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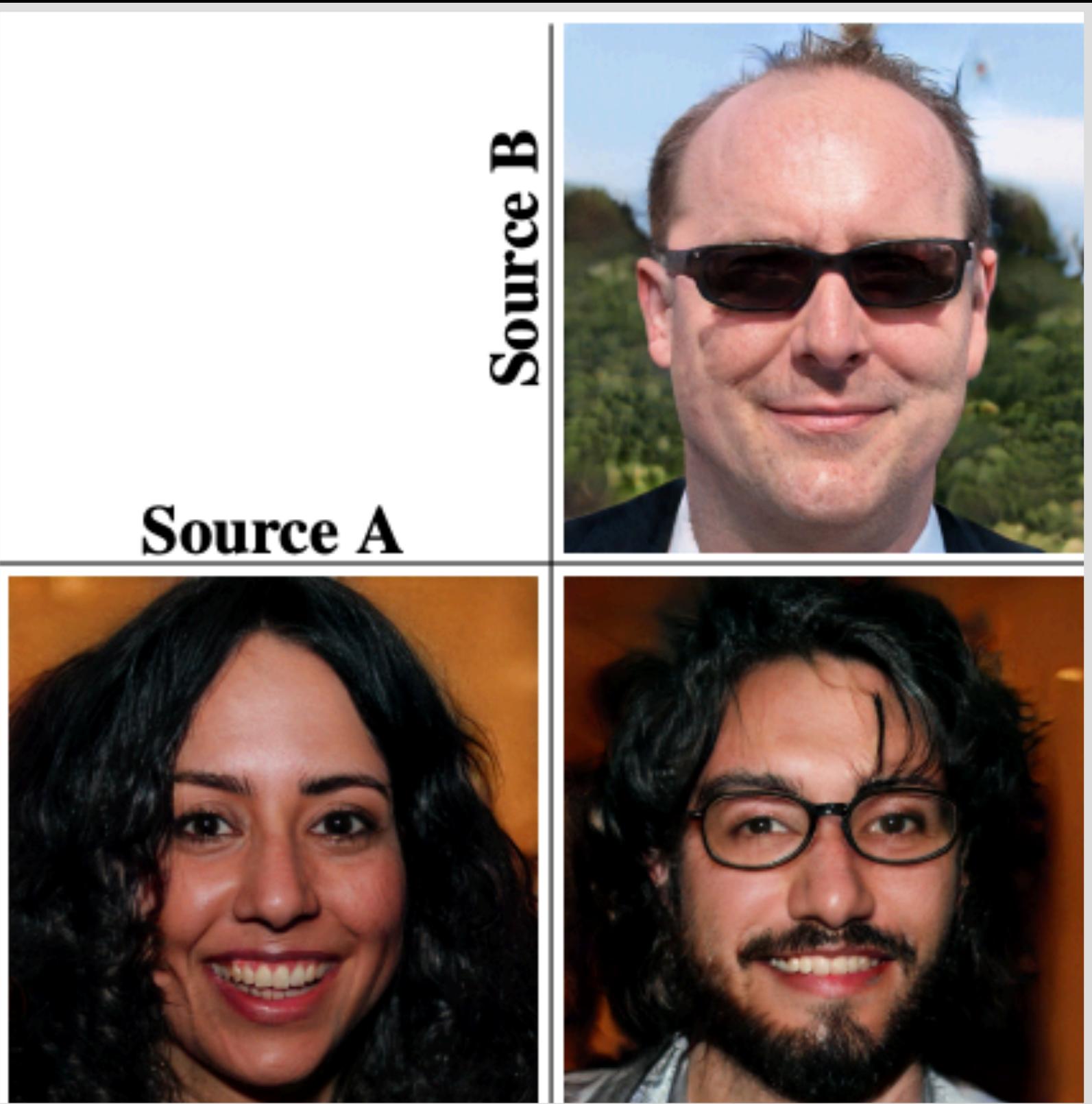
# Generative Adversarial Networks

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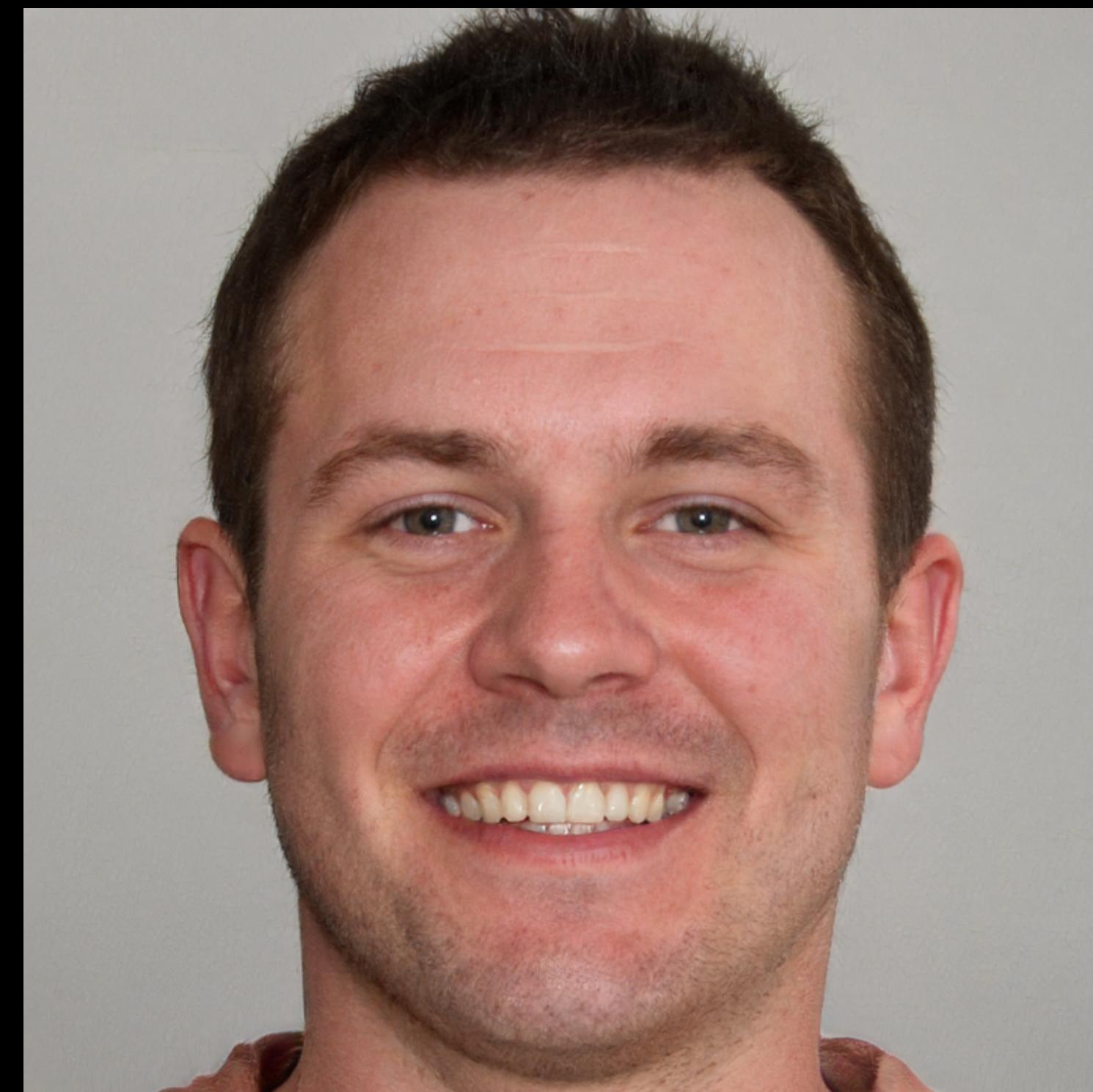
L03 - Deep Learning for Life Sciences Course

# Generative Adversarial Networks (GANs)

Creating content



# Which face is fake ?



Karras et al., 2019. *Analyzing and improving the image quality of stylegan*.



# Generative Adversarial Networks (GANs)



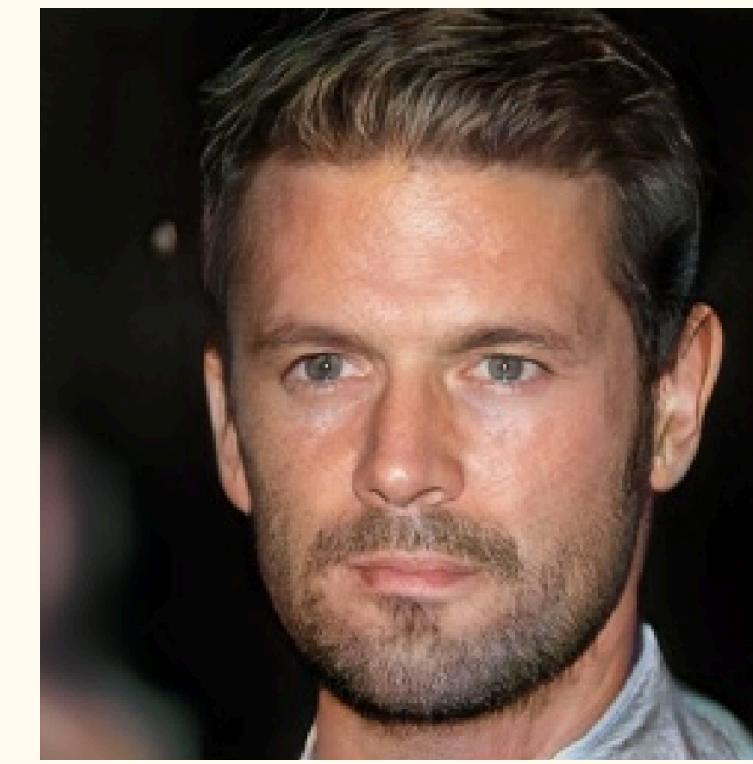
2014



2015



2016



2017



2018

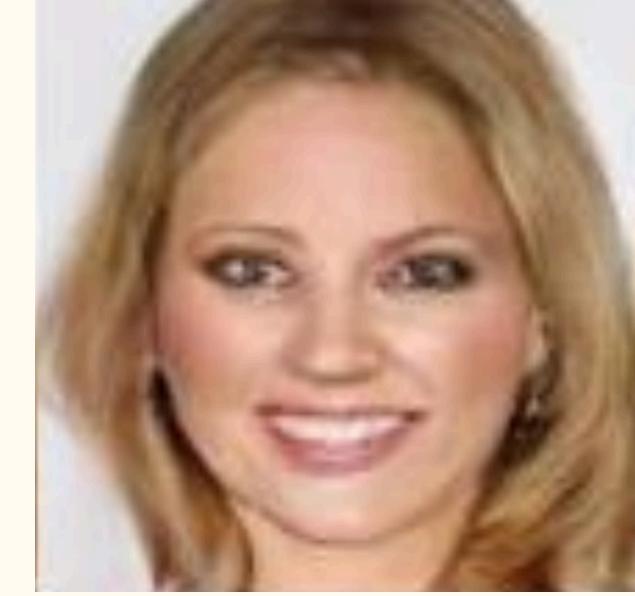


2019

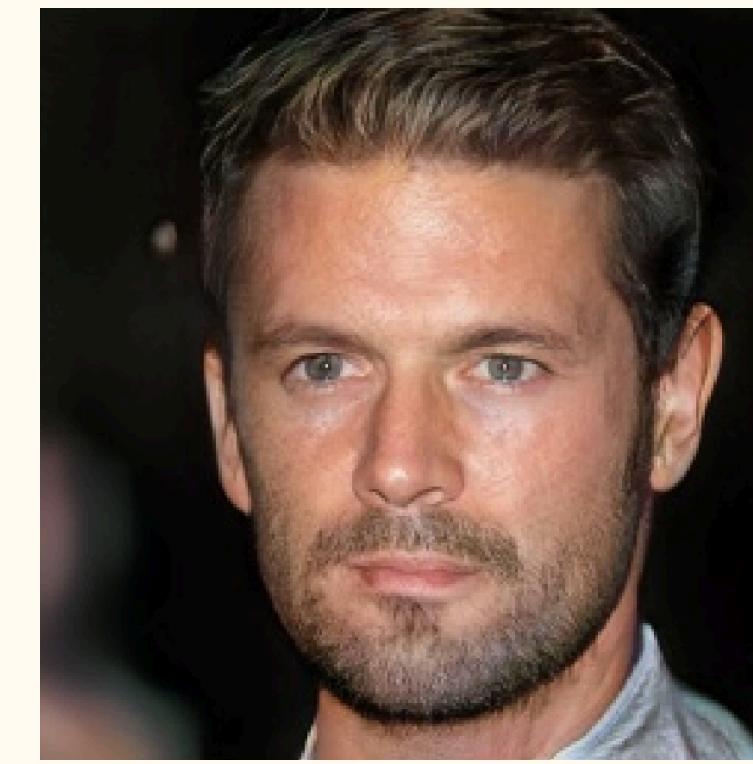
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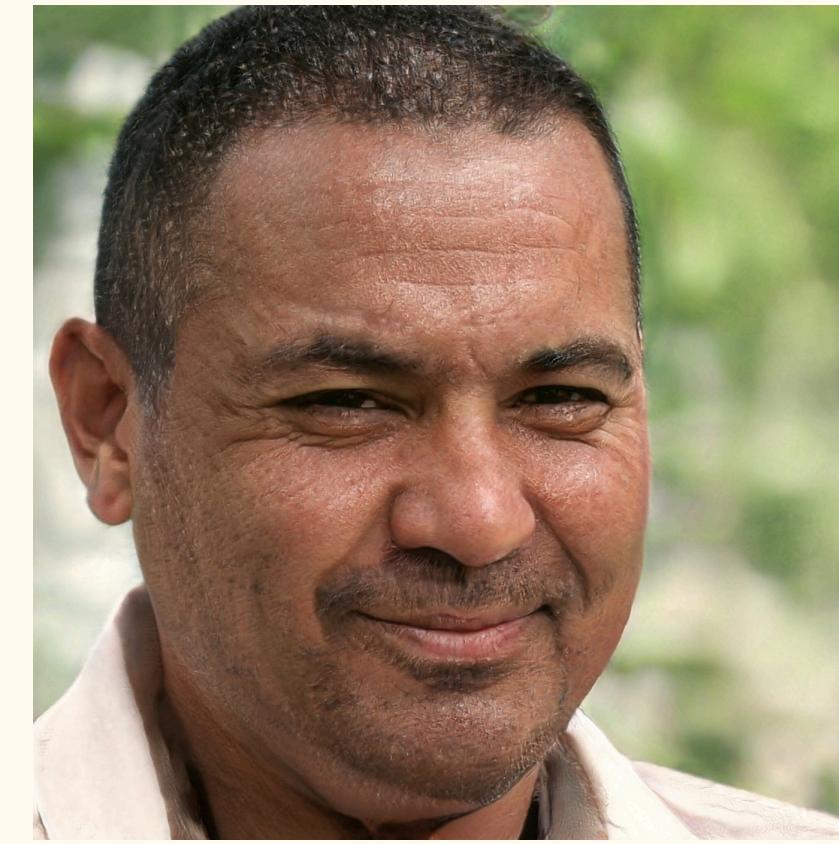
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- Generative modelling → progress in facial image generation

# Generative Adversarial Networks (GANs)



2014



2015



2016



2017



2018



2019

- Generative modelling → progress in facial image generation
- Newer and more sophisticated methods every year

# Supervised Learning

# Supervised Learning

1	...	...
2	...	...
3	...	...

Training Data

# Supervised Learning

	1	...	...
1		...	...
2		...	...
3		...	...

Training Data

	...	...	...
1		...	...
2		...	...
3		...	...

Labels

# Supervised Learning

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Training Data

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Predictions

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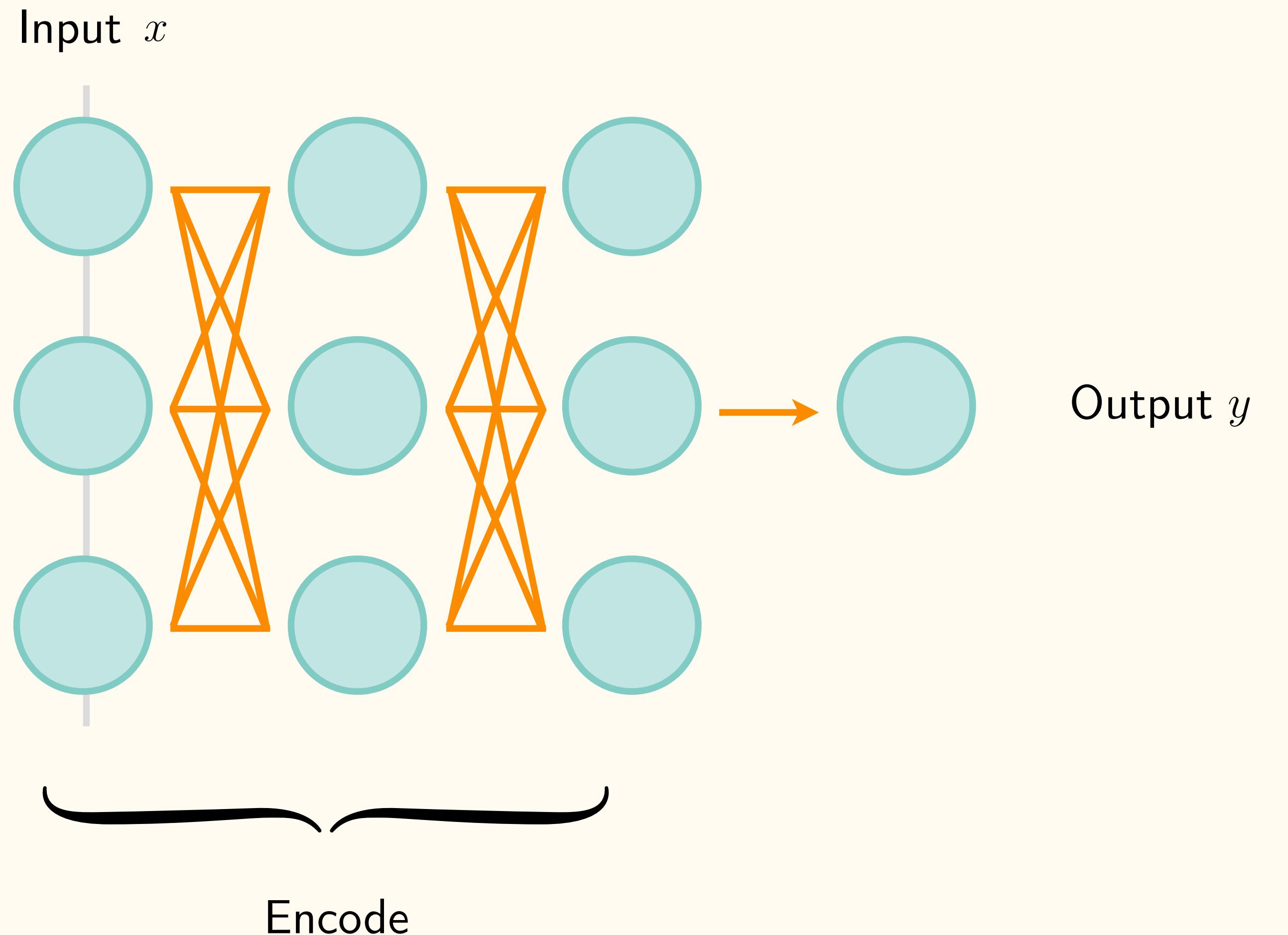
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So far we've seen models which:

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- Instead of taking a sample as *input*, they produce a sample as *output*.

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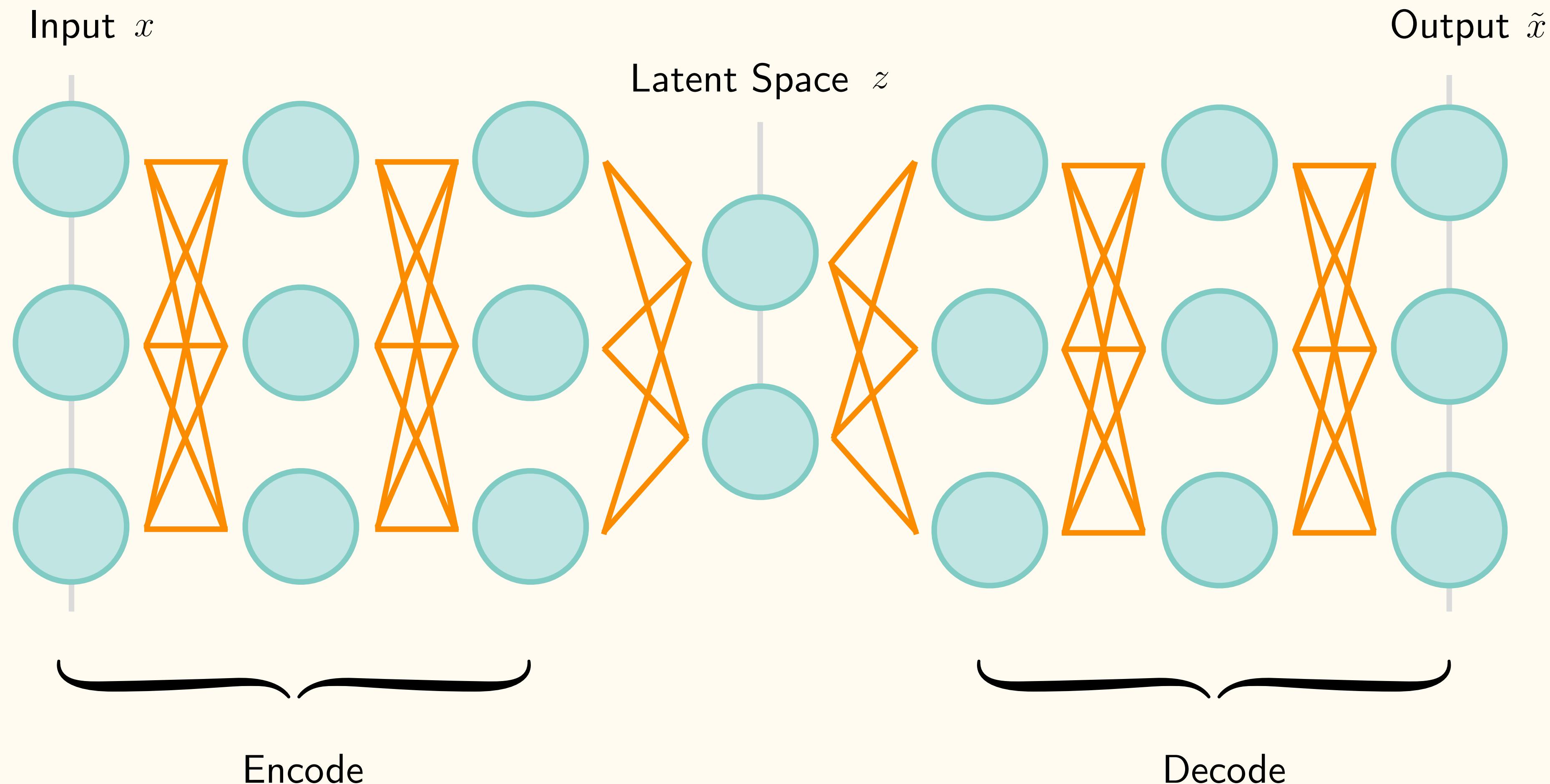
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**probability distribution**
- Its job is to produce new samples from that same probability distribution.

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- What if we take *random vectors* in the latent space (picking a random value for each component of the vector) and pass them through the decoder ?
- ▶ If everything goes well, the decoder should produce a completely *new sample* that *resembles* the ones it was trained on.

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  - ▶ Not for *arbitrary* ones.

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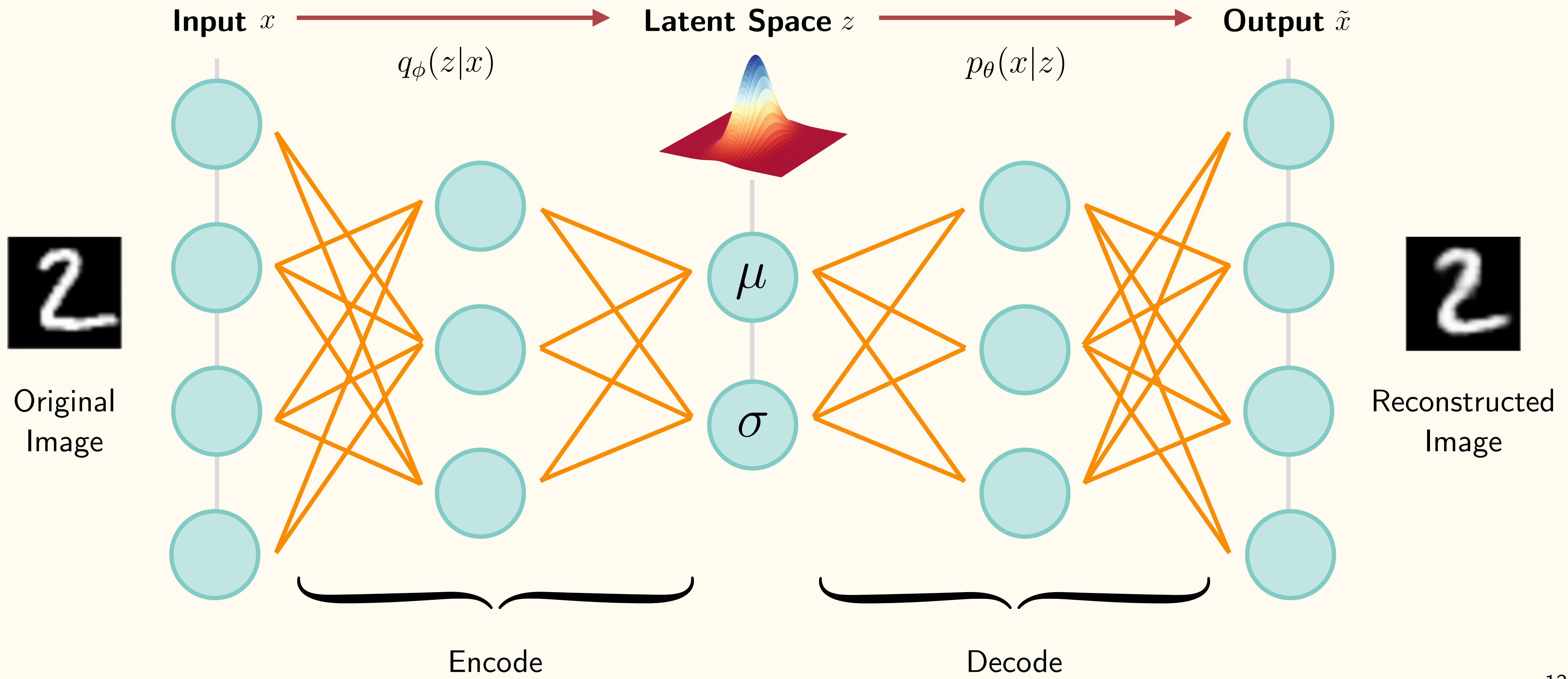
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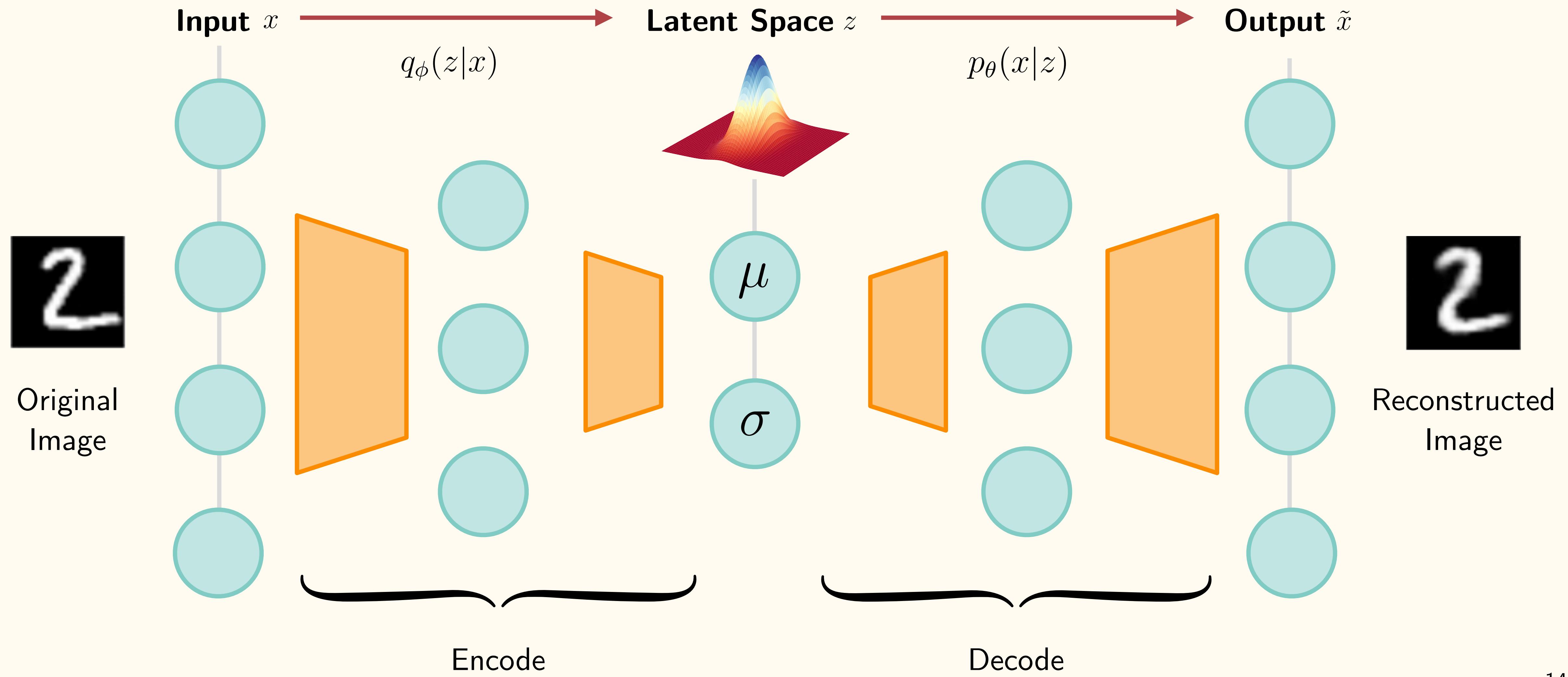
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- We add random noise to the latent vector
  - ▶ Prevents decoder from being too sensitive to details

# Variational Auto-Encoder (VAE)

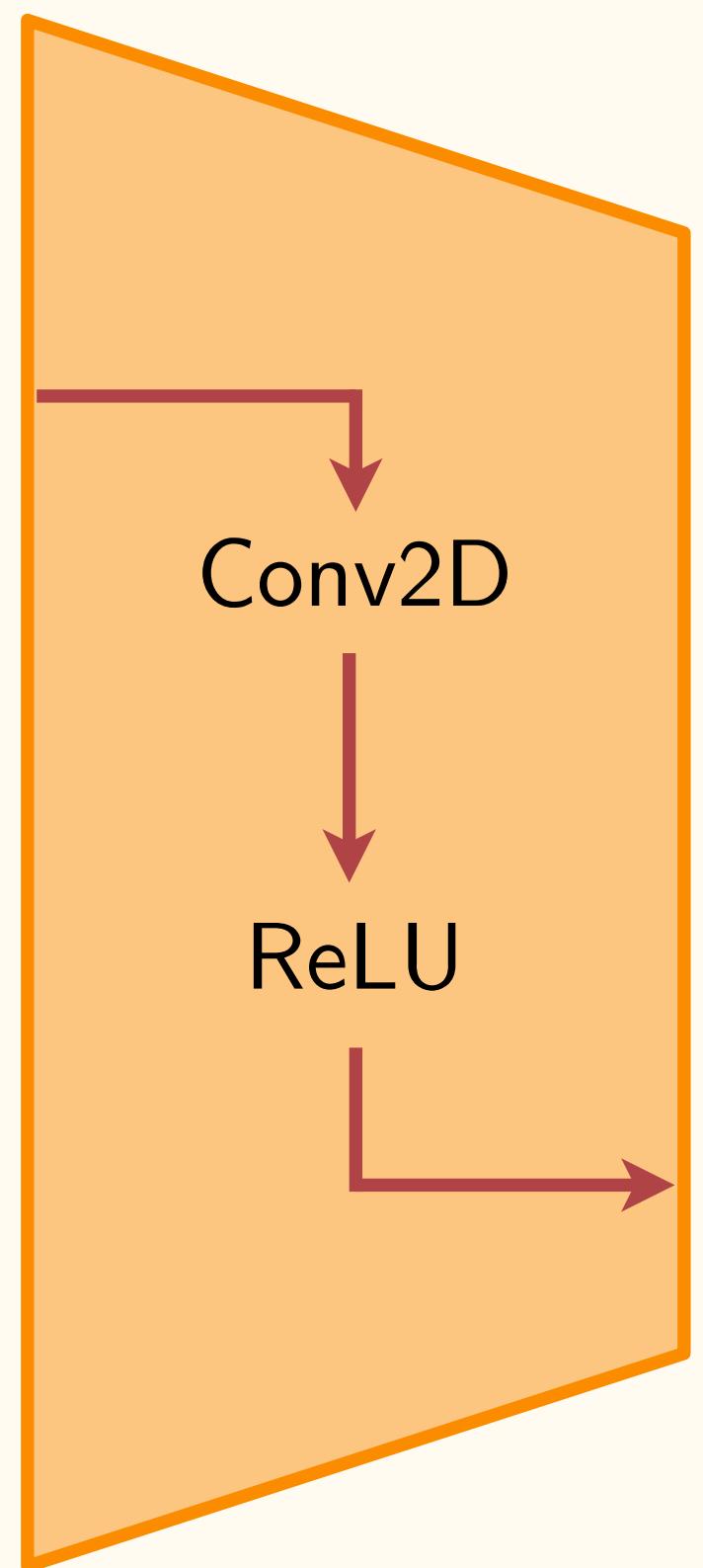


# Simplified VAE Representation

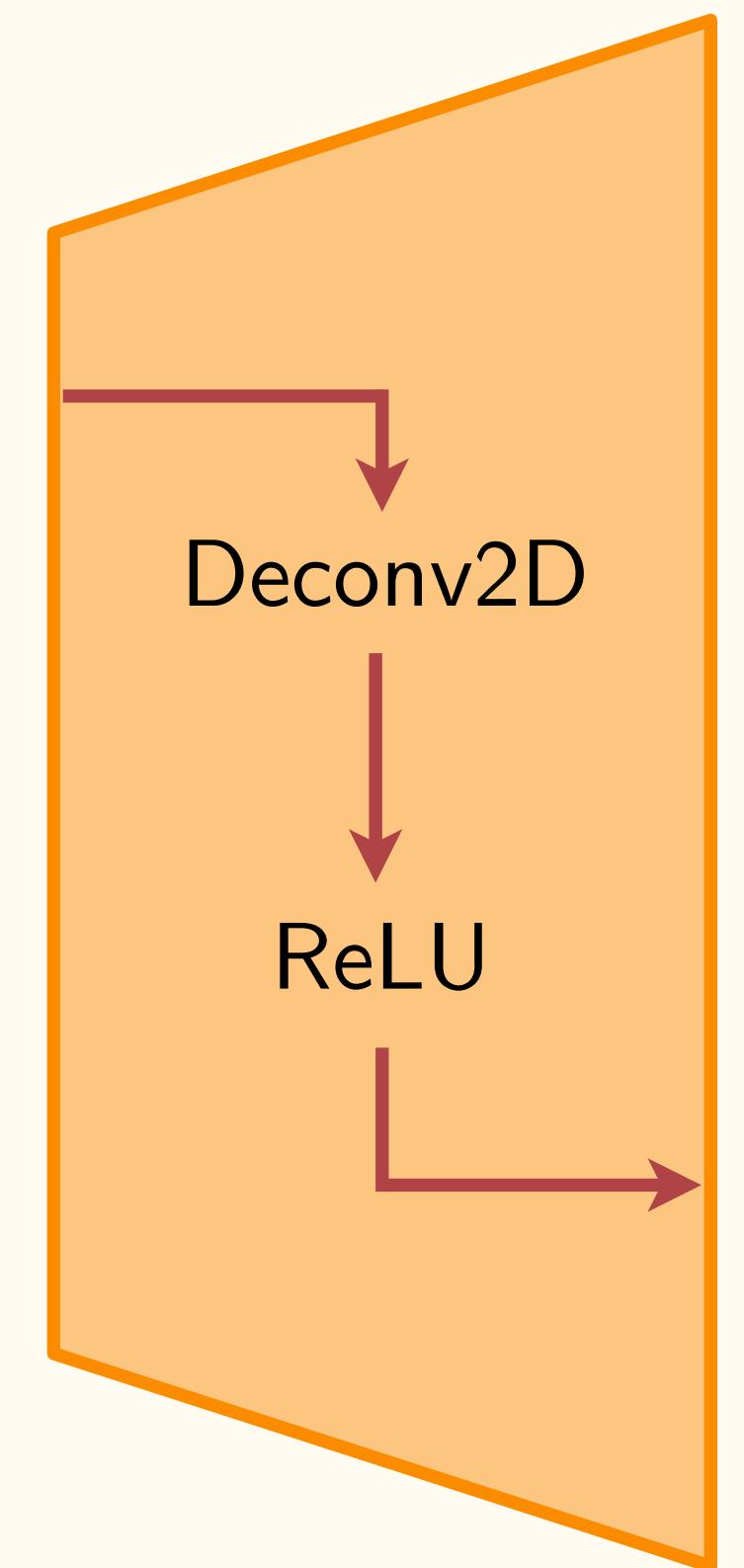


# Encoder-Decoder

**Encode**

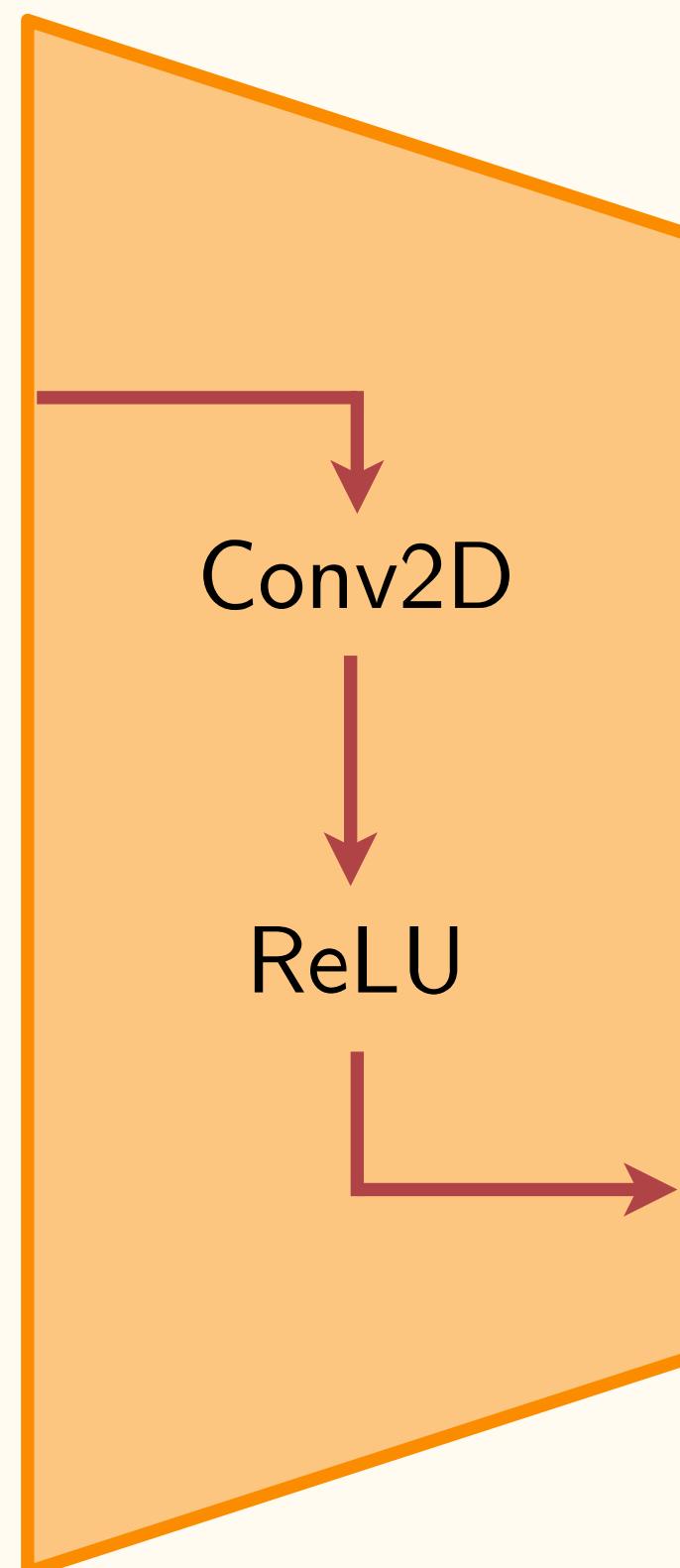


**Decode**



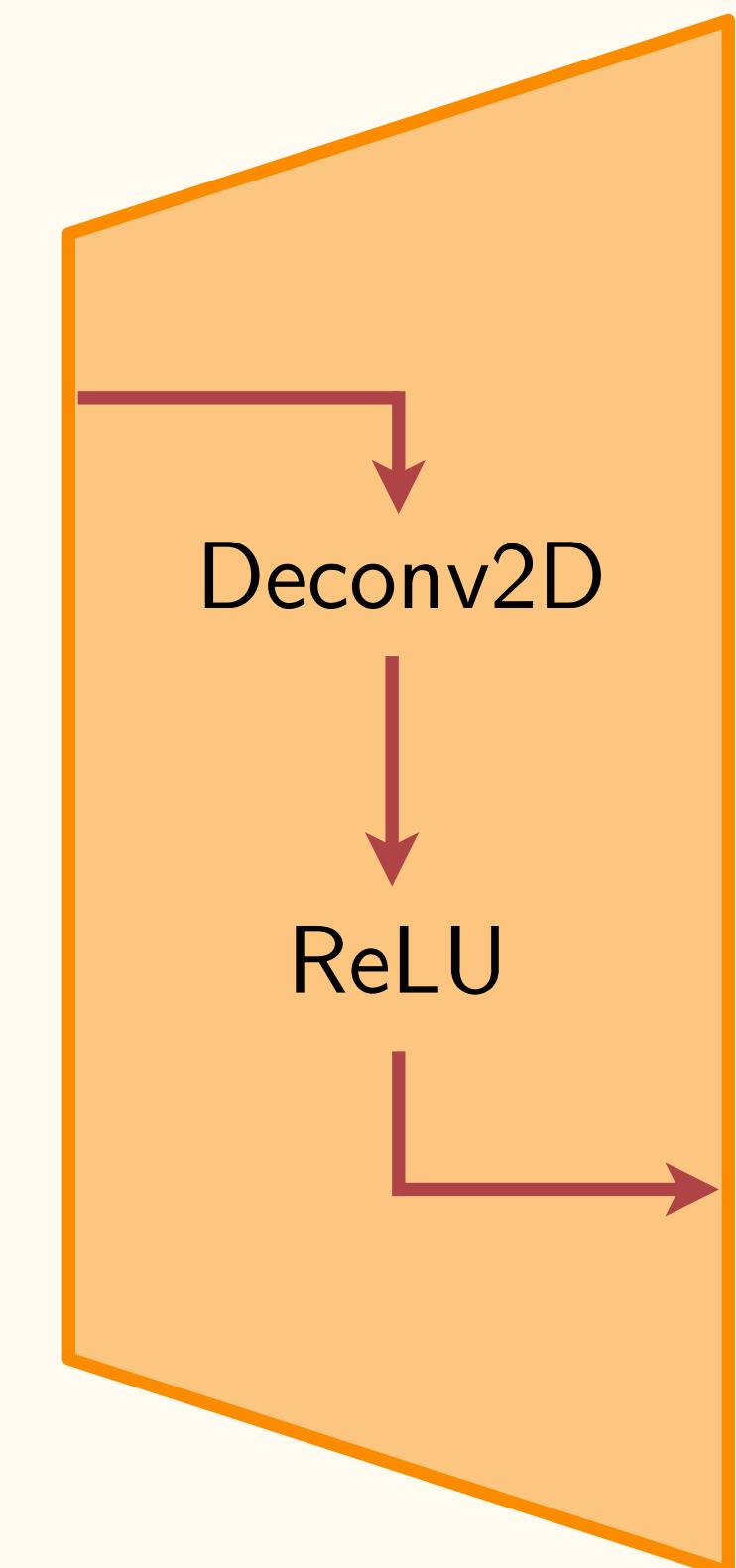
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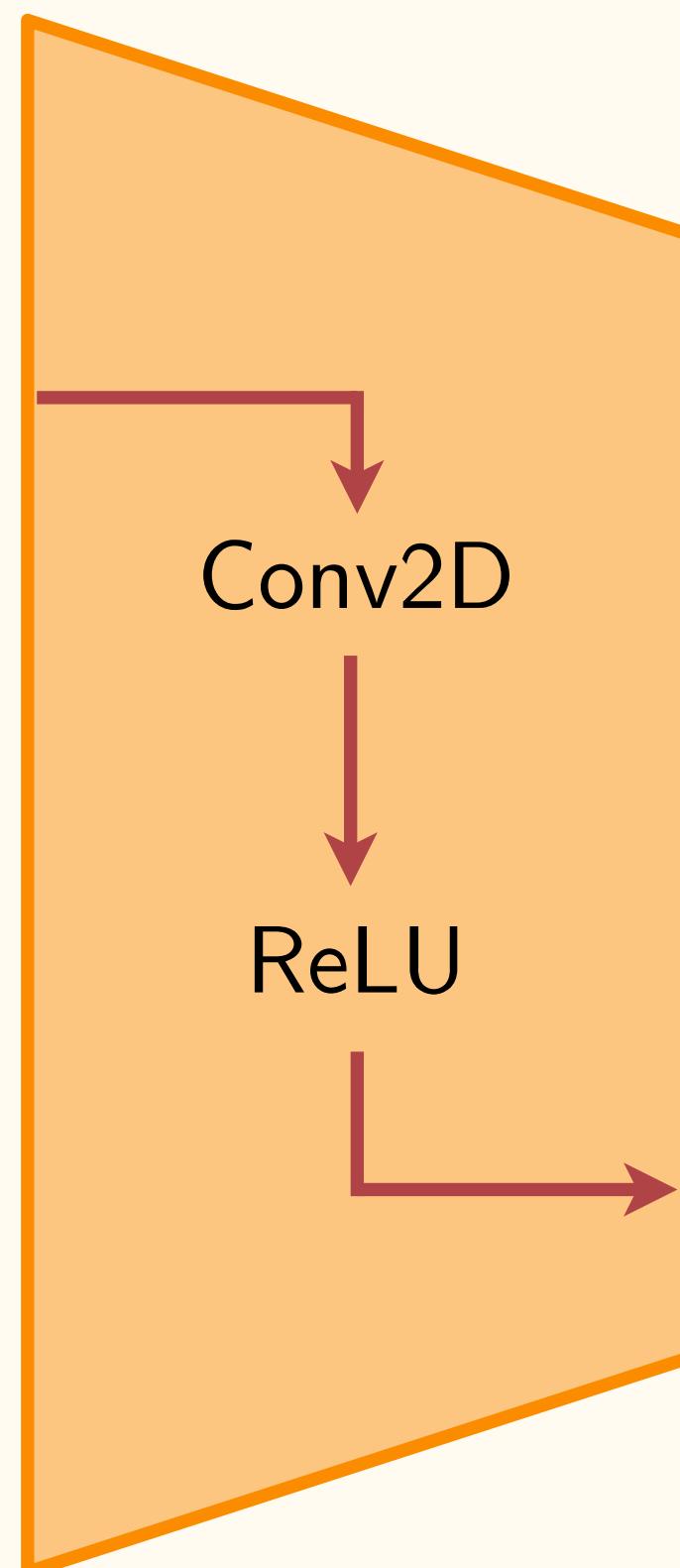
- An **encoder** is just a convolutional operation coupled with an activation function

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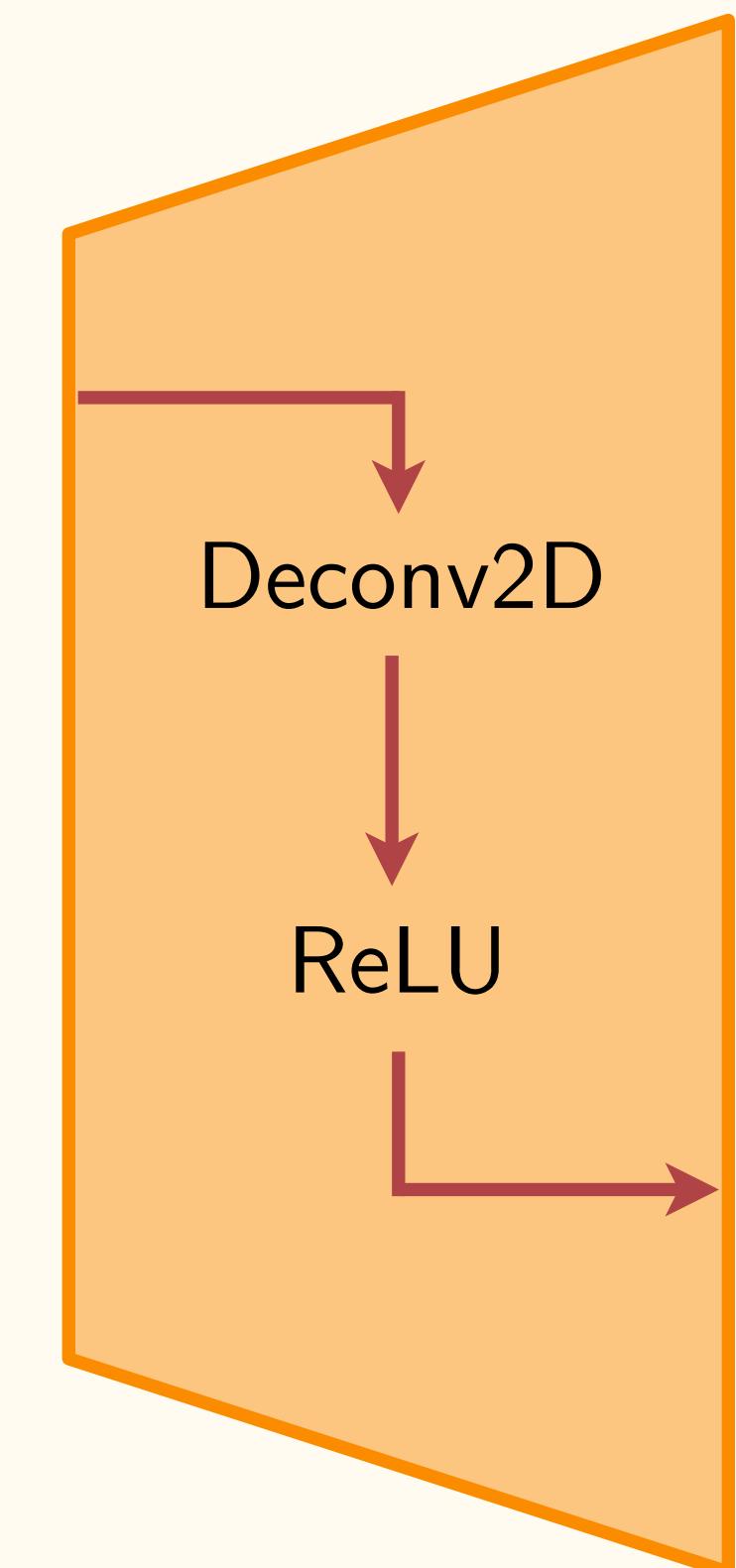
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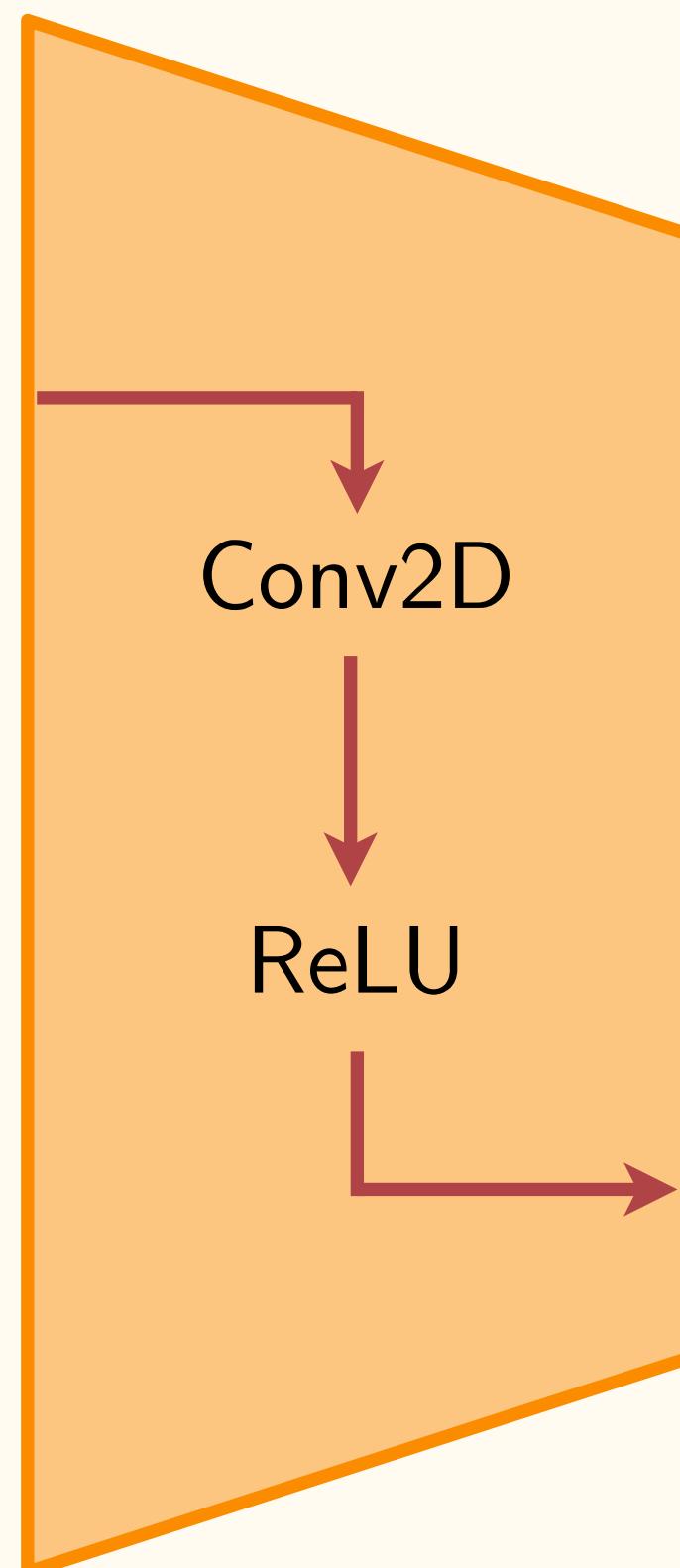
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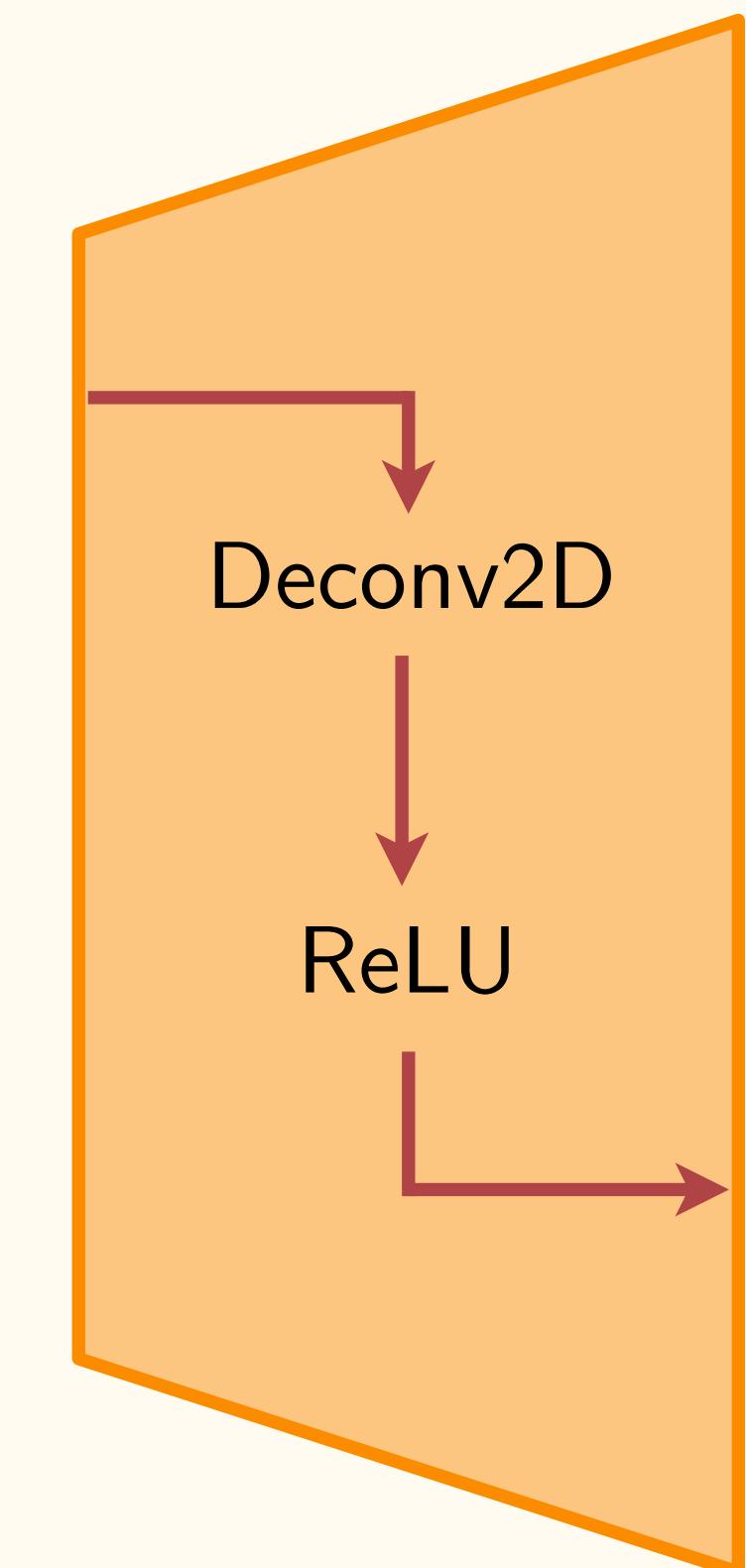


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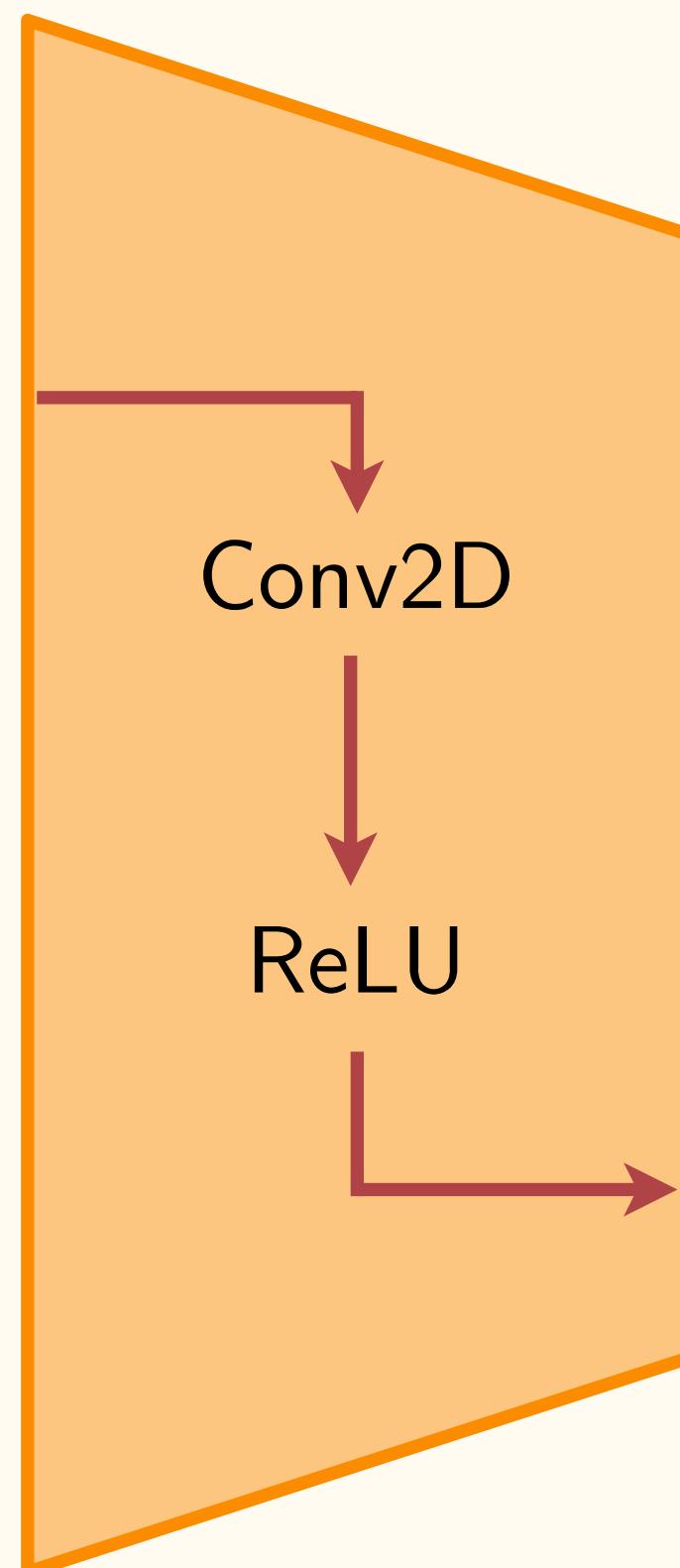
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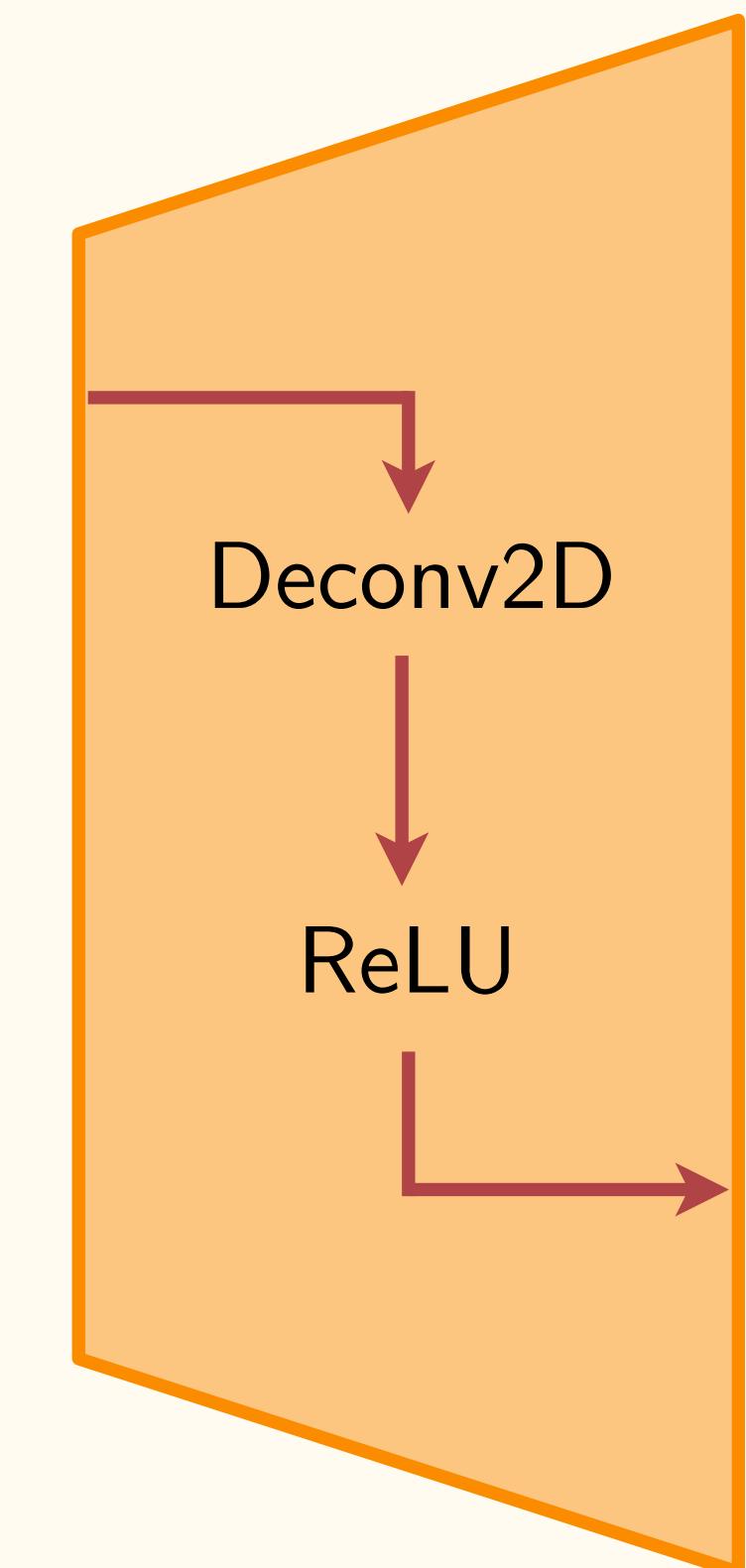
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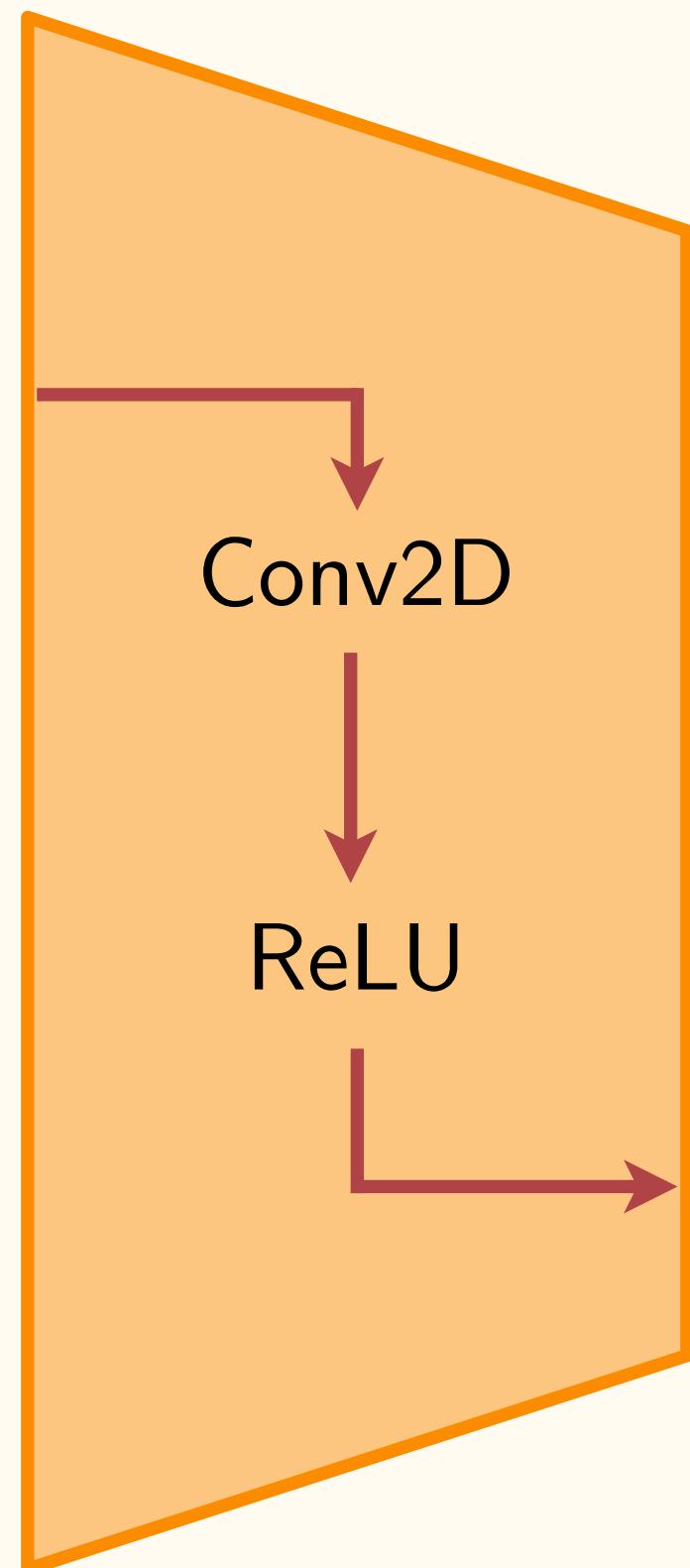
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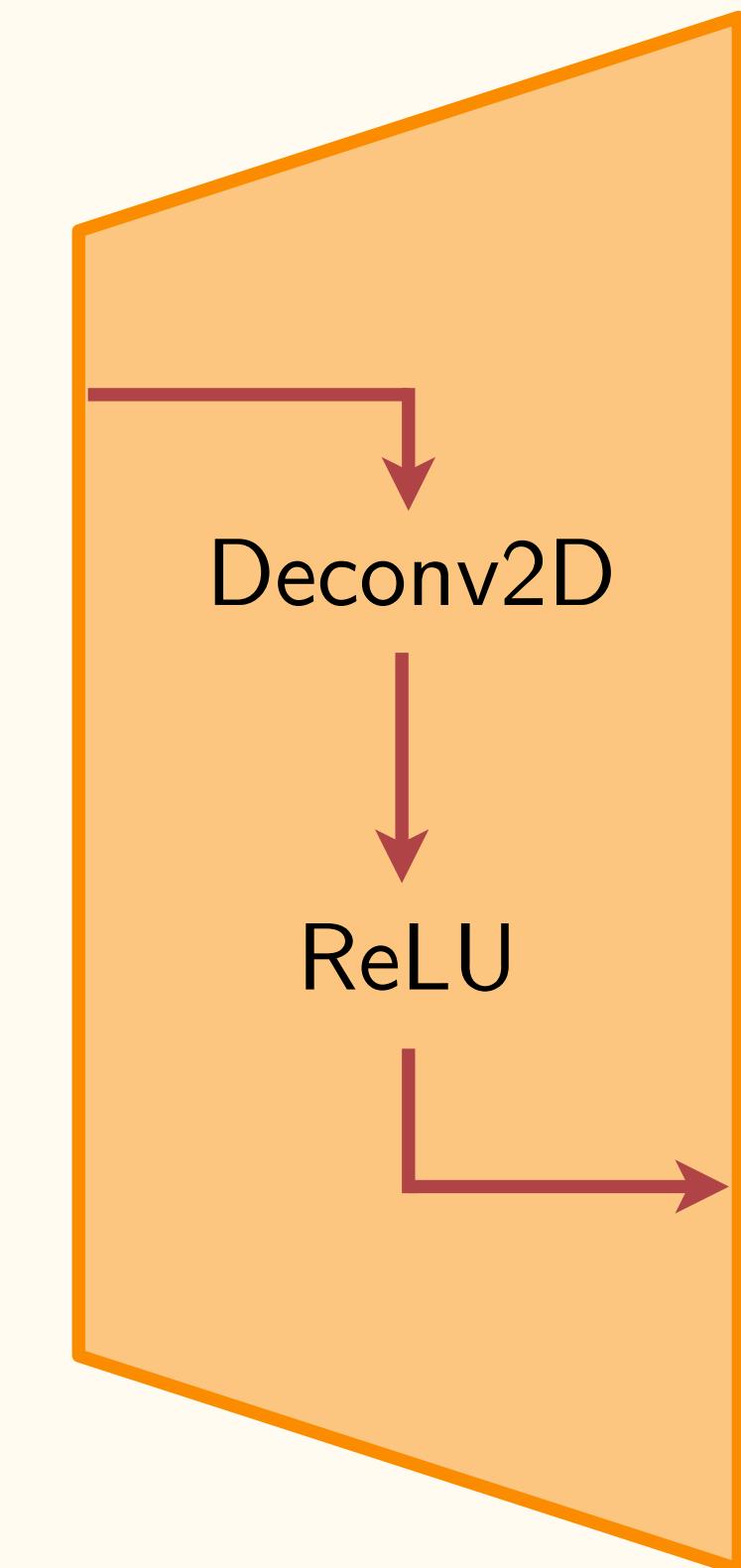
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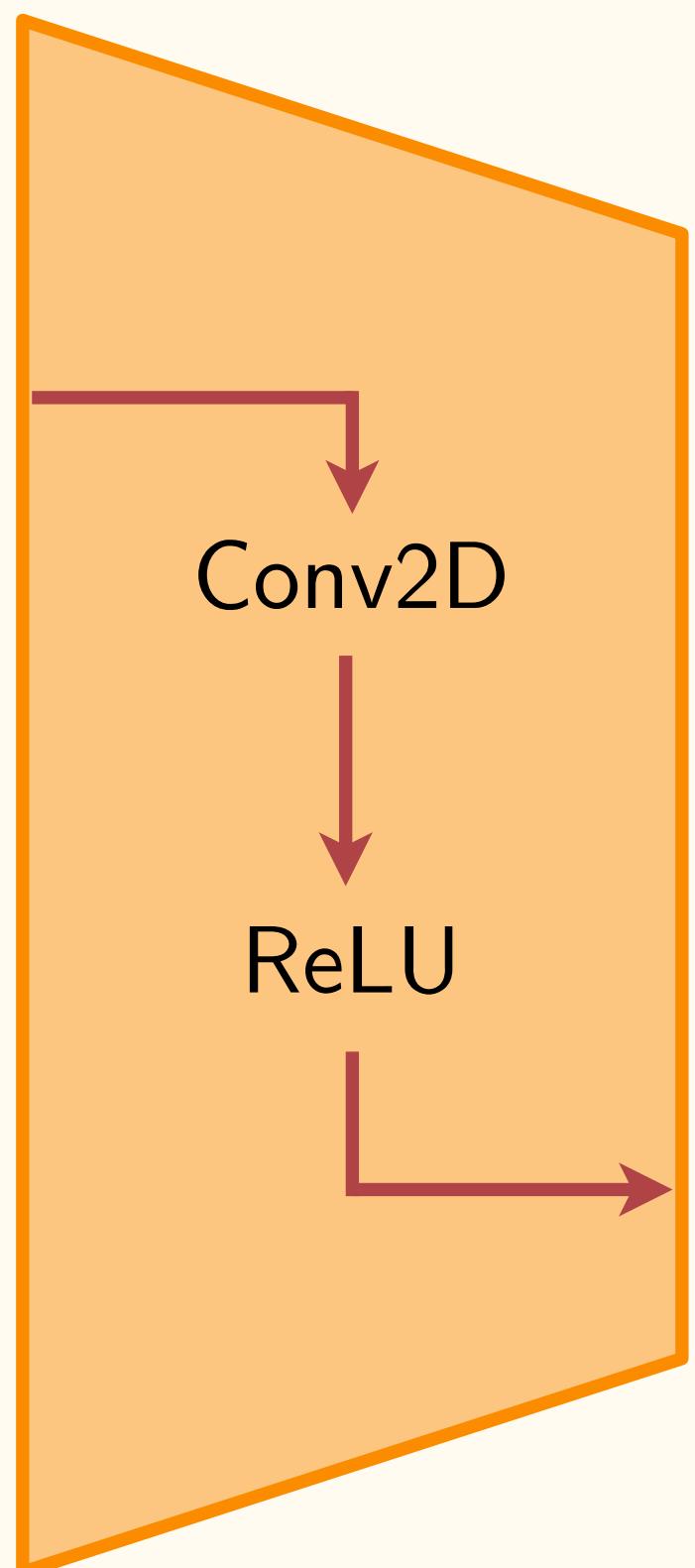
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- An **encoder** is just a convolutional operation coupled with an activation function
- A **decoder** is de-convolutional operation and activation function
- De-conv2D is just a **transposed** Conv2D

# Encoder-Decoder

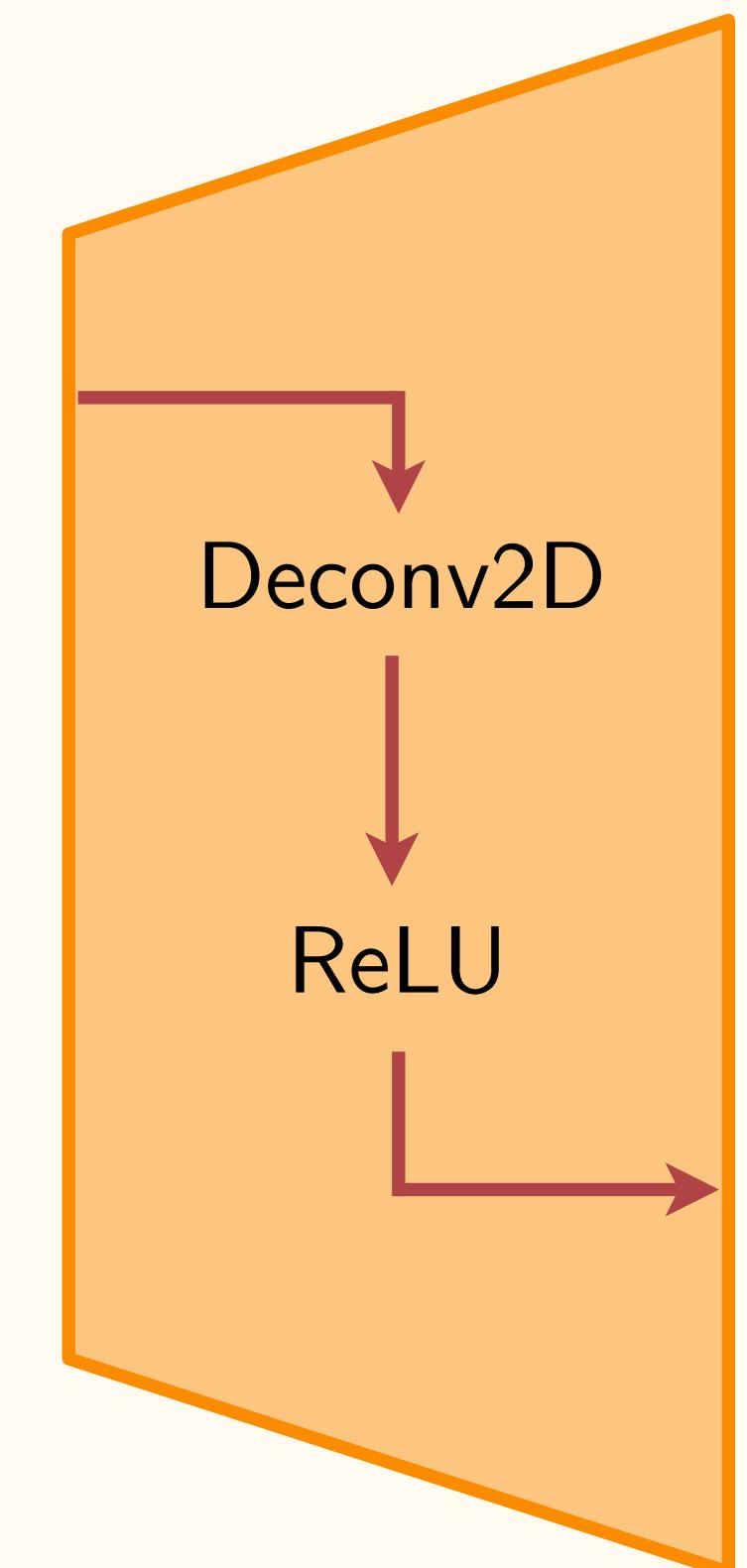
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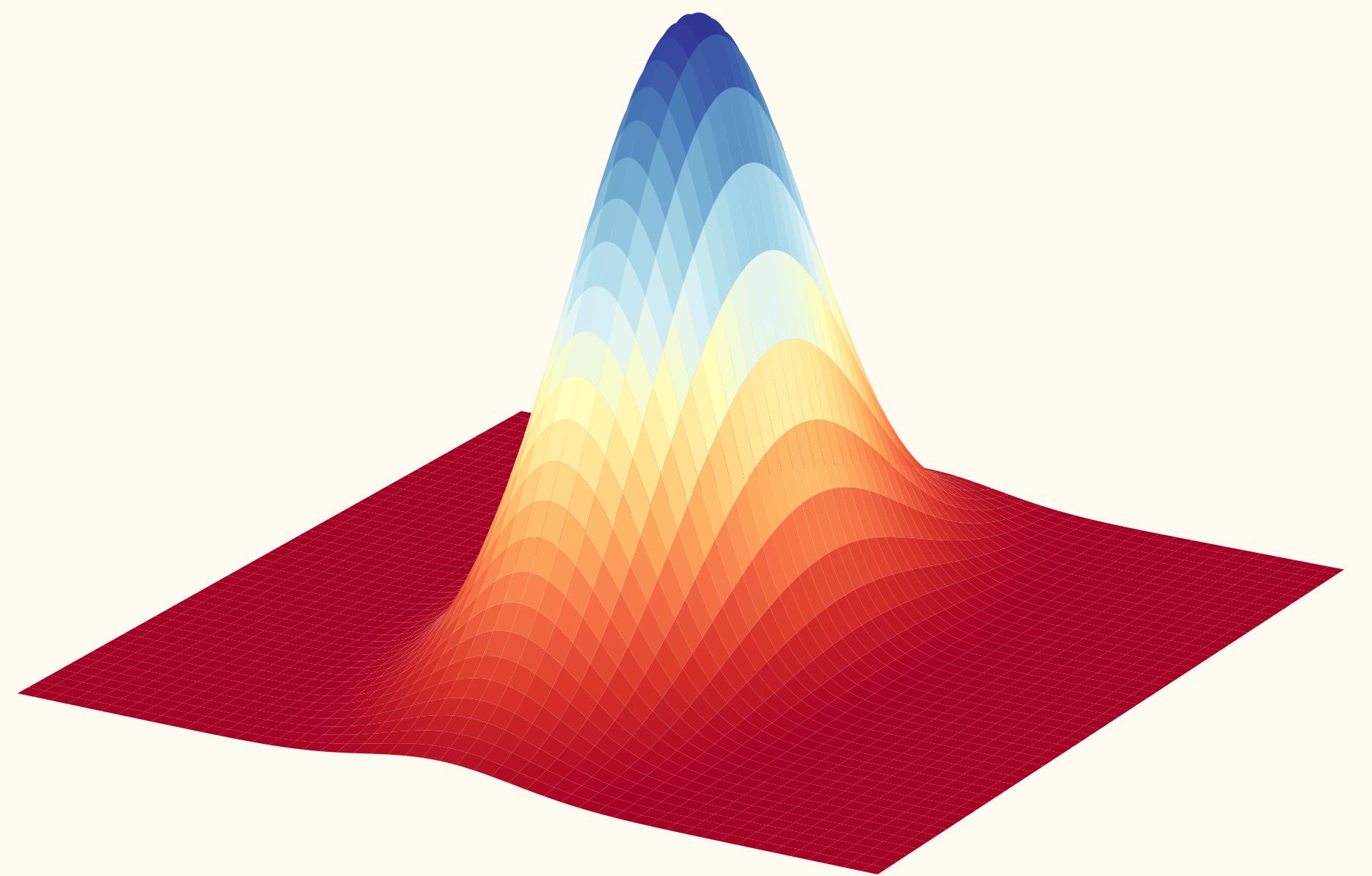
```
# Encoder  
tf.nn.conv2d()  
tf.nn.relu()
```

```
# Decoder  
tf.nn.conv2d_transpose()  
tf.nn.relu()
```

Decode

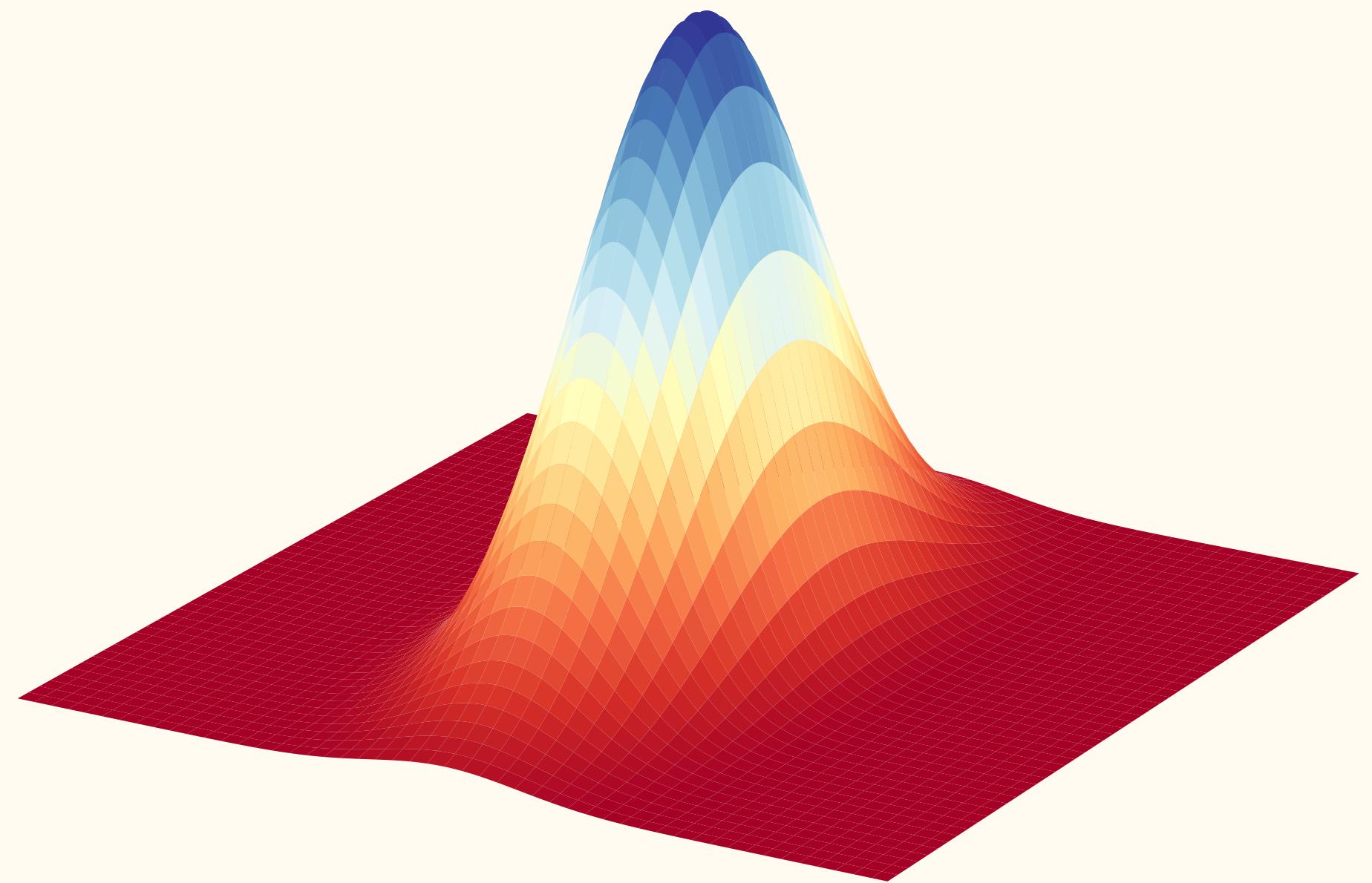


# Latent Distribution



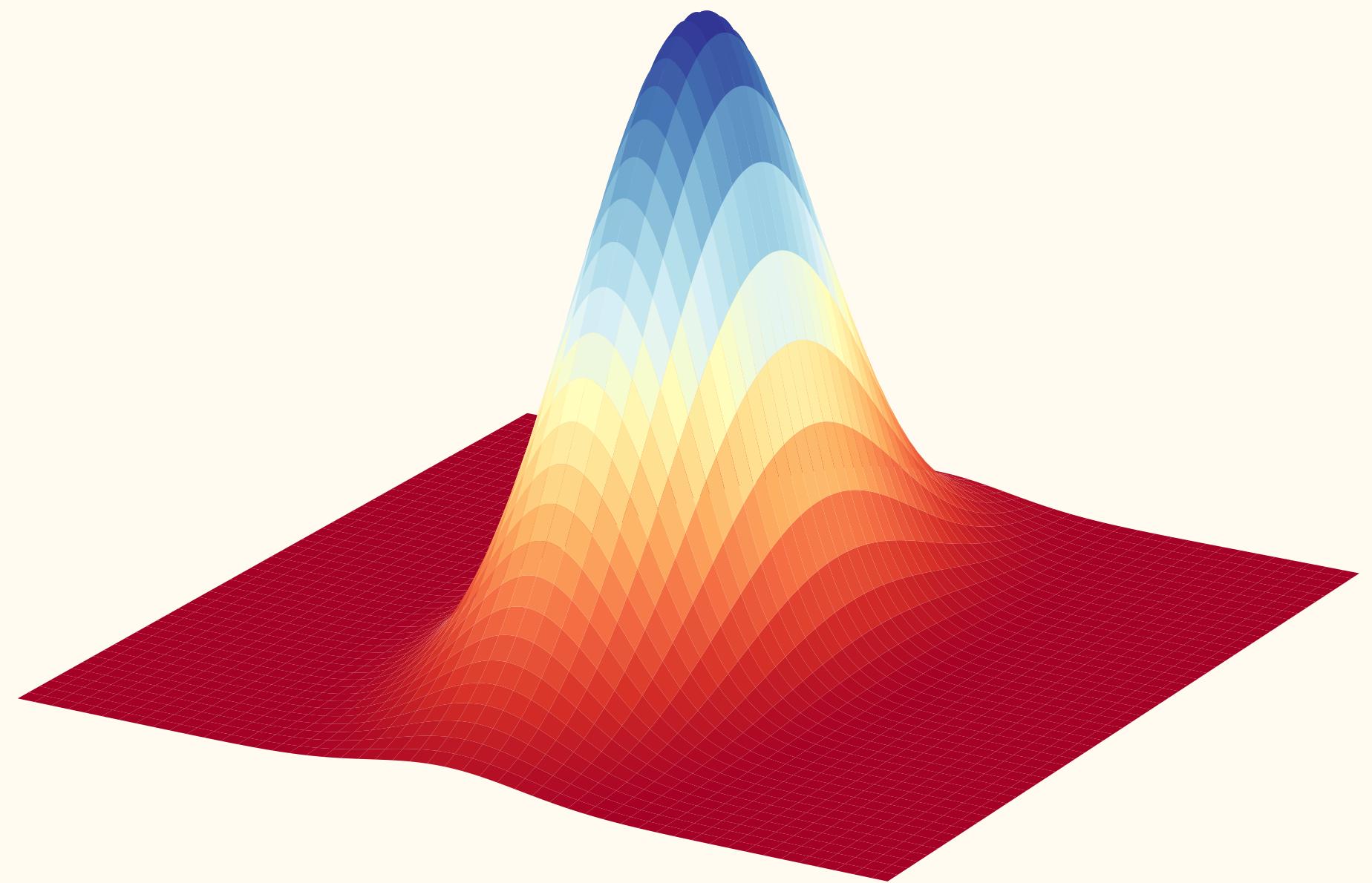
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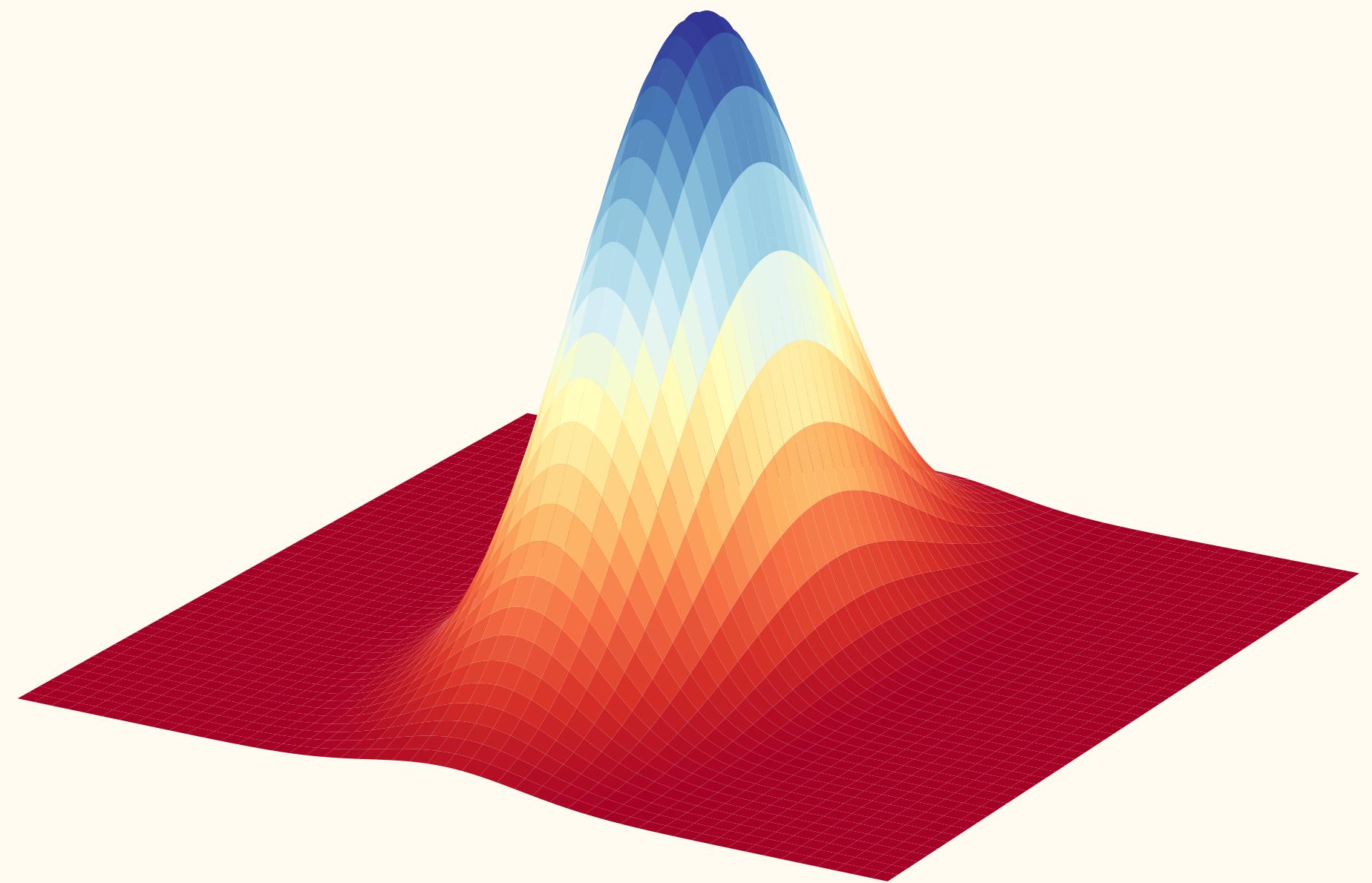
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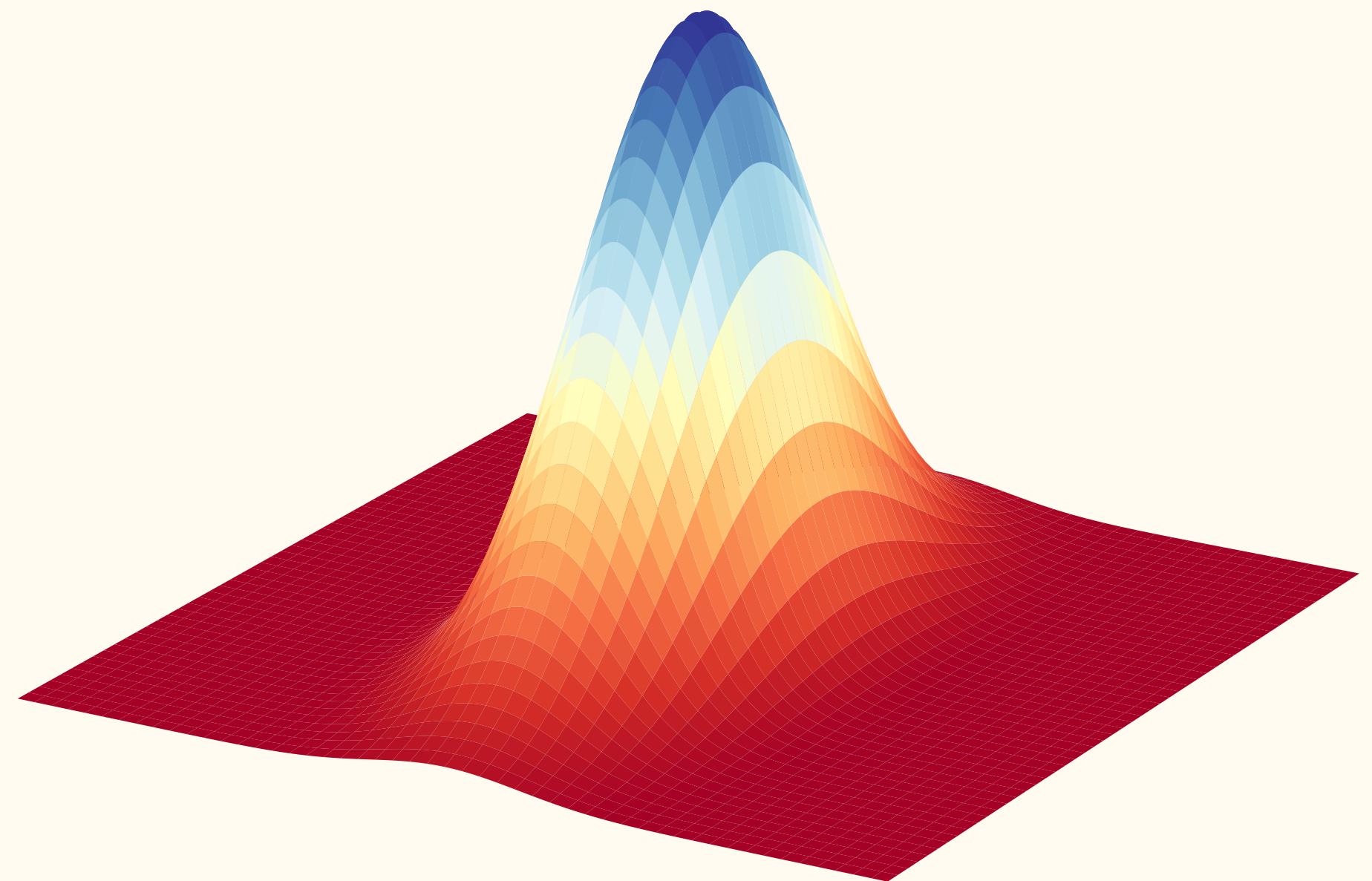


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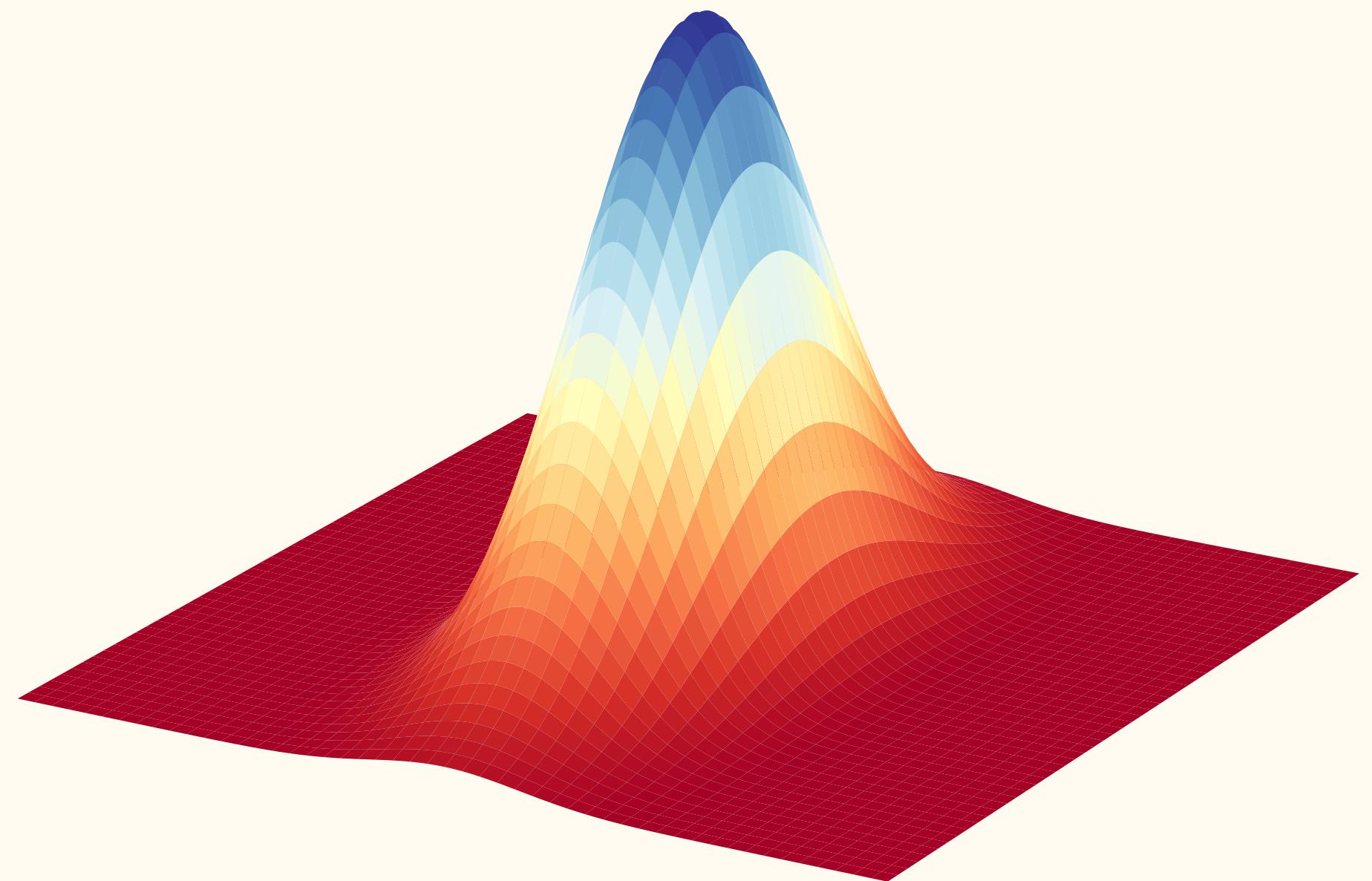


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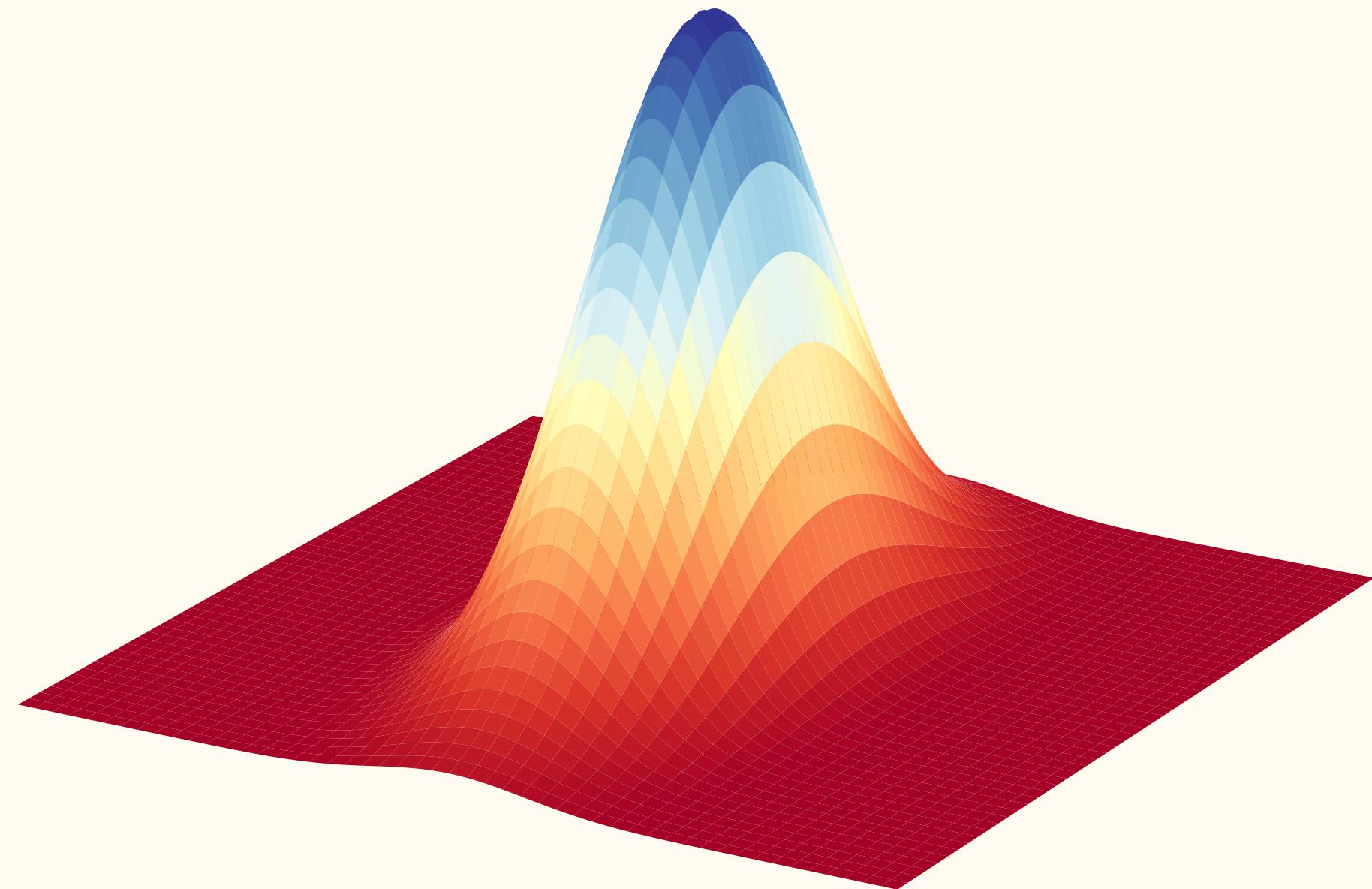
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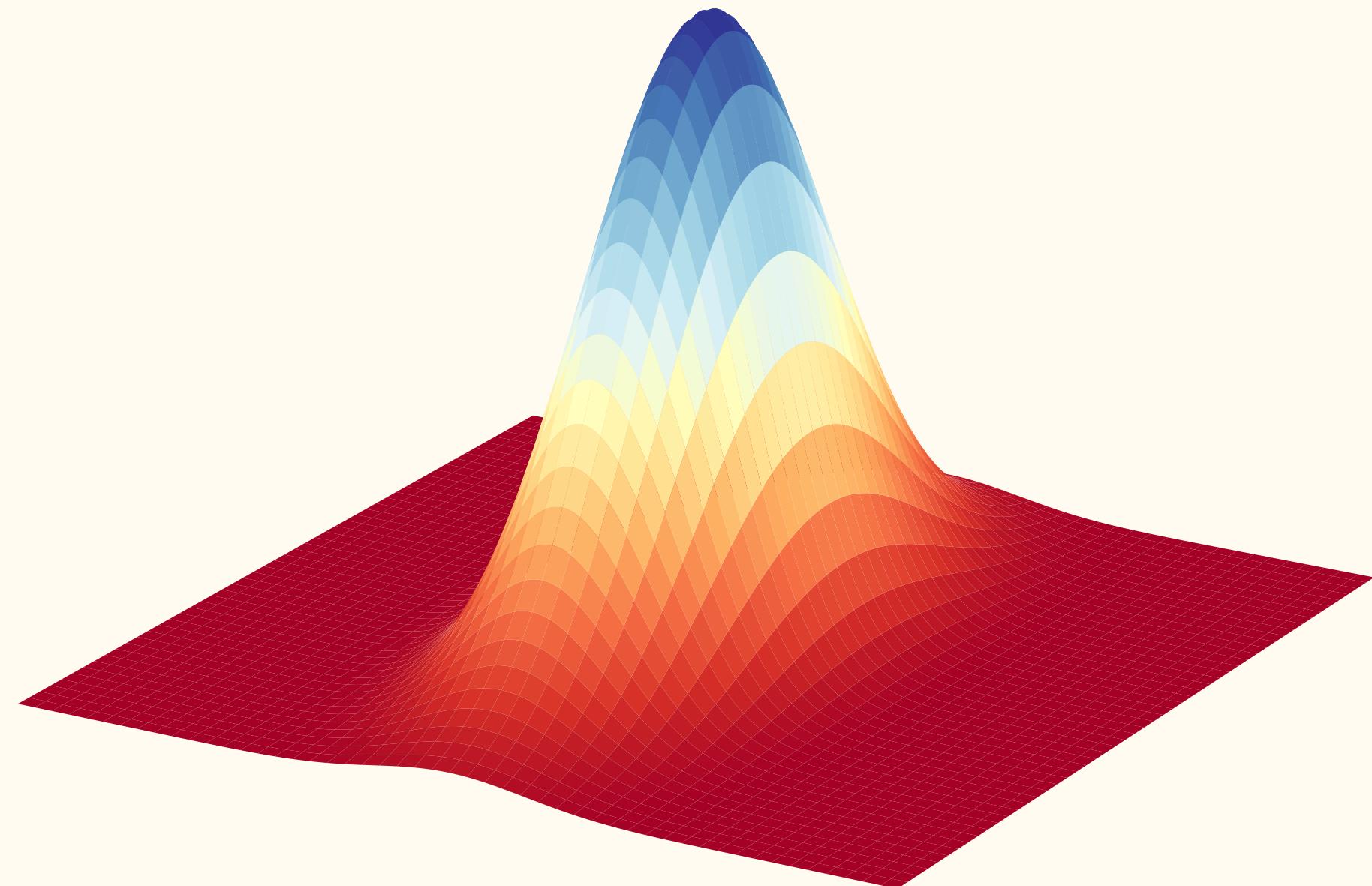
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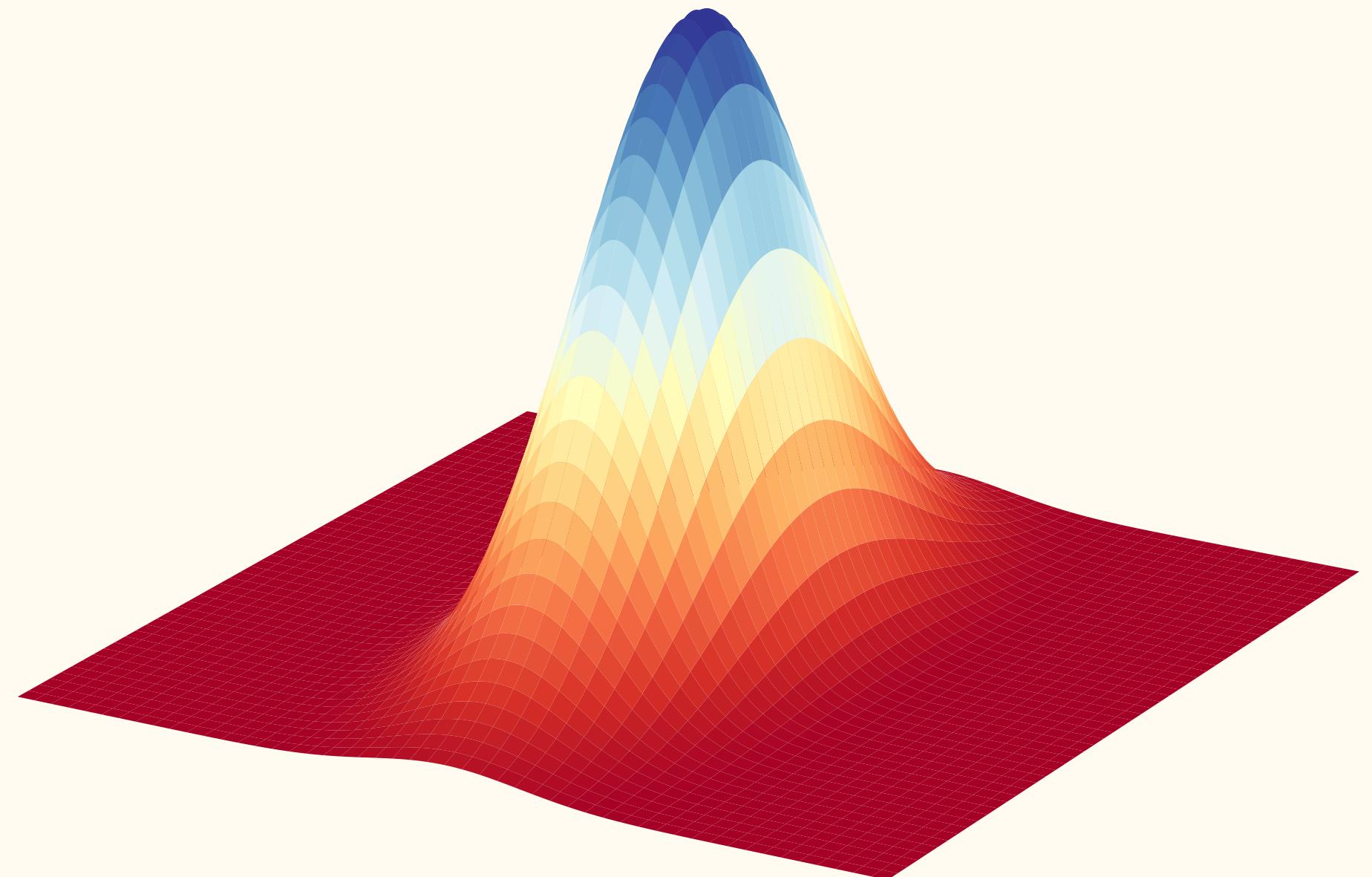
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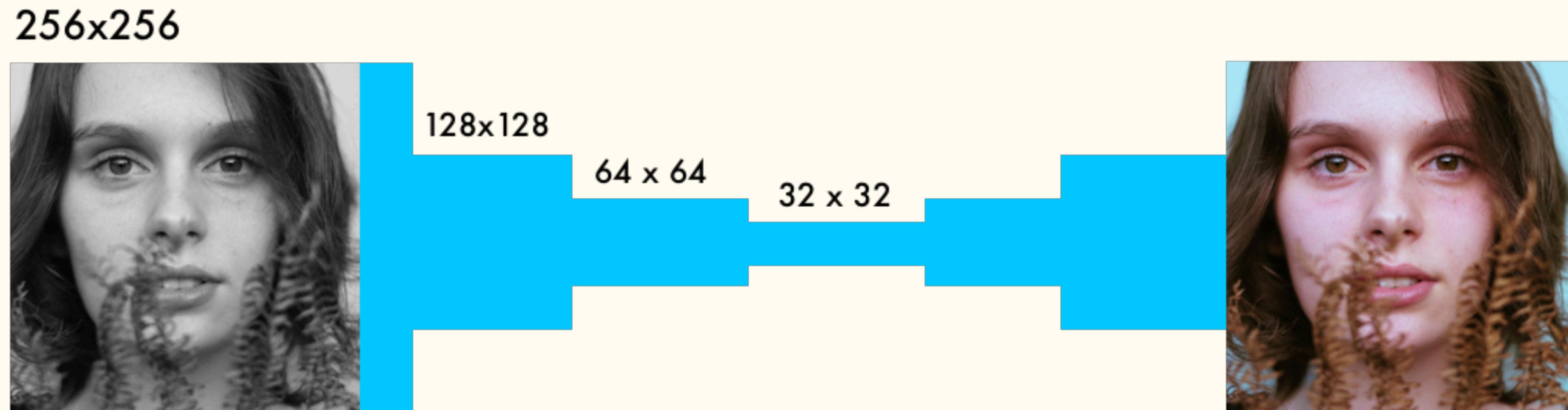


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- Remember: we **sample** from the distribution  $z \rightarrow$  lossy reconstruction

# VAE Applications

Colorize B&W images

- Encoder-Decoder architecture
- Inception ResNet V2 Classifier



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  - ▶ Passes random vectors into the generator
  - ▶ Directly evaluates the outputs on how well they follow the expected distribution

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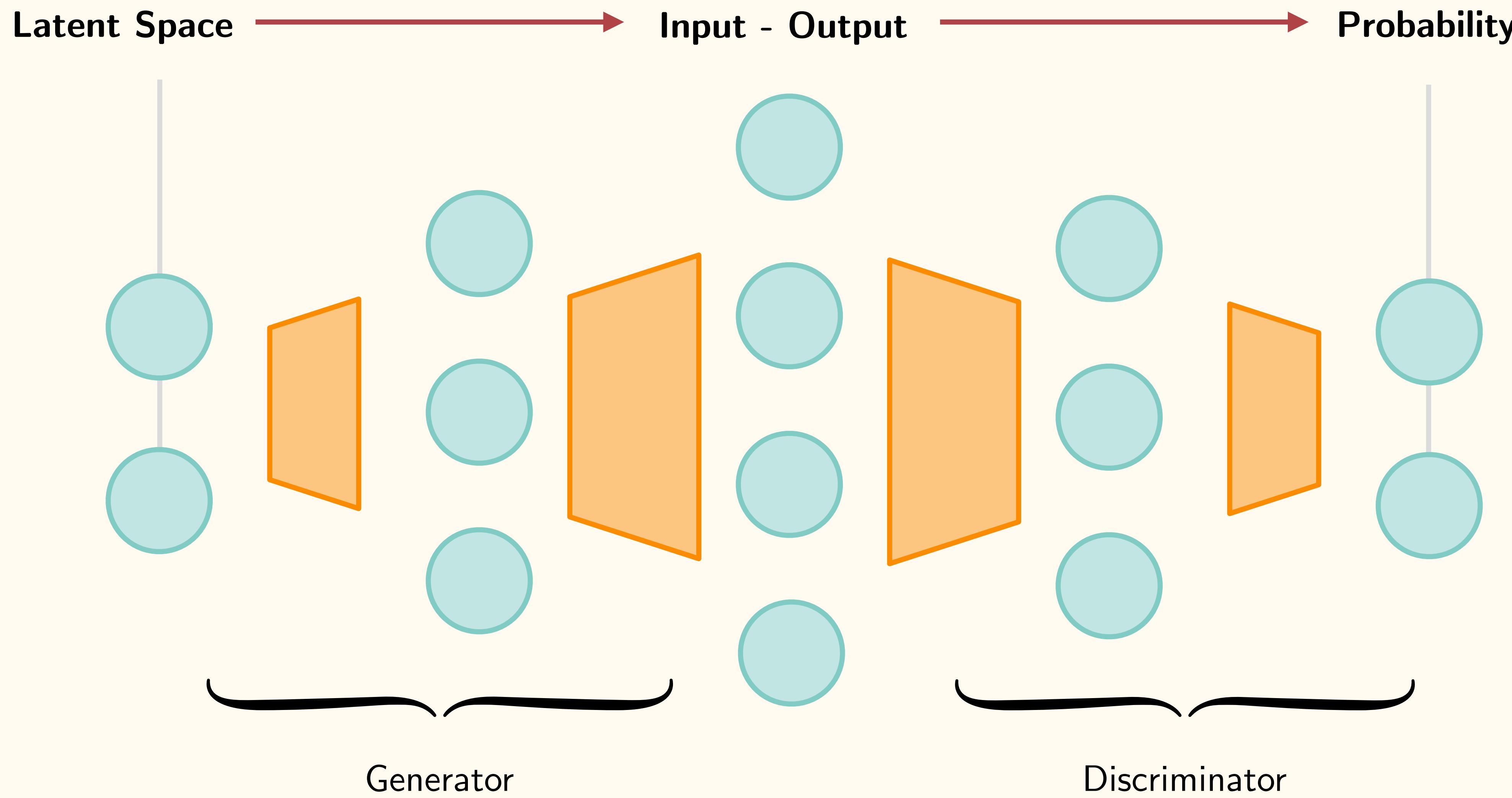


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  - GAN learns the loss function from the data.



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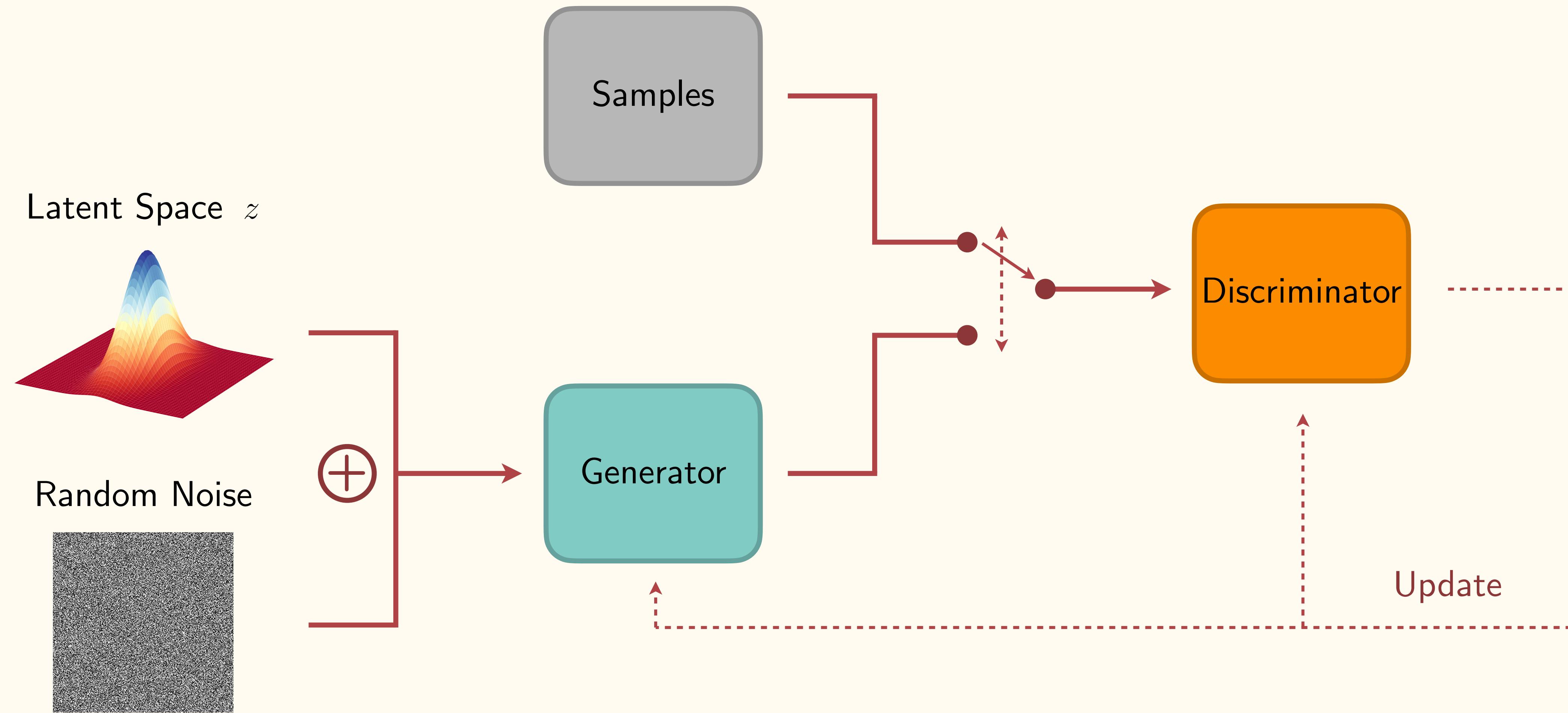
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  - The generated samples from real training samples
  - It takes a sample as input and outputs a **probability** of being a real sample
    - ▶ This acts as a loss function for the generator.

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Generative *Adversarial* Networks

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Generative *Adversarial* Networks

# GAN Applications

Colorize B&W images

- Even more advanced and realistic
- GAN based architecture



# VAE vs GANs

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Roughly:

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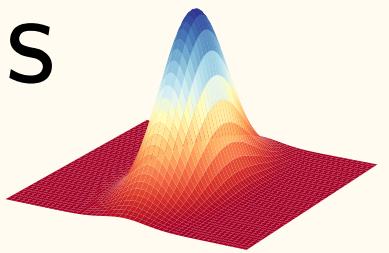
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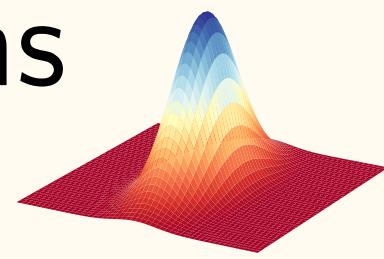
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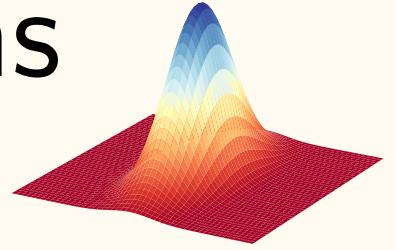
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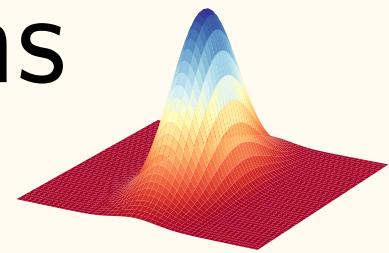
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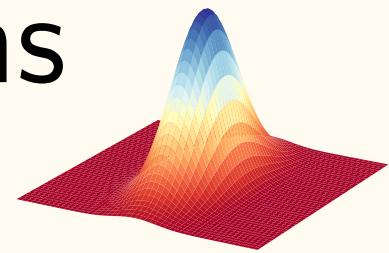


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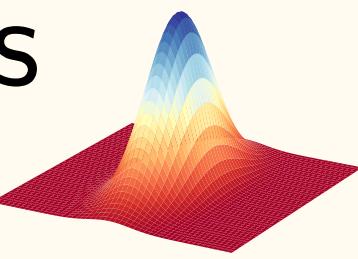
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Very active field of research → Things changing constantly !

# Application: Predicting Drug-Target Binding Affinity

<sup>1</sup> Zhao Lingling et al., 2020. *GANsDTA: Predicting Drug-Target Binding Affinity Using GANs*. Frontiers in Genetics, Volume 10.

# Application: Predicting Drug-Target Binding Affinity

- Challenging in Drug Discovery

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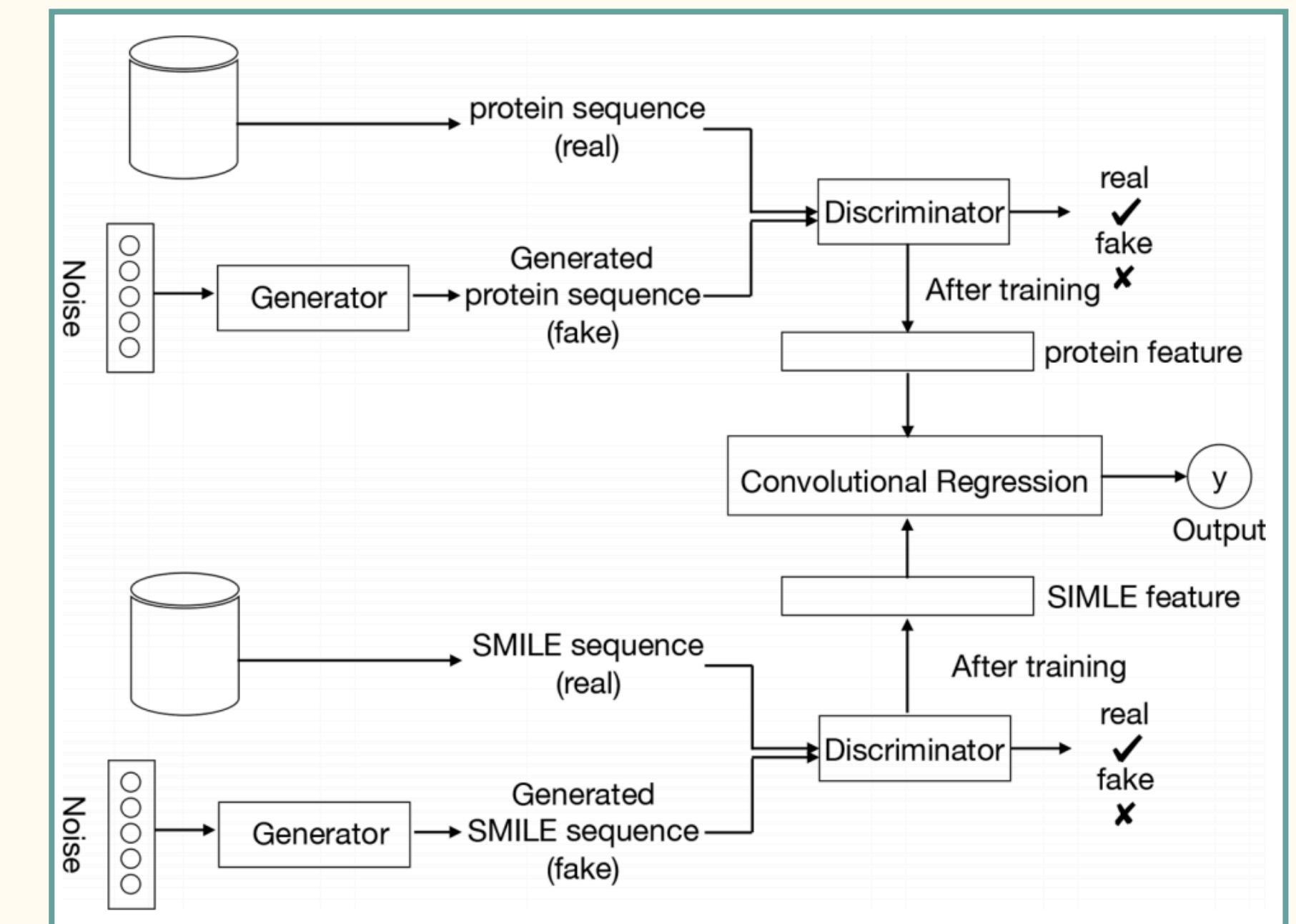
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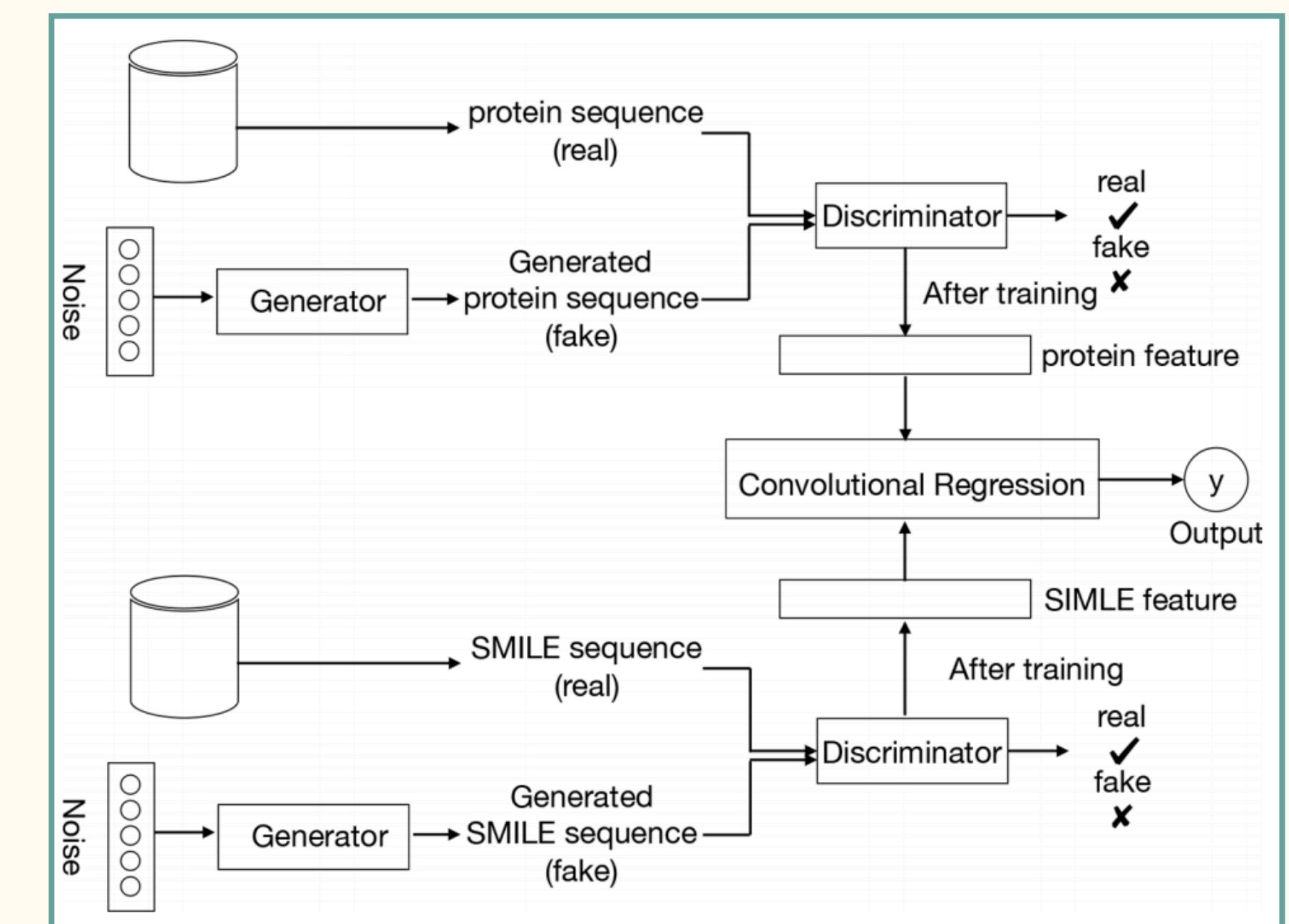
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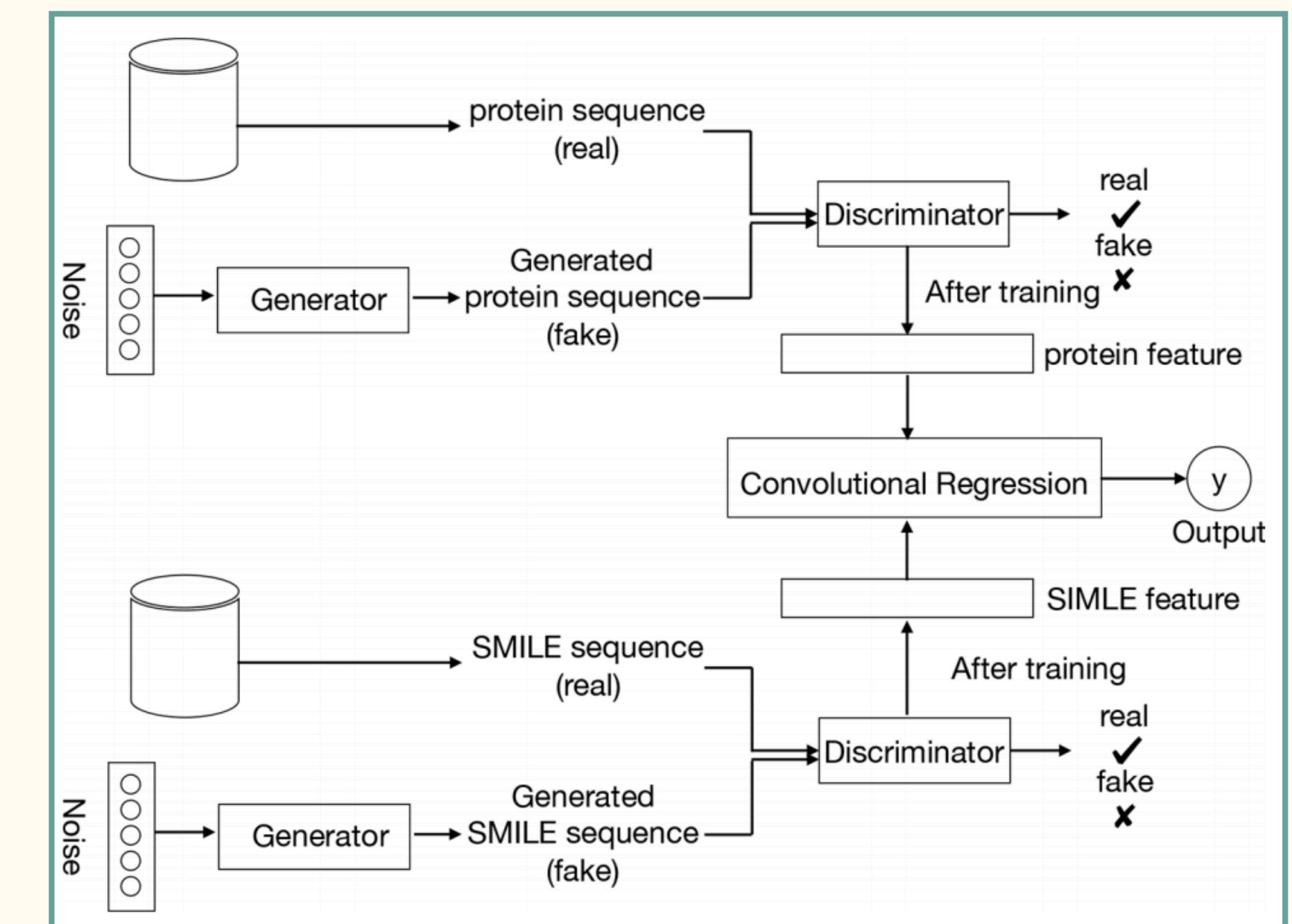
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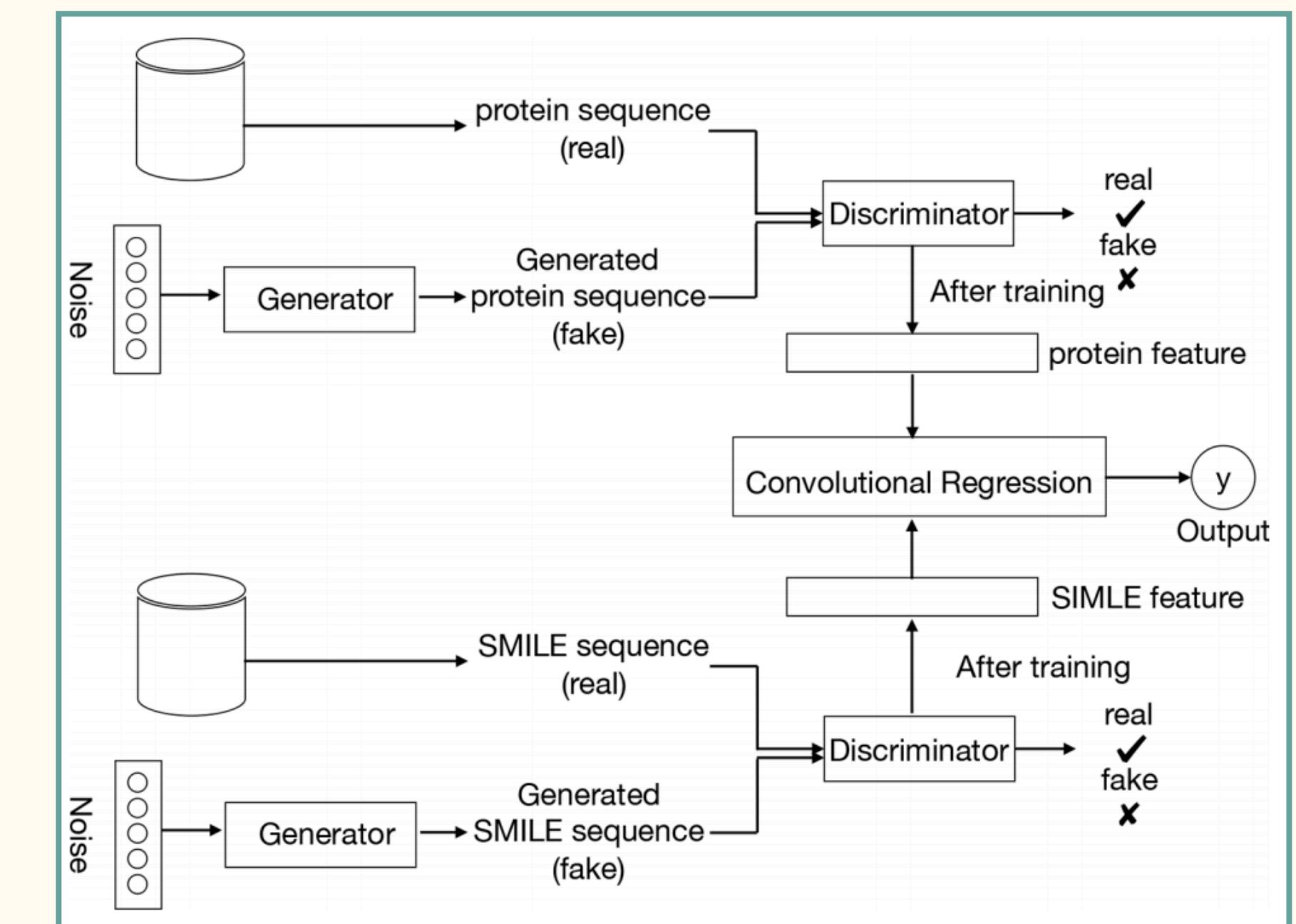
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1. Train the GANs on the unlabelled data set
  - Compound SMILES and protein sequences are encoded



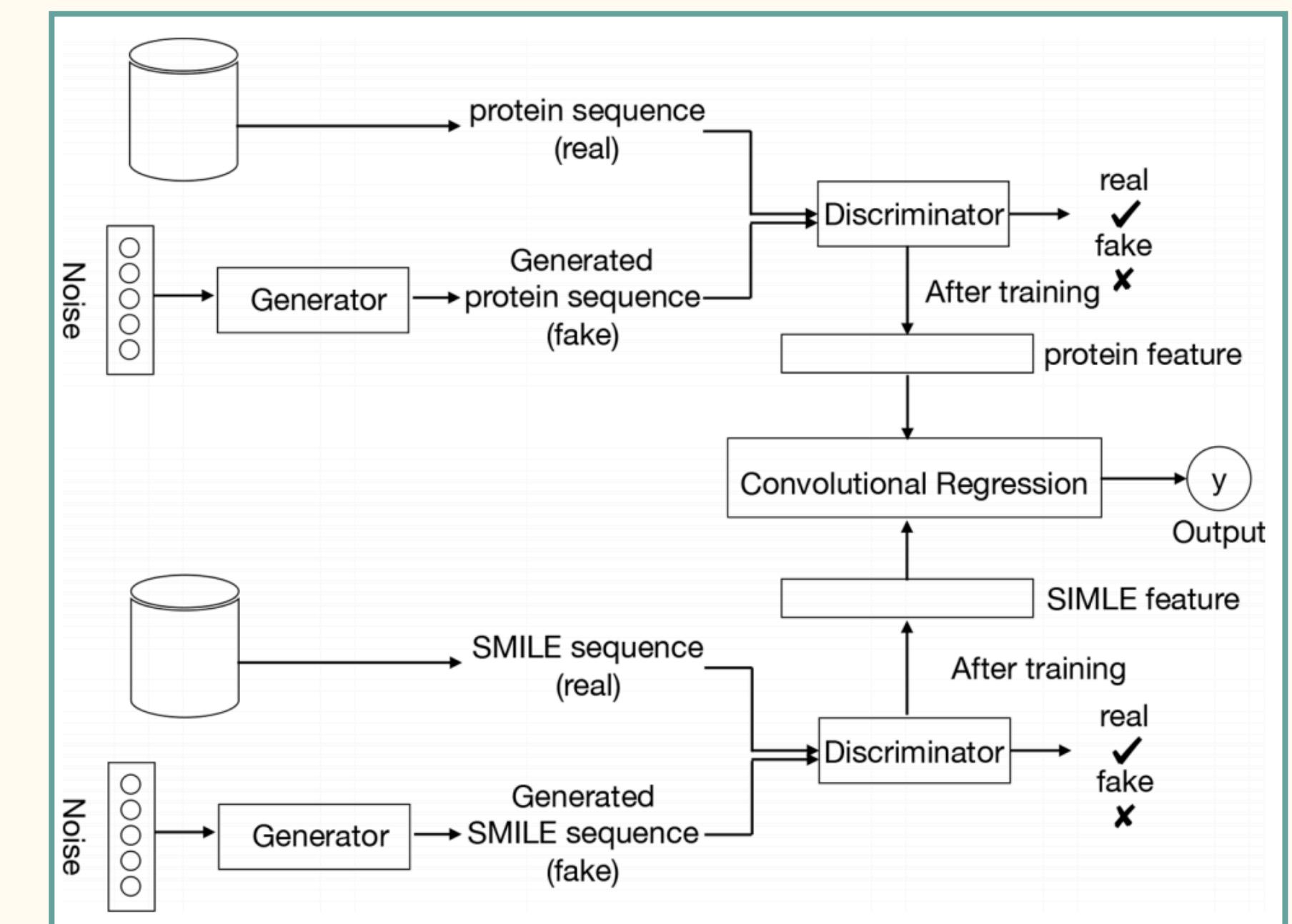
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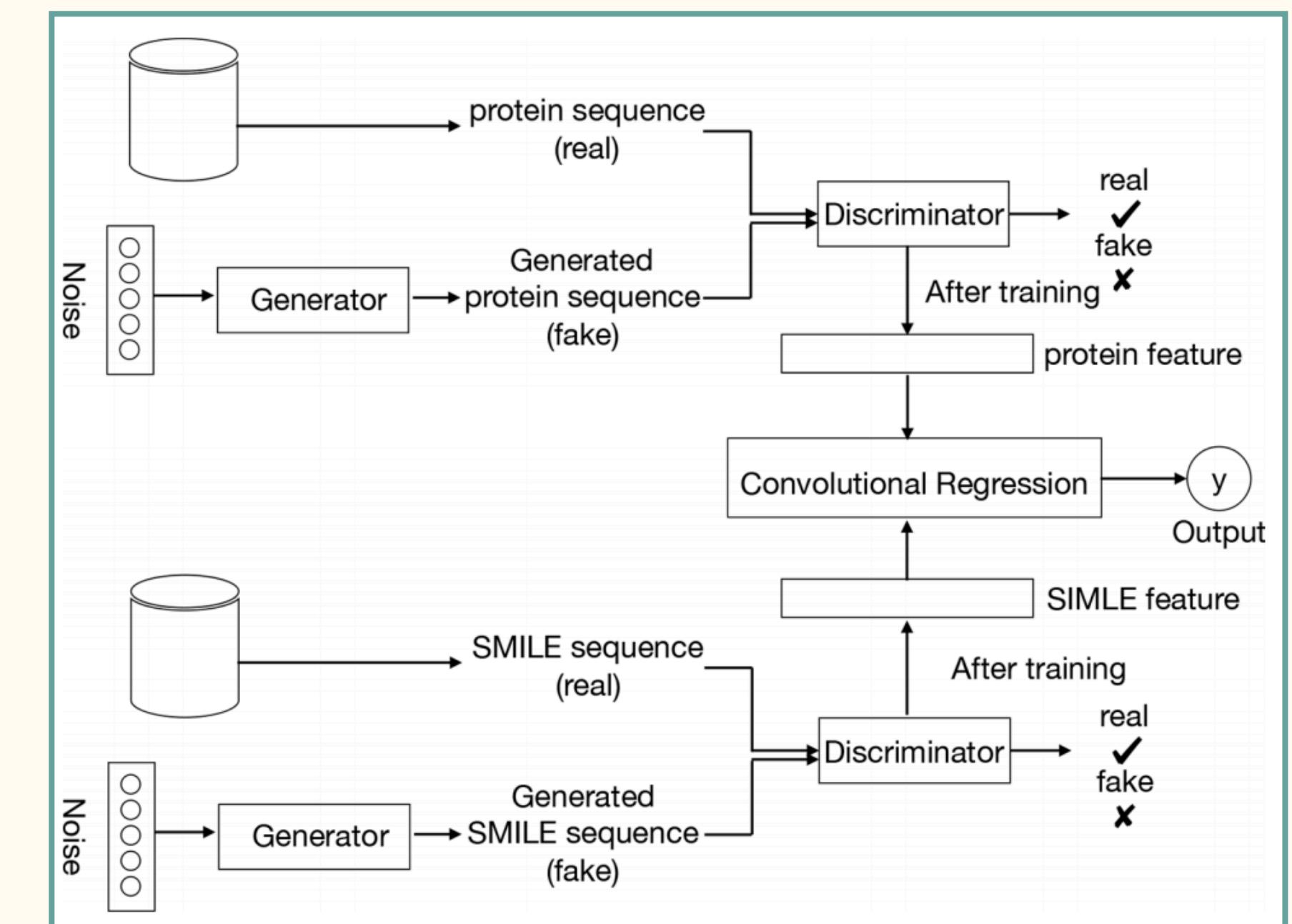
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1. Train the GANs on the unlabelled data set
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2. Two independent GANs are applied



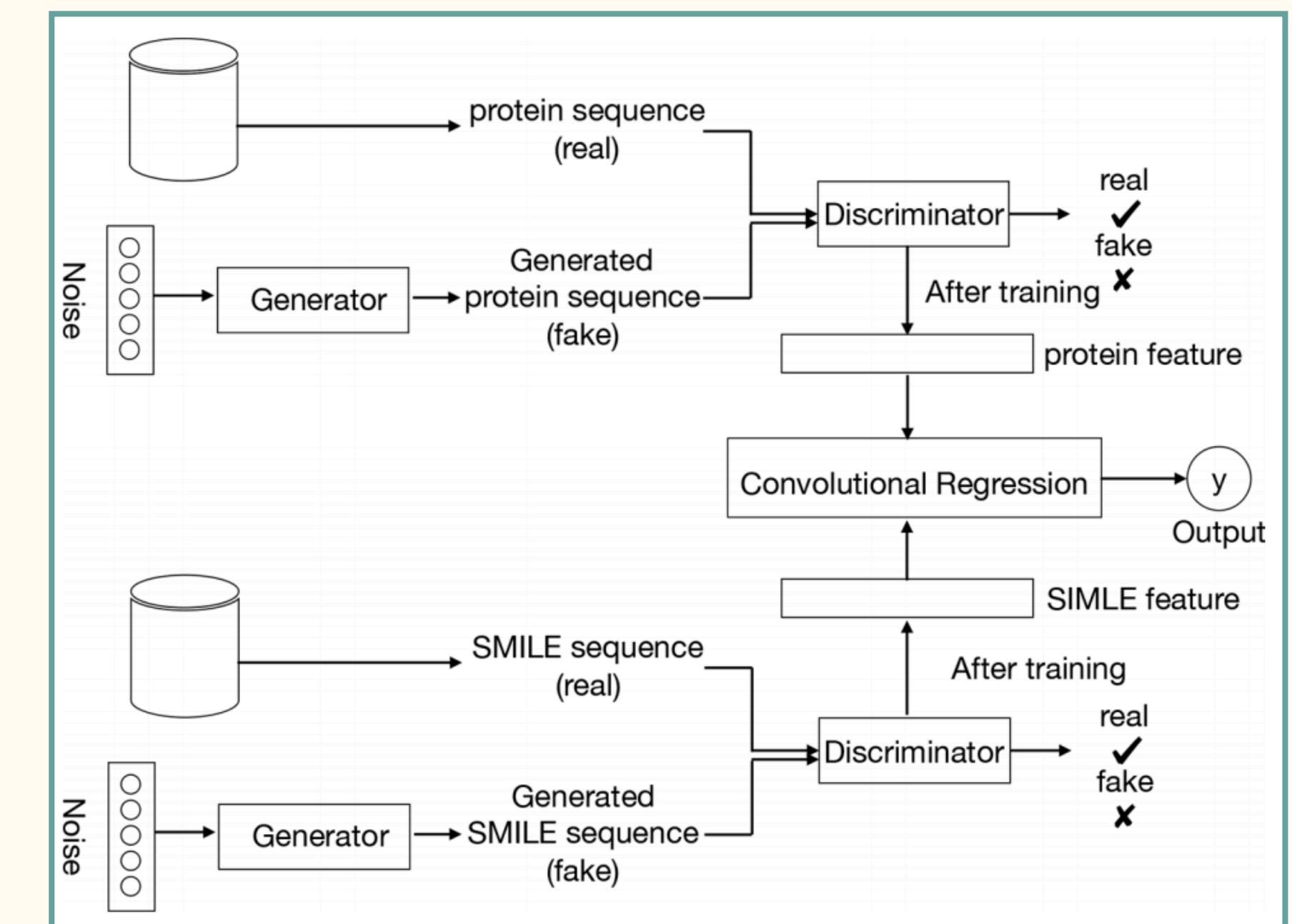
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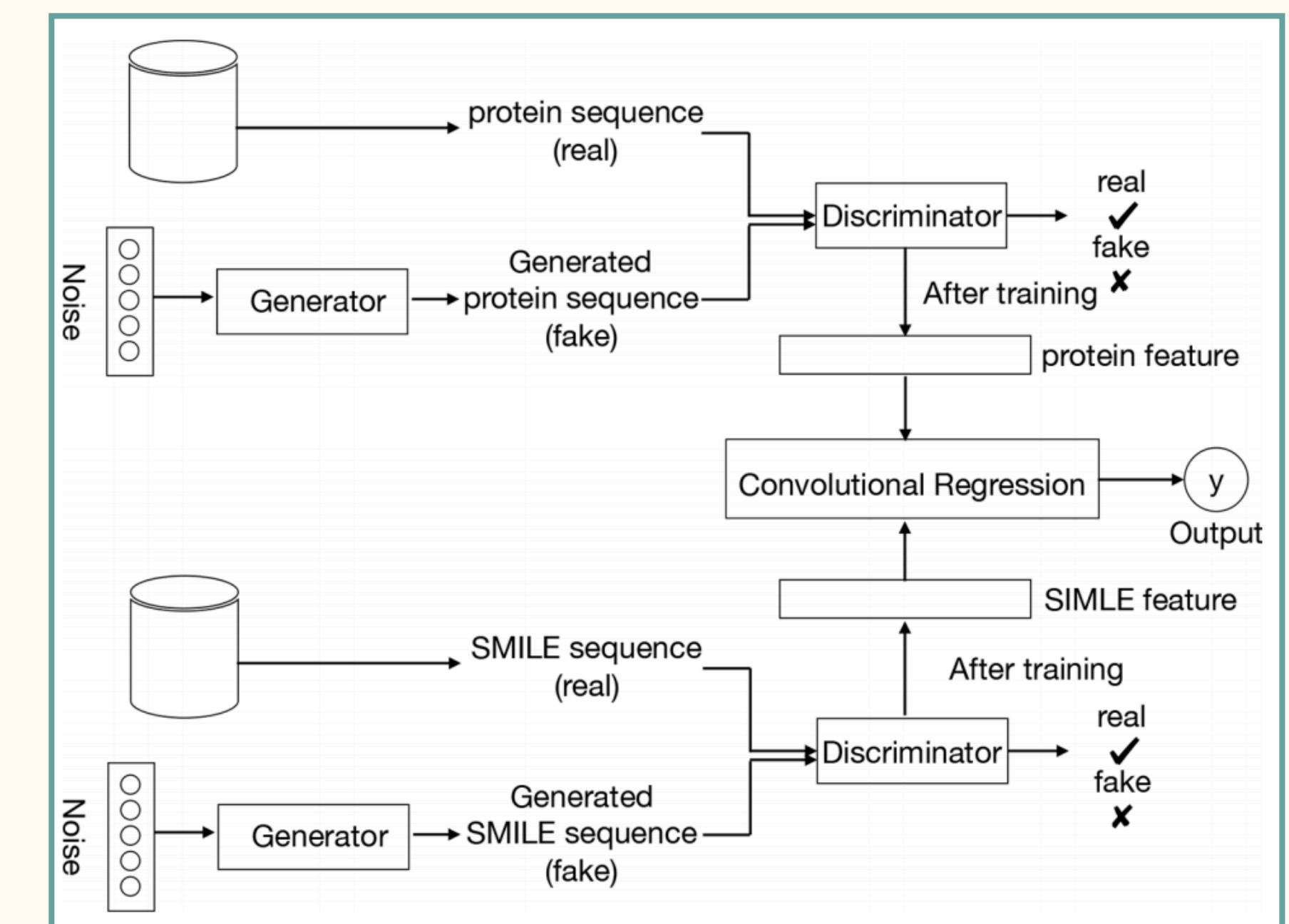
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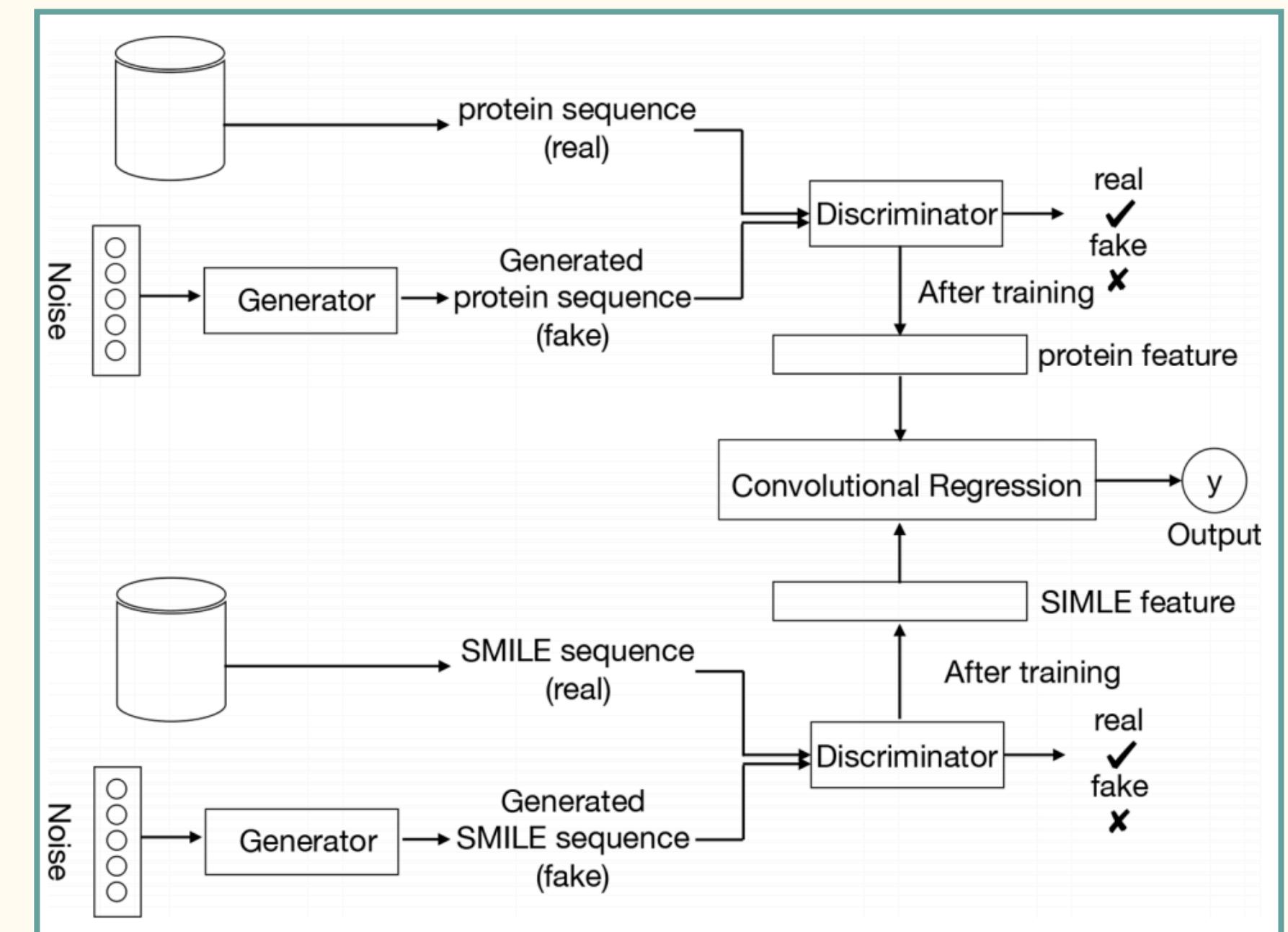
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3. Use GANs' trained discriminator



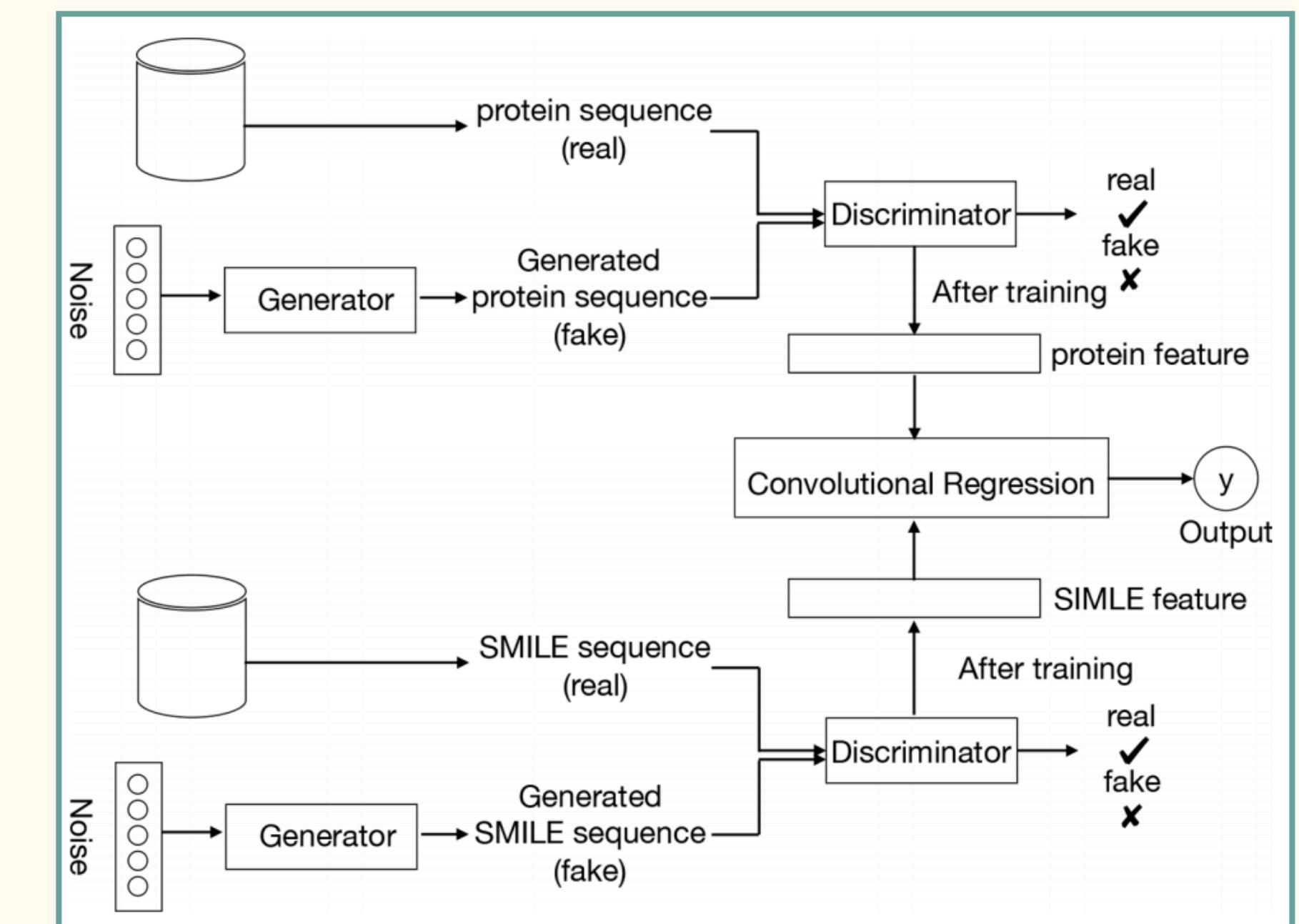
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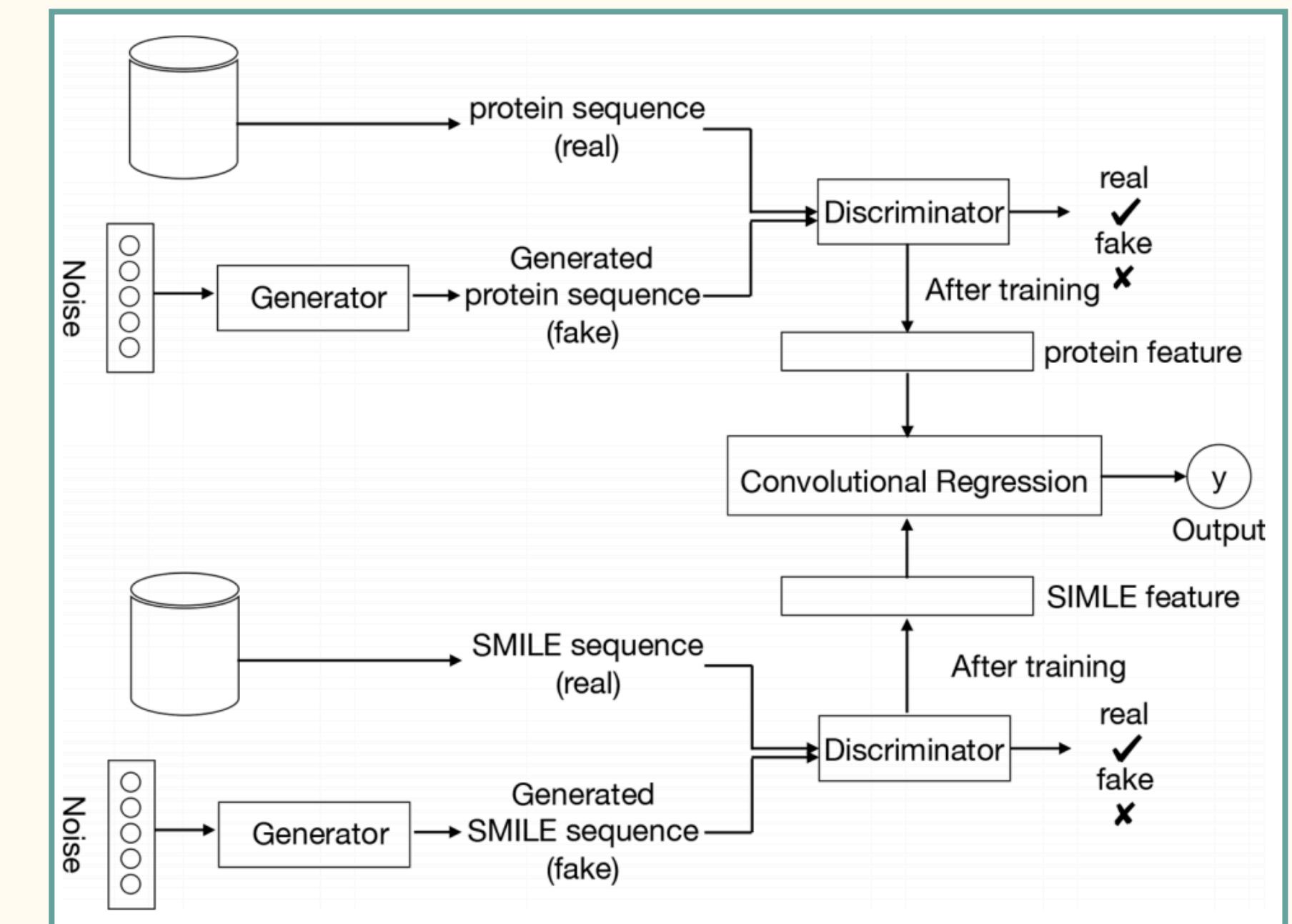
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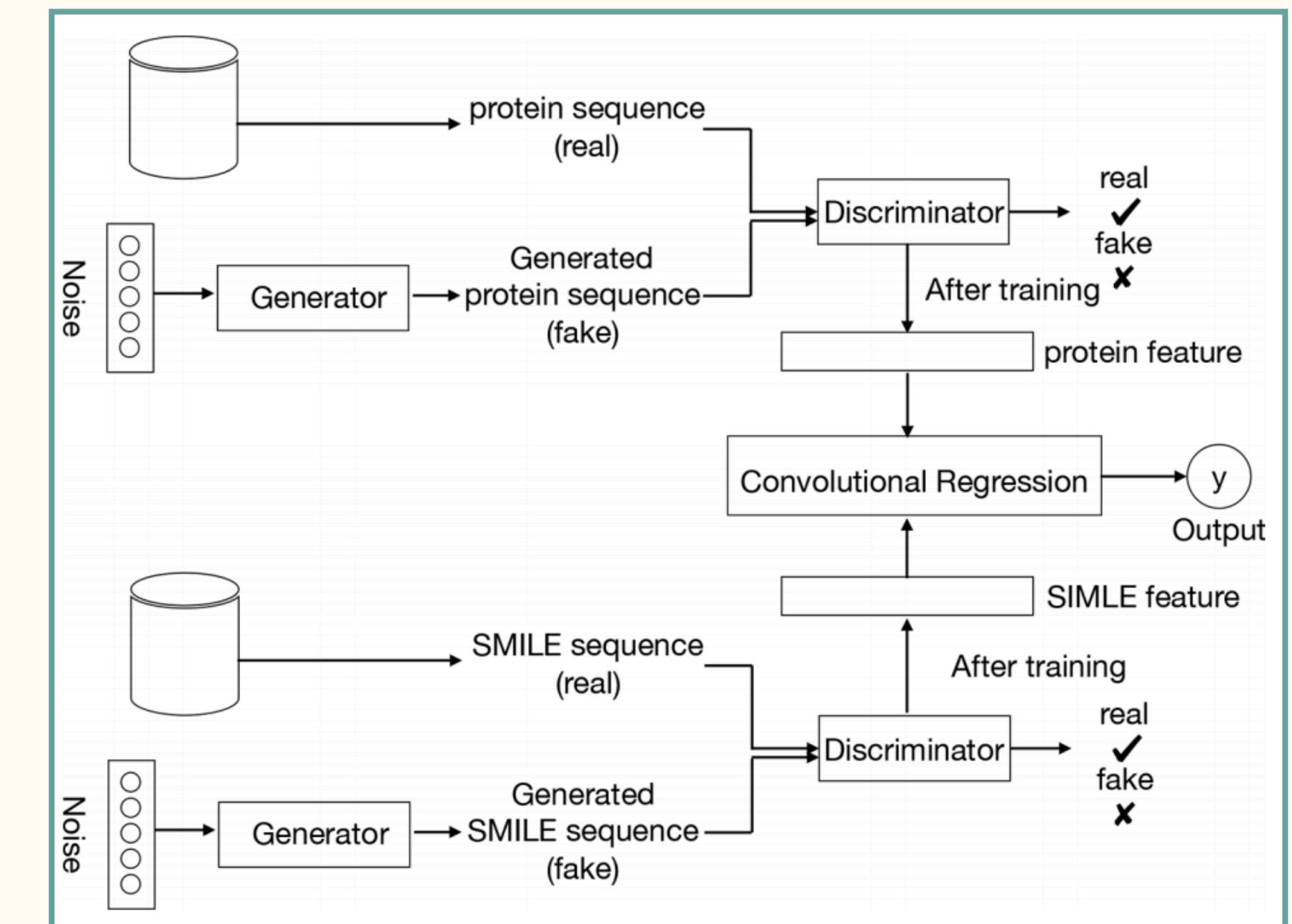
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4. Train a convolutional regression based on this feature



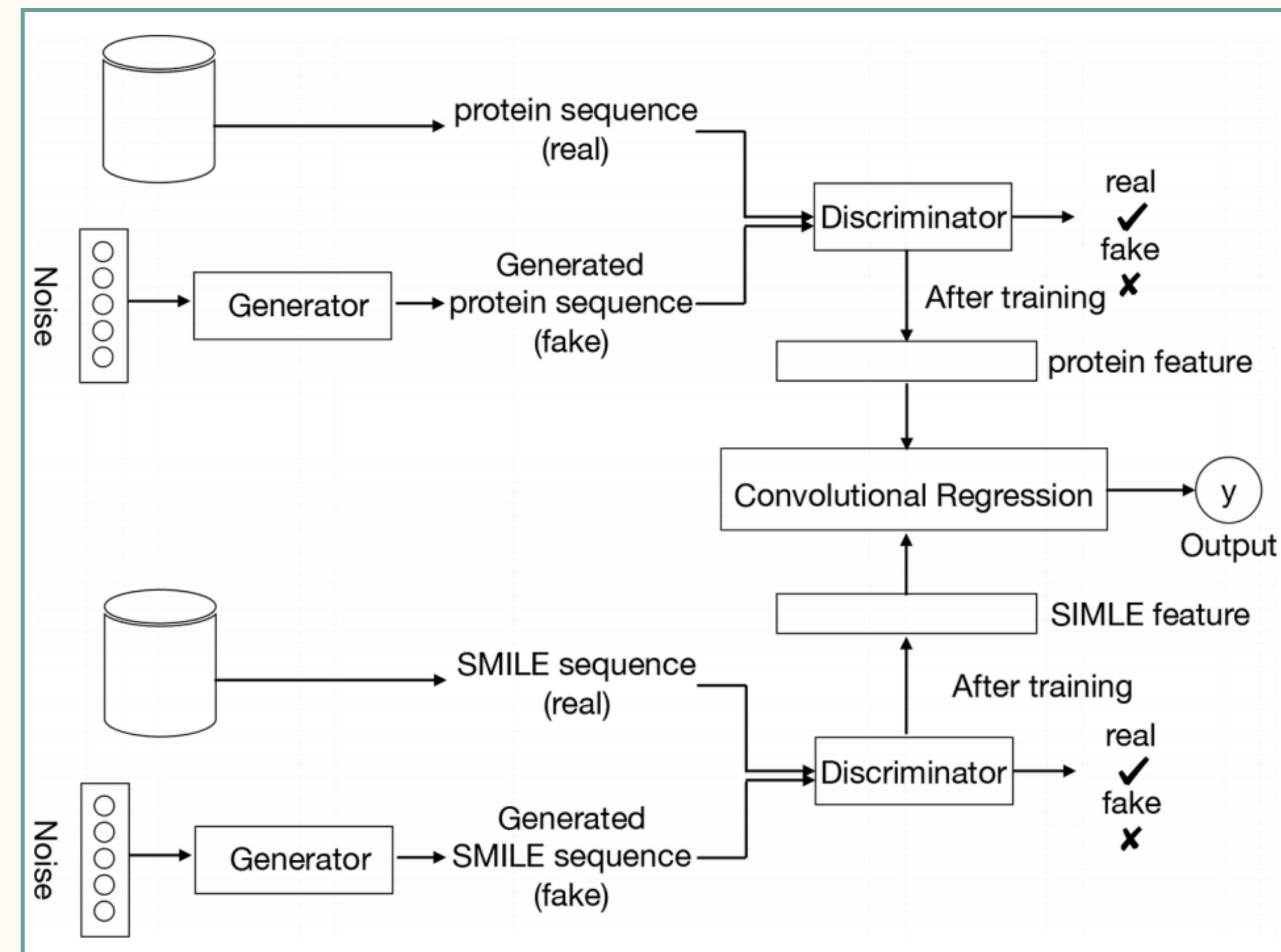
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4. Train a convolutional regression based on this feature
  - ▶ Predict the DT binding affinity



# Application: Predicting Drug-Target Binding Affinity

Pipeline:



# Future Work

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- Remember the progress !

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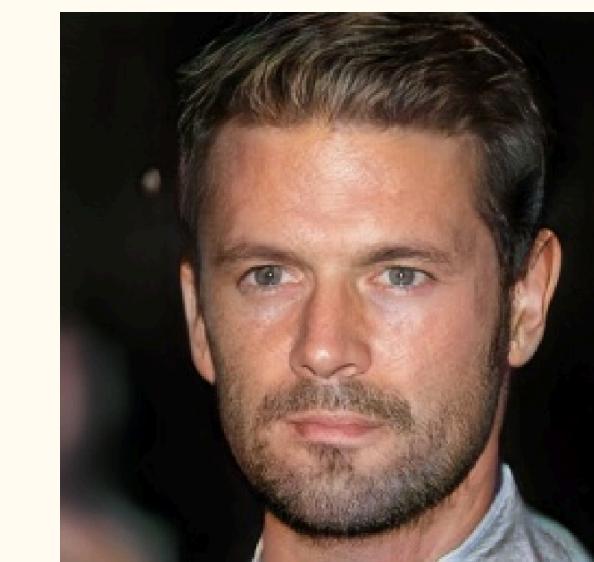
2014



2015



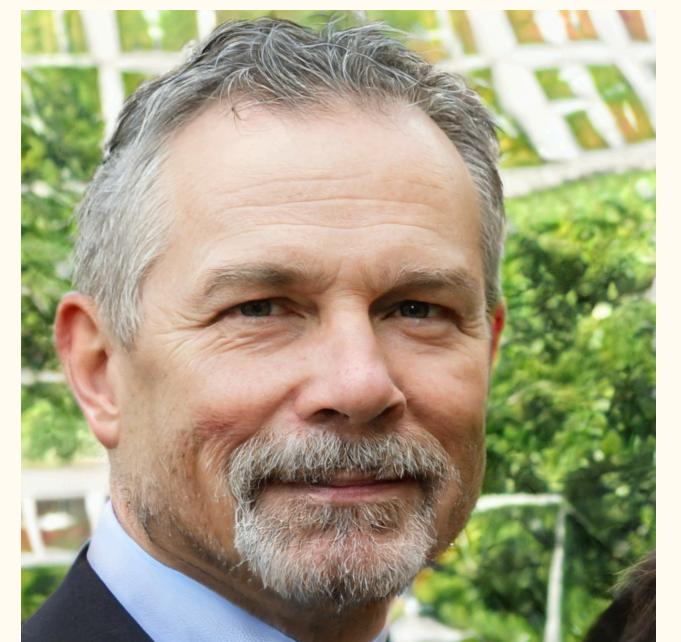
2016



2017



2018



2019

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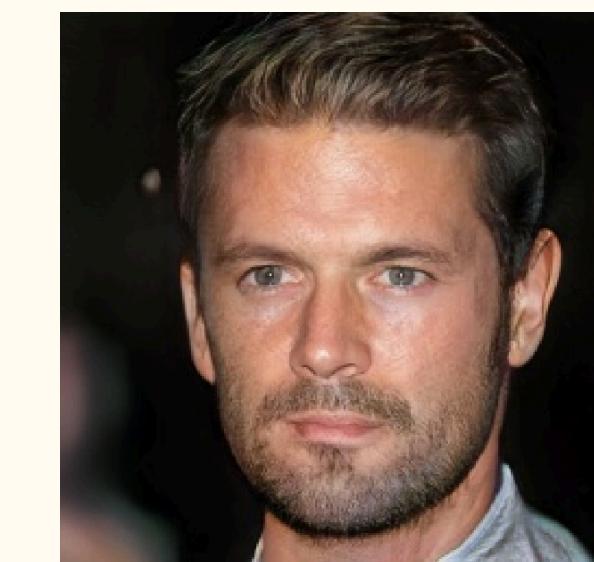
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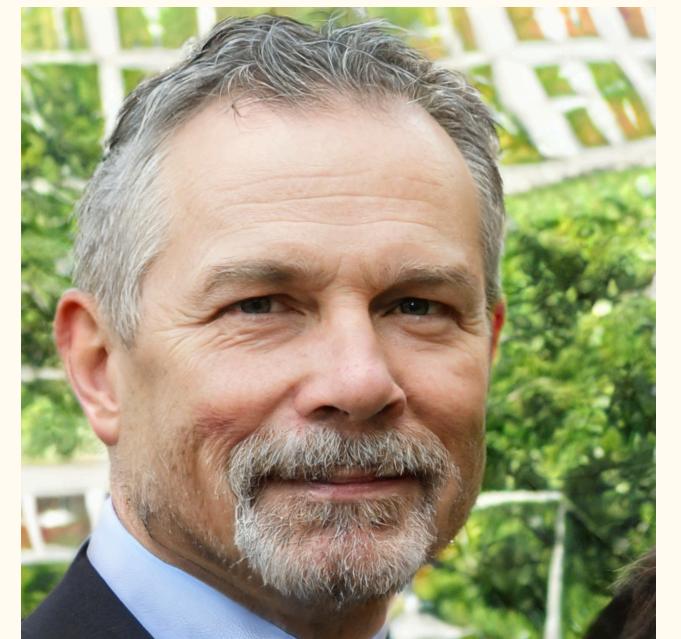
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- Next: generative videos



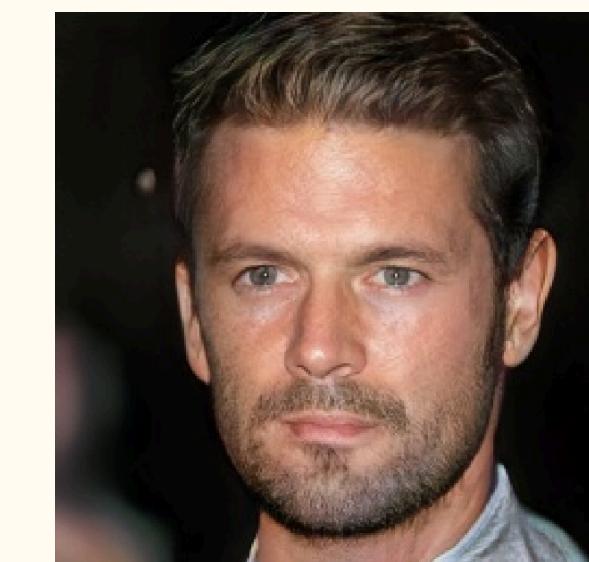
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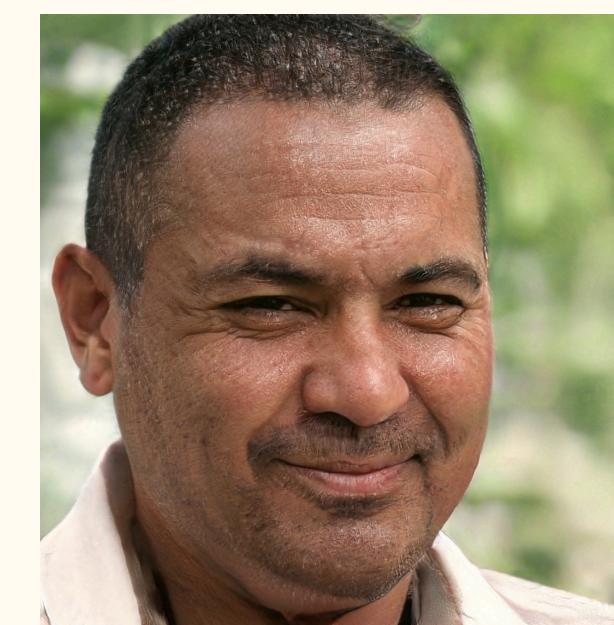
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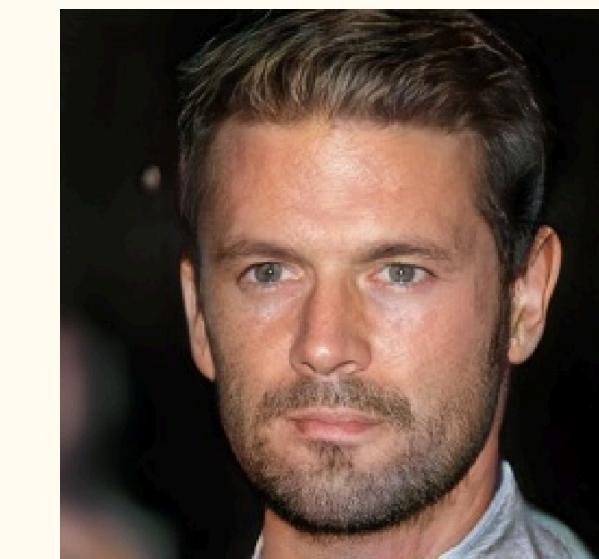
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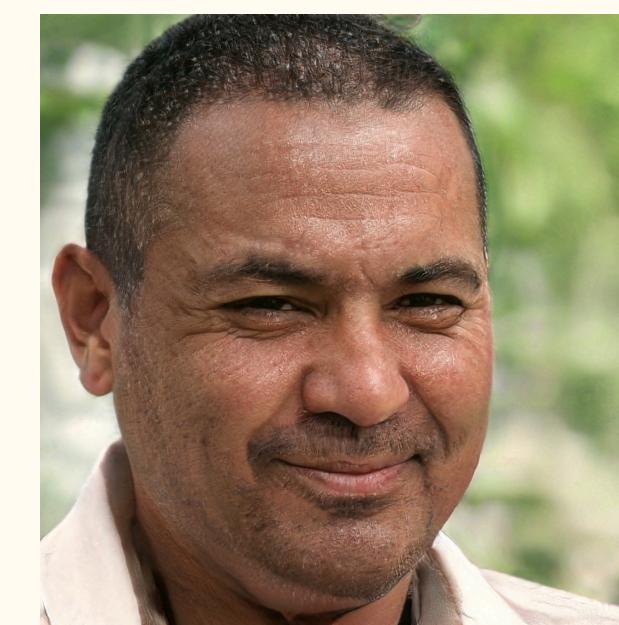
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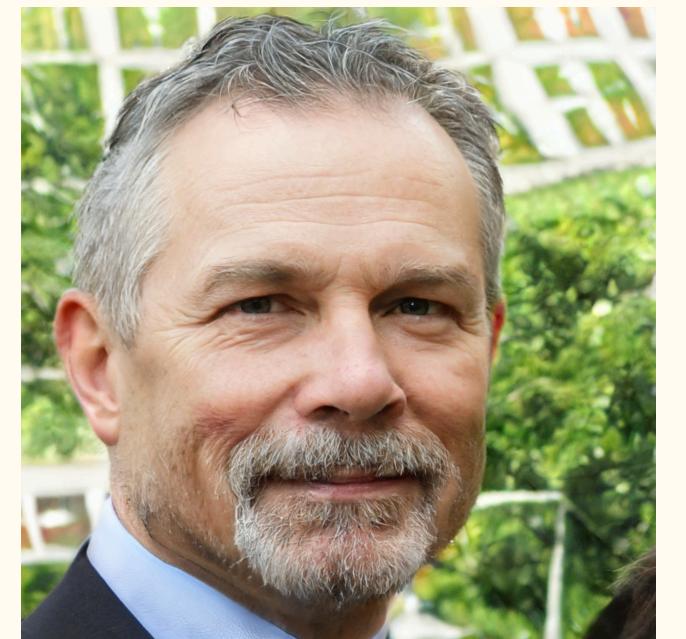
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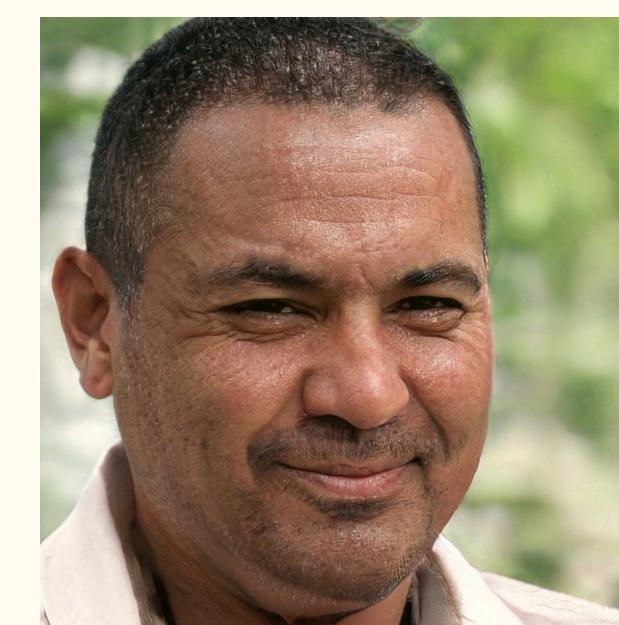
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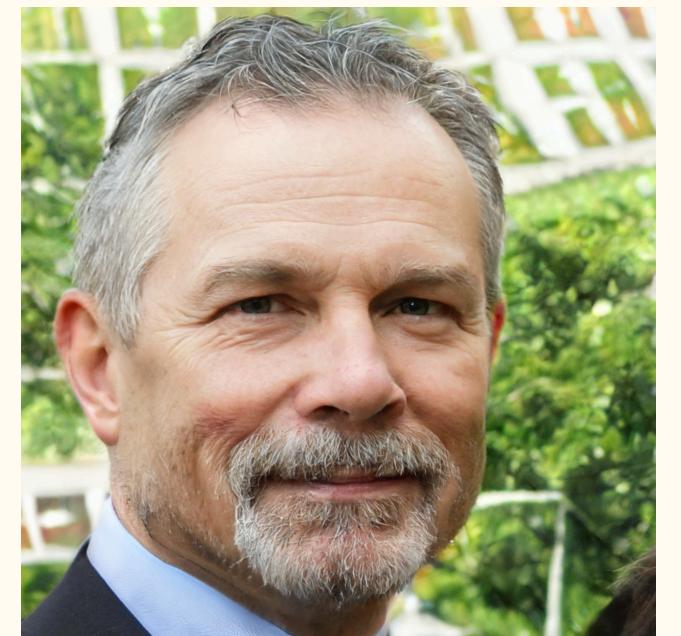
2016



2017



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  - ▶ Deepfakes ?
- Evolving quickly



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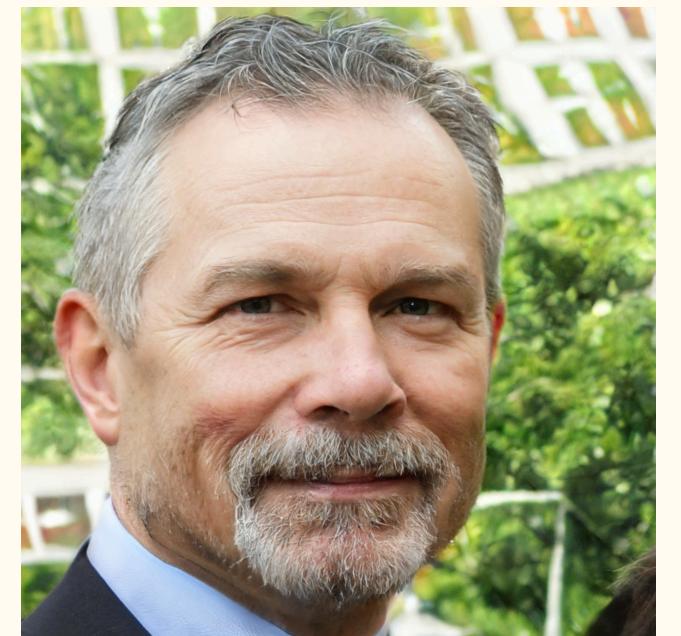
2016



2017



2018



2019

# Thank you !



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Ackruti Trade Center, MIDC, Mumbai, IND



[www.acubeit.com](http://www.acubeit.com)



+91 9892512129



[prakash@acubeit.com](mailto:prakash@acubeit.com)