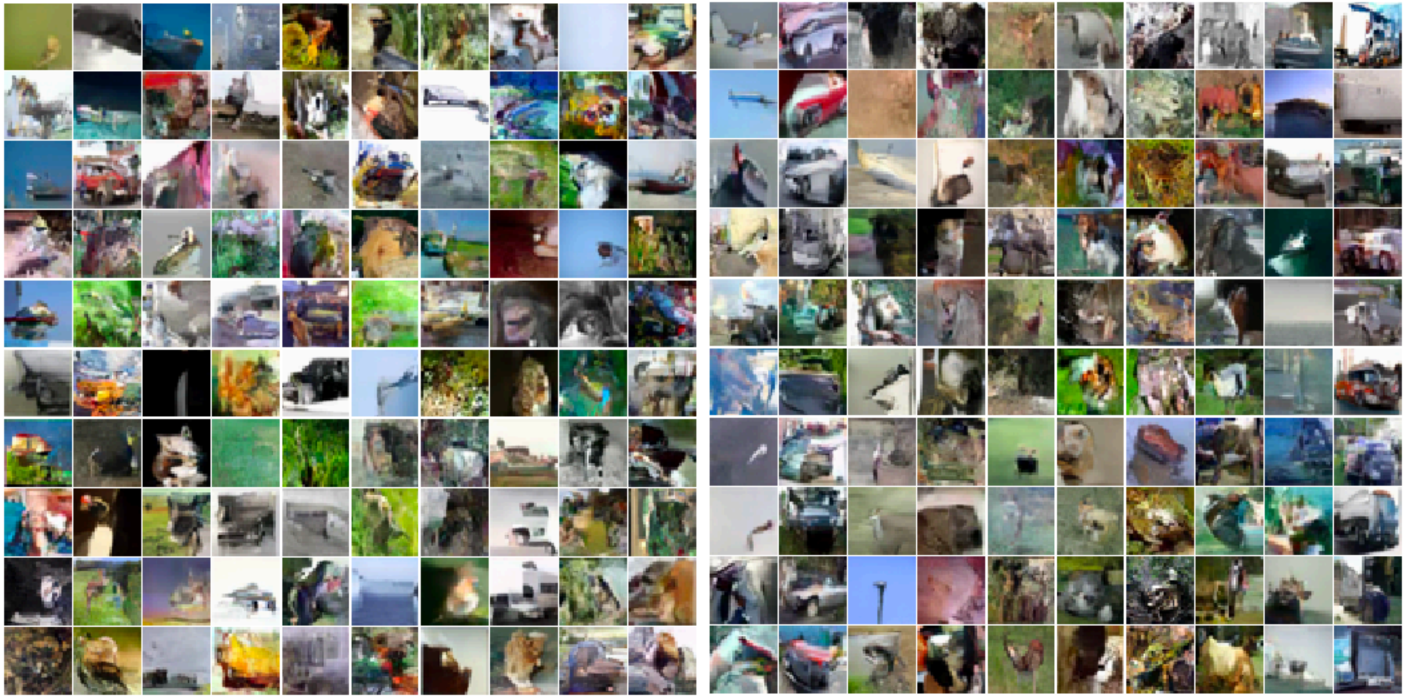


Easy!
Long-range dependencies!
No training issues!

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?

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)

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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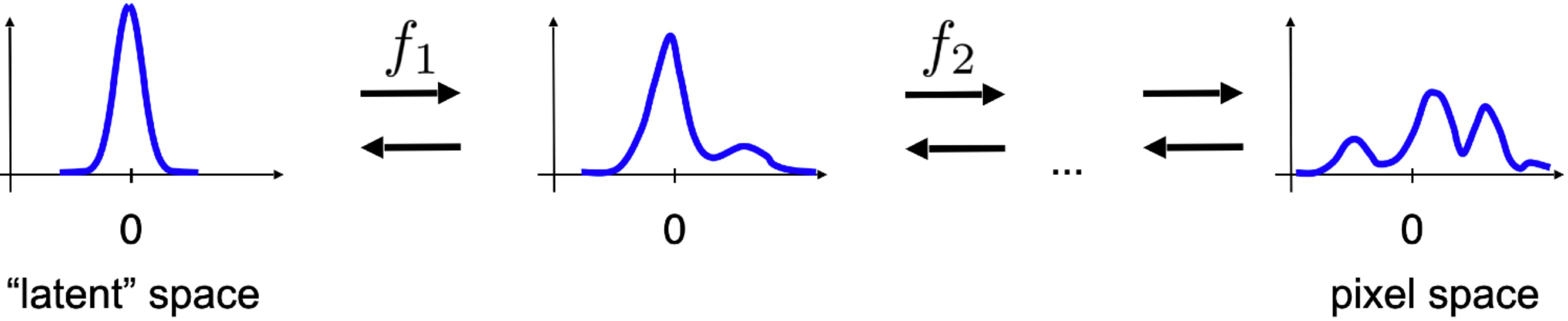

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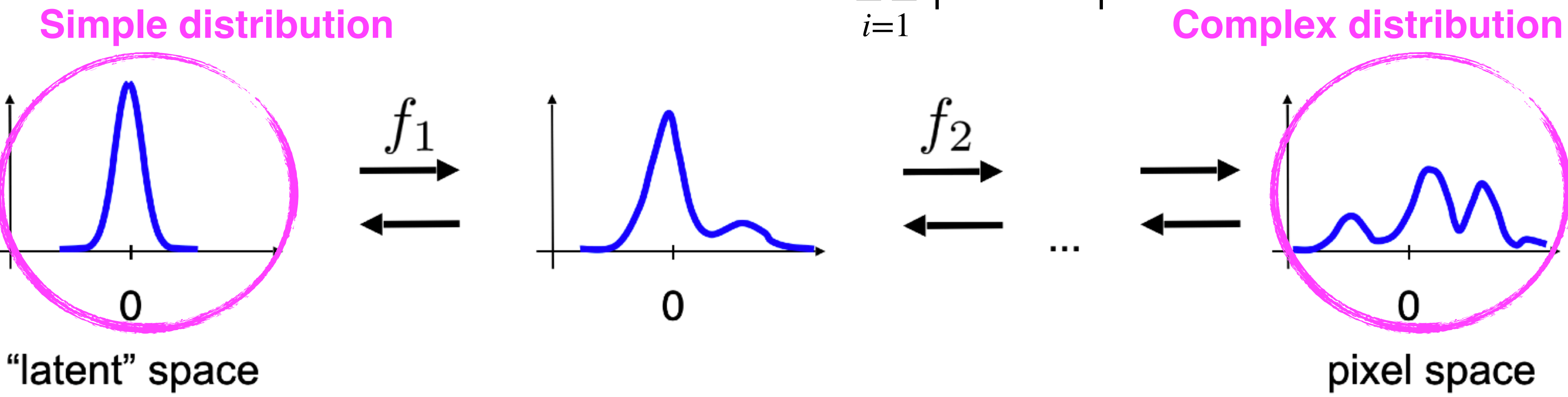

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Known, e.g., Gaussian

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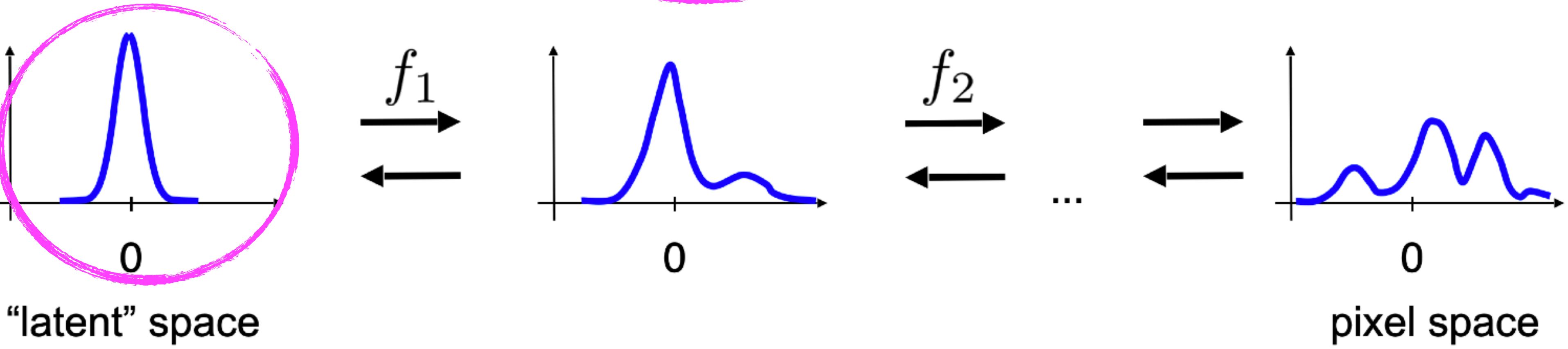

We change a random variable **x** to another random variable **z** using **invertible** transformations, $\mathbf{x}, \mathbf{z} \in \mathbb{R}^D$:

Jacobian must be tractable

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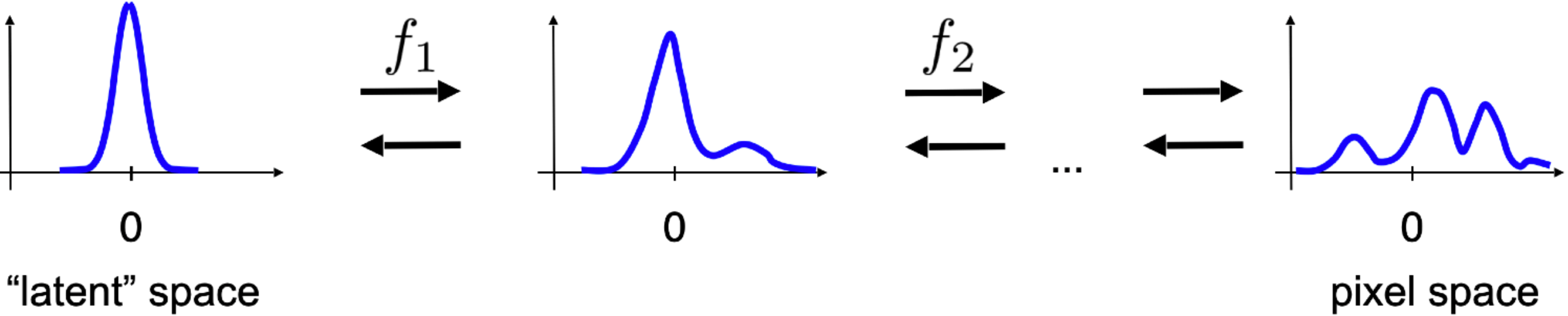

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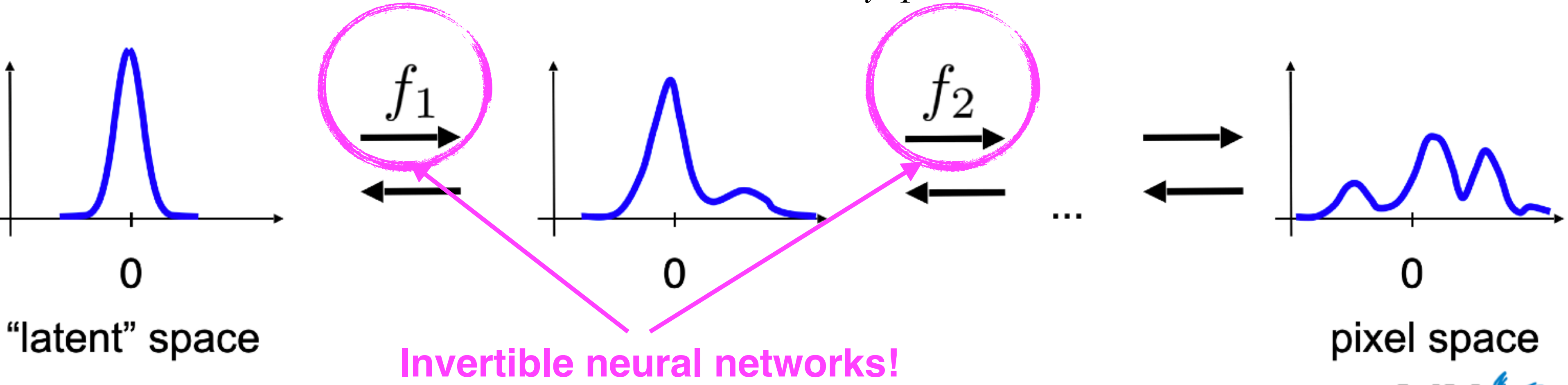

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Training objective:

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

Two main components

1) **Coupling layer**:

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

is invertible by design:

$$\mathbf{x}_b = \big(\mathbf{y}_b - t(\mathbf{y}_a)\big) \odot \exp\big(-s(\mathbf{y}_a)\big)$$
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2) **Permutation layer**

Two main components

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Jacobian is tractable!

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

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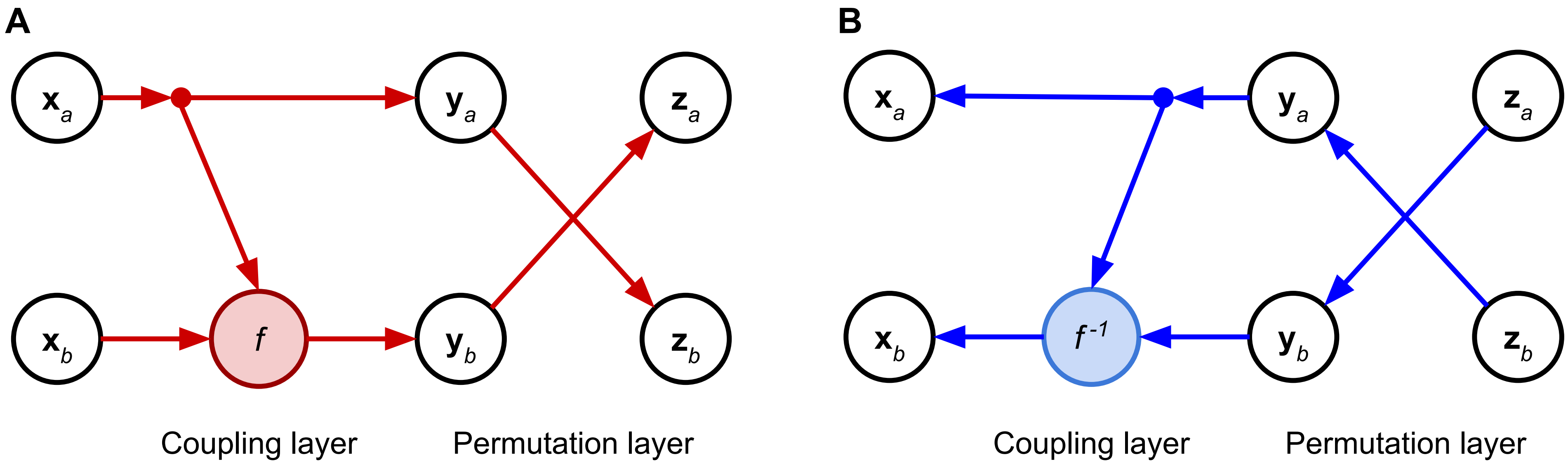
2) **Permutation layer** $\det(\mathbf{J}) = 1$

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*

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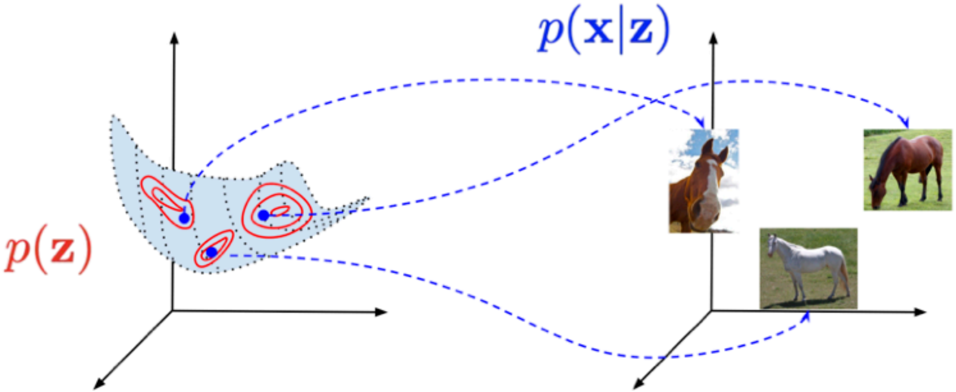
Let's consider a **latent variable model** where we distinguish:

- **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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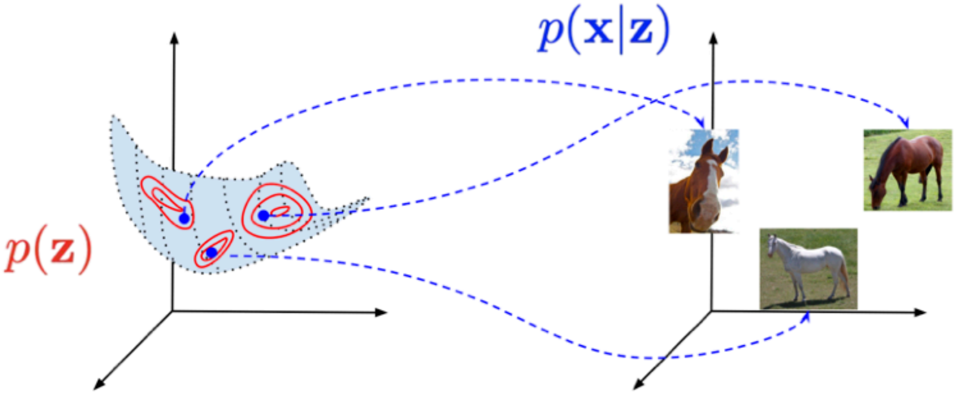

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$$\ln p(\mathbf{x}) = \ln \int p(\mathbf{x}\,|\,\mathbf{z}) p(\mathbf{z}) \, \mathrm{d}\mathbf{z}$$

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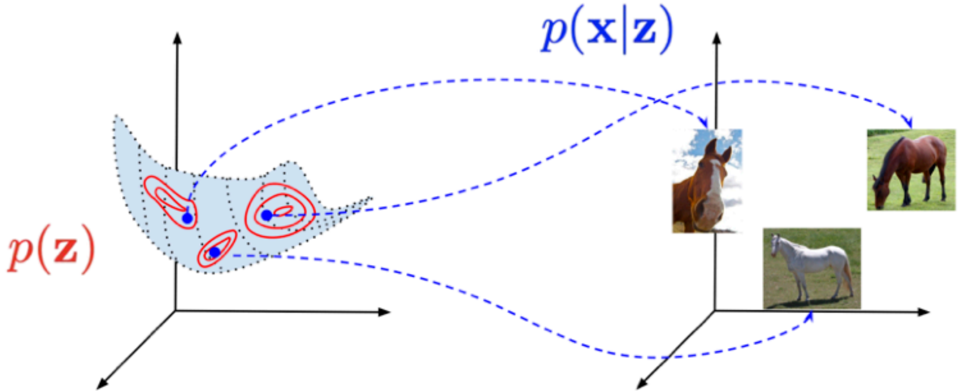

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The integral is intractable…

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Variational posteriors

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VARIATIONAL AUTO-ENCODERS

$$
\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

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ELBO: Evidence Lower Bound

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

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

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

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VARIATIONAL AUTO-ENCODERS

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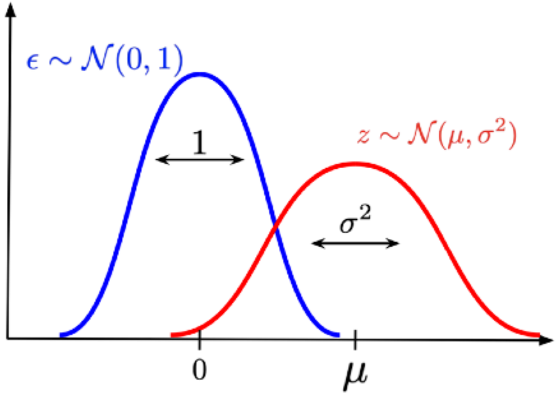
In other words, a single parameterization for each new input **x**.

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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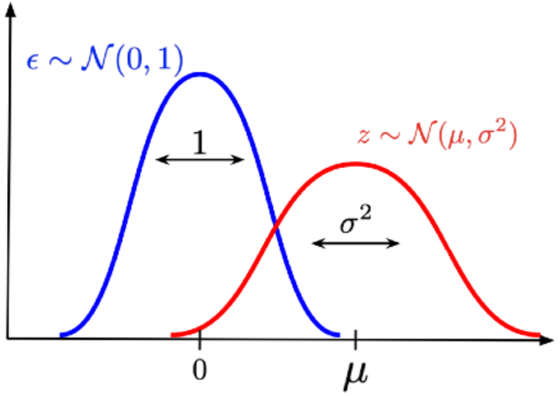
Moreover, we use **reparameterization trick**:

It reduces the variance of the gradients.

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

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



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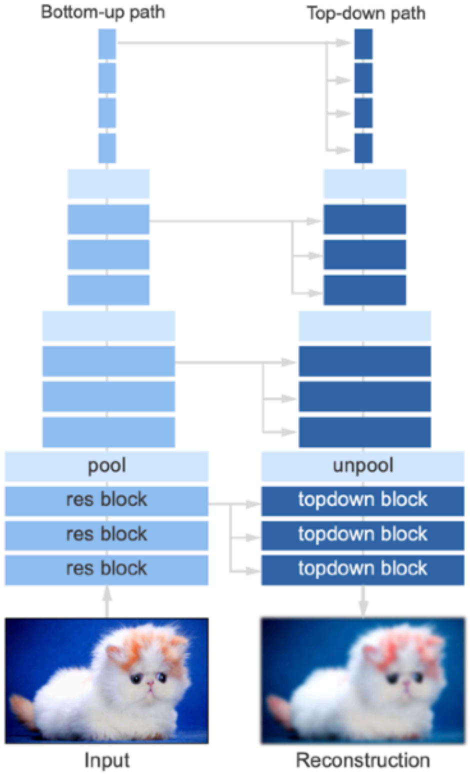
VARIATIONAL AUTO-ENCODERS

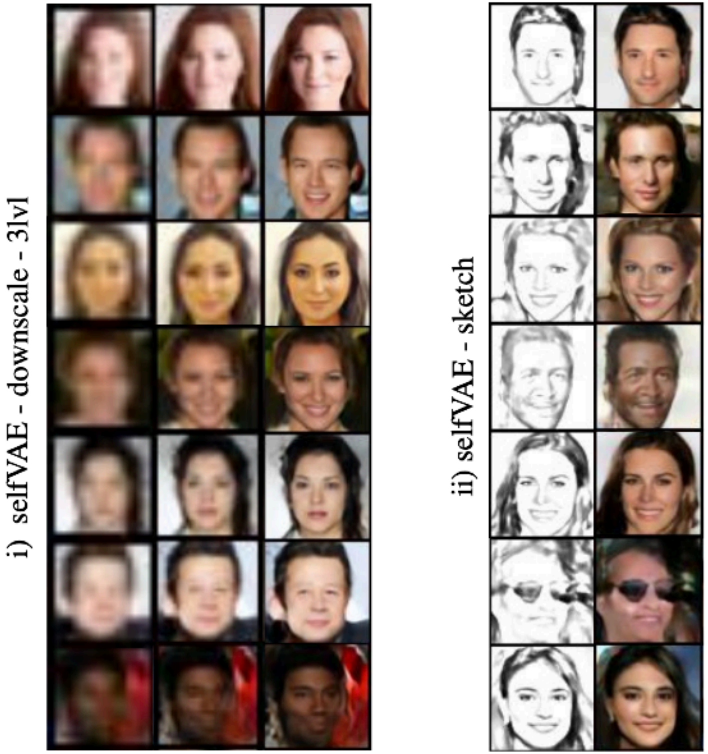
Generations



Very Deep VAE

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

VARIATIONAL AUTO-ENCODERS



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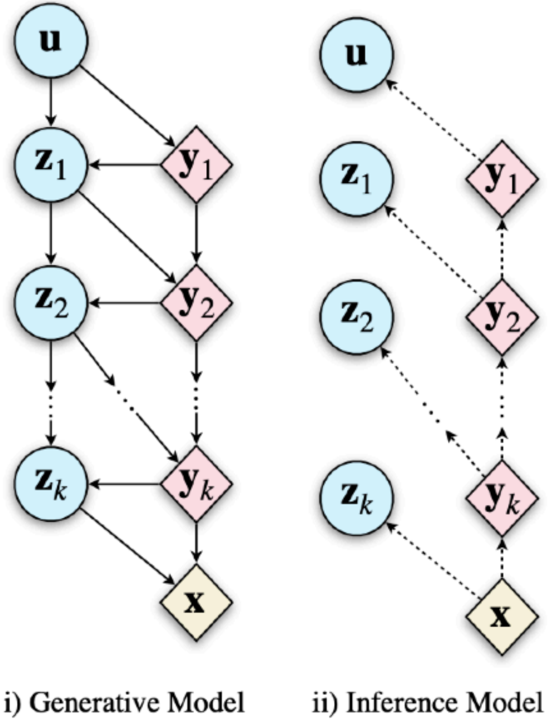

Hierarchical VAE

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

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

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

- Important directions:
  - ➡ Better uncertainty quantification
  - ➡ New parameterization (new neural networks)
  - ➡ Out-of-Distribution
  - ➡ Continual learning

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], [Link]
- **Hybrid modeling**: [Link]

THANK YOU FOR YOUR ATTENTION

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