Session 6: Deep Generative Models: VAEs and GANs

Matthew Willetts and Alexander Camuto

Outline

Unsupervised learning

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Unsupervised learning

Autoencoders

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Autoencoders

Generative Adversarial Networks

Unsupervised learning

Unsupervised learning

Generic goal of unsupervised learning is to **find underlying structrure** in data. Specific goals include:

- clustering: group similar observations together;
- reducing the dimensionality for visualization;
- building a better representation of data for a downstream supervised task;
- learning a likelihood function, e.g. to detect anomalies;
- generating new samples similar to past observations.

Unsupervised learning

For complex data (text, image, sound, ...), there is plenty of hidden latent structure we hope to capture:

- **Image data**: find low dimensional semantic representations, independent sources of variation;
- **Text data**: find fixed size, dense semantic representation of data.

Unsupervised learning

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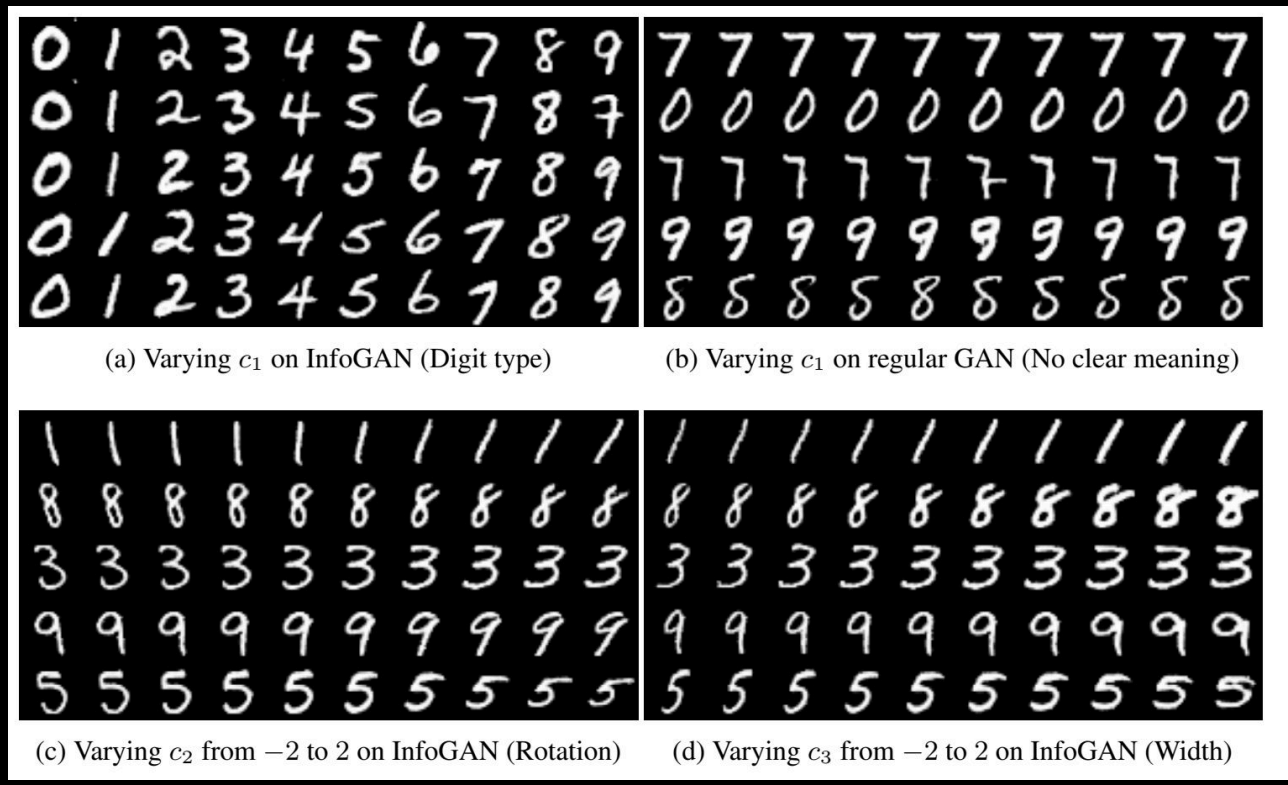
Latent space might be used to help build more efficient human labeling interfaces.

=> Goal: reduce labeling cost via active learning.

Graal of unsupervised learning

A low dimension space which captures all the **variations** of data and **disentangles** the different latent factors underlying the data.



(a) Varying c_1 on InfoGAN (Digit type)

(b) Varying c_1 on regular GAN (No clear meaning)

(c) Varying c_2 from -2 to 2 on InfoGAN (Rotation)

(d) Varying c_3 from -2 to 2 on InfoGAN (Width)

Chen, Xi, et al. Infogan: Interpretable representation learning by information maximizing generative adversarial nets. NIPS, 2016.

Self-supervised learning

find smart ways to **build supervision** without labels, exploiting domain knowledge and regularities

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Can we do the same for other domains?

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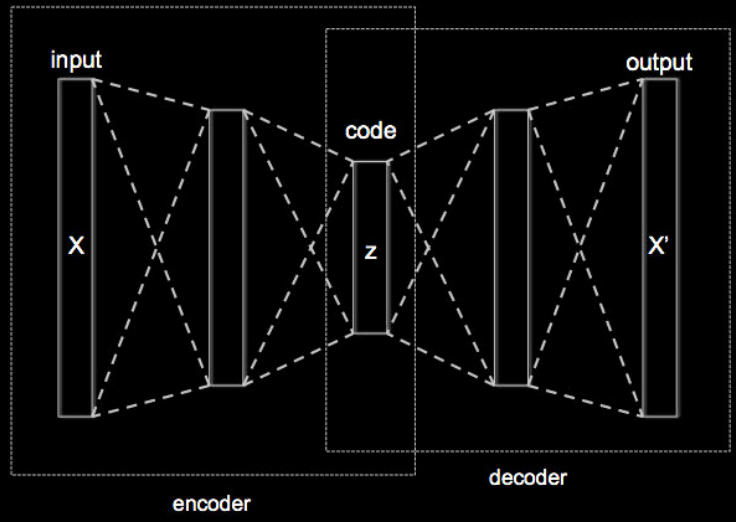
- **Image:** exploit spatial context of an object
- **Sound, video:** exploit temporal context

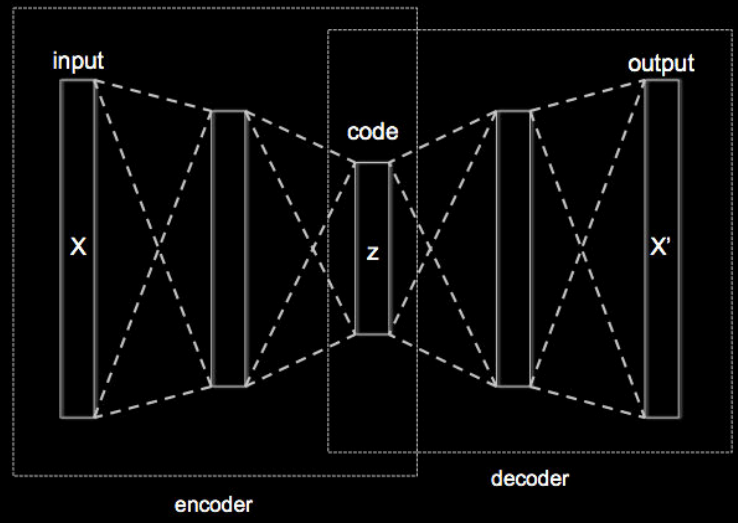
No direct **accuracy** measure: usually tested through a downstream task

Autoencoders

Autoencoder



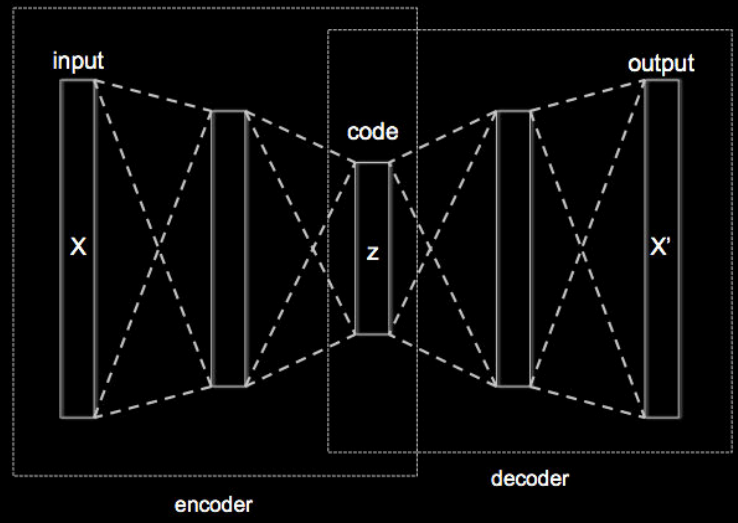
Autoencoder



Supervision : reconstruction loss of the input, usually:

$$l(x, f(x)) = ||f(x) - x||_2^2$$

Autoencoder



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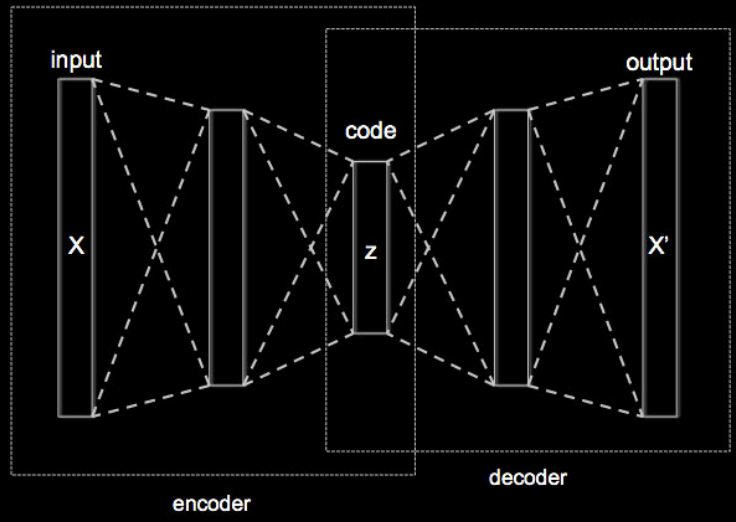
Binary crossentropy is also used

Autoencoder



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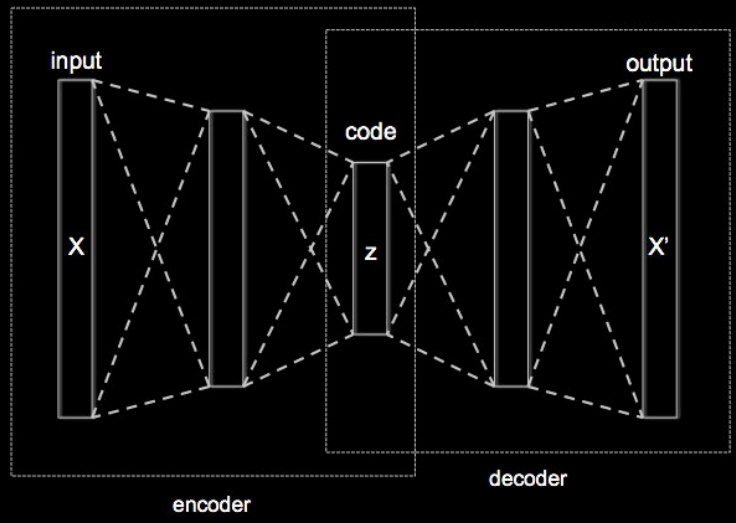

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Encoder and decoder can have arbitrary architecture (CNNs, RNNs...)

Sparse/Denoising Autoencoder

Adding a sparsity constraint on activations:

$$||encoder(x)||_1 \sim \rho, \rho = 0.05$$

Learns sparse features, easily interpretable

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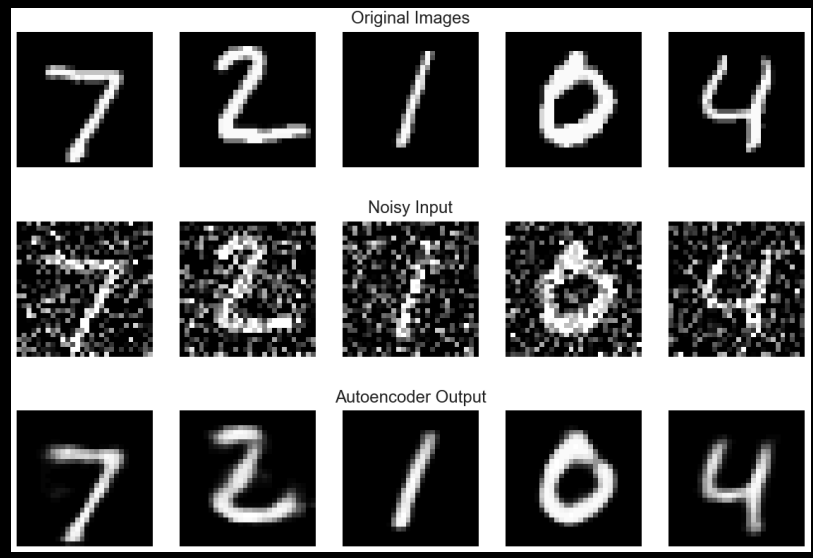
Denoising Autoencoder: train features for robustness to noise.



Uses and limitations

After **pre-training** use the latent code $\mathbf{z}$ as input to a classifier instead of $\mathbf{x}$

Semi-supervised learning simultaneous learning of the latent code (on a large, unlabeled dataset) and the classifier (on a smaller, labeled dataset)

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Limitations :

- Direct autoencoder fails to capture good representations for complex data such as images
- The generative model is usually of very poor quality (very blurry for images for instance)

Reality Check

For image features, **ImageNet pretraining** is still **much better** than unsupervised models

Pretraining Method	Supervision	Pretraining time	Classification	Detection	Segmentation
ImageNet [26]	1000 class labels	3 days	**78.2%**	**56.8%**	**48.0%**
Random Gaussian	initialization	< 1 minute	53.3%	43.4%	19.8%
Autoencoder	-	14 hours	53.8%	41.9%	25.2%
Agrawal *et al.* [1]	egomotion	10 hours	52.9%	41.8%	-
Doersh *et al.* [7]	context	4 weeks	55.3%	**46.6%**	-
Wang *et al.* [39]	motion	1 week	**58.4%**	44.0%	-
Ours	context	14 hours	56.5%	44.5%	**29.7%**

- Results shown after fine-tuned the network on **Pascal VOC dataset**
- The "ours" method is feature representation based on context inpainting

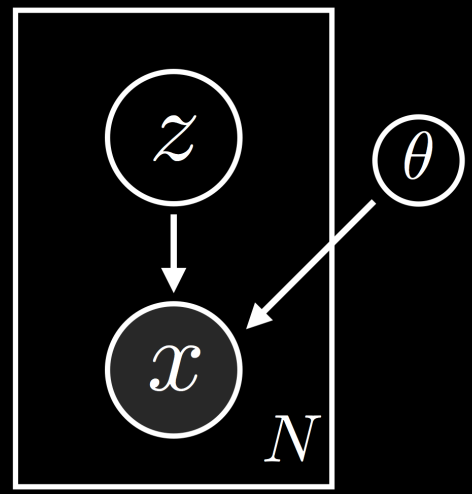
Pathak, Deepak, et al. Context encoders: Feature learning by inpainting. CVPR 2016.

Variational Autoencoders

Variational Autoencoders (VAE)

Assume the data samples $\mathbf{x}^{(i)}$ are generated by the model:

$$p_{\theta^*}(\mathbf{x}, \mathbf{z}) = p_{\theta^*}(\mathbf{z}) \cdot p_{\theta^*}(\mathbf{x}|\mathbf{z})$$



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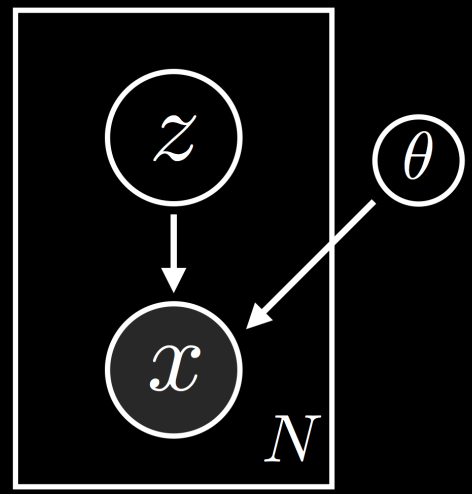

- $\mathbf{x}$ is an observed r.v. with values in $\mathbb{R}^n$;
- $\mathbf{z}$ is a latent r.v. with values in $\mathbb{R}^d$;

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- True continuous parameters $\boldsymbol{\theta}^*$ are unknown;
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But this high dimensional integral cannot be estimated efficently.

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But this high dimensional integral cannot be estimated efficently.

Auto-Encoding Variational Bayes, Diederik P Kingma, Max Welling

Variational Autoencoders (VAE) - Imp.

Imagine we try to estimate $p_\theta(\mathbf{x})$ by marginalising out $\mathbf{z}$:

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{z}) \cdot p_\theta(\mathbf{x}|\mathbf{z}) \, \mathrm{d}\mathbf{z} = \mathbb{E}_{p_\theta(\mathbf{z})} \, p_\theta(\mathbf{x}|\mathbf{z})$$

But instead introduce $\frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})}$ into the integral:

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{z}) \cdot p_\theta(\mathbf{x}|\mathbf{z}) \cdot \frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} \, \mathrm{d}\mathbf{z} = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \, \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

This is importance sampling - by picking a q distribution with continuous parameters ϕ that is well-peaked around high values of the joint distribution we can get an estimate of $p_\theta(\mathbf{x})$ with fewer samples.

Variational Autoencoders (VAE) - Imp.

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{z}) \cdot p_\theta(\mathbf{x}|\mathbf{z}) \cdot \frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} \, \mathrm{d}\mathbf{z} = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

Can we bound this? Yes, apply Jensen's Inequality:

$$\mathbb{E}\, f(x) \geq f(\mathbb{E}\, x)$$

where $f(\cdot) = -\log(\cdot)$:

$$-\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \geq -\log \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} = -\log p_\theta(\mathbf{x})$$

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

Variational Autoencoders (VAE) - Imp.

Expand this out

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) + \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log \frac{p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) - \mathrm{D}_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}))$$

$$\log p_\theta(\mathbf{x}) \geq \mathcal{L}(x)$$

$$\mathcal{L}(x) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) - \mathrm{D}_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}))$$

We call $\mathcal{L}(x)$ the Evidence Lower Bound, because it is. If we now take gradients wrt θ, ϕ we will be increasing the lower bound of the evidence of our model.

First though, another view:

Variational Autoencoders (VAE) - KL

We wish we had the true posterior $p_\theta(\mathbf{z}|\mathbf{x})$ but that's really hard. We'd have to divide the joint by the marginal, we don't have that.

Instead, introduce a family of approximate (variational) posteriors on the latent variable: $q_\phi(\mathbf{z}|\mathbf{x})$ with continuous parameters ϕ:

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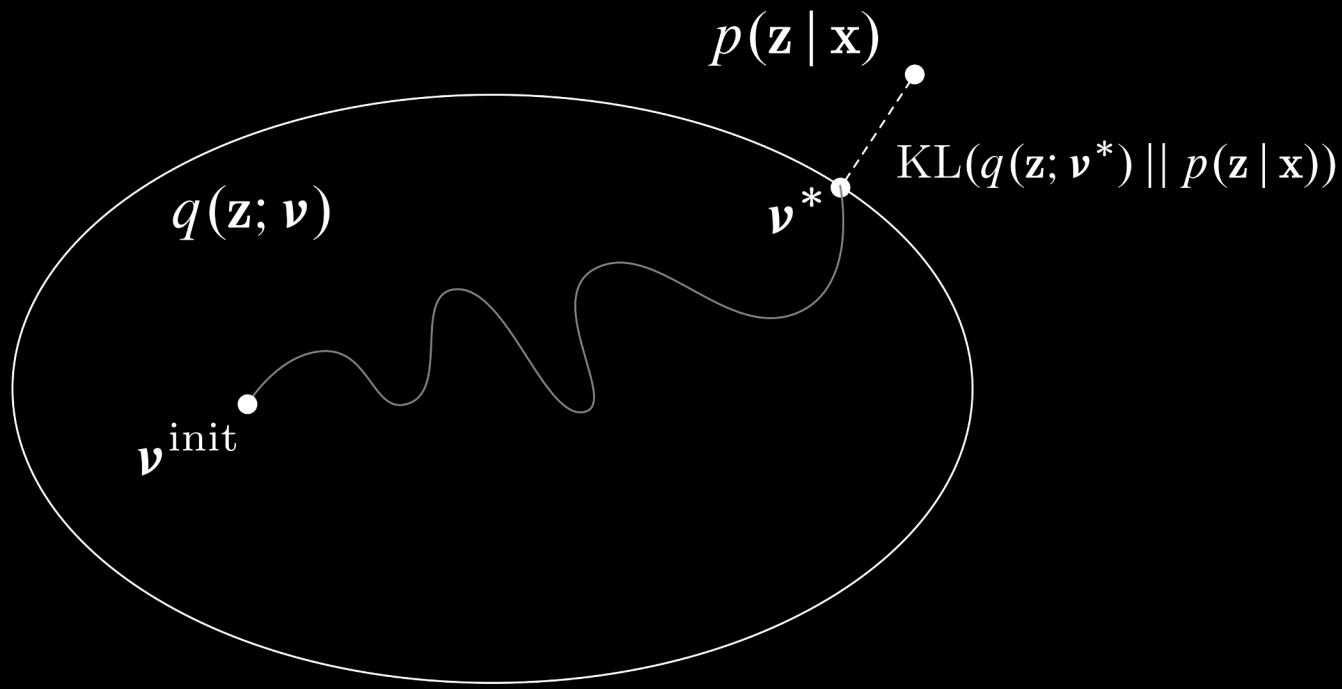
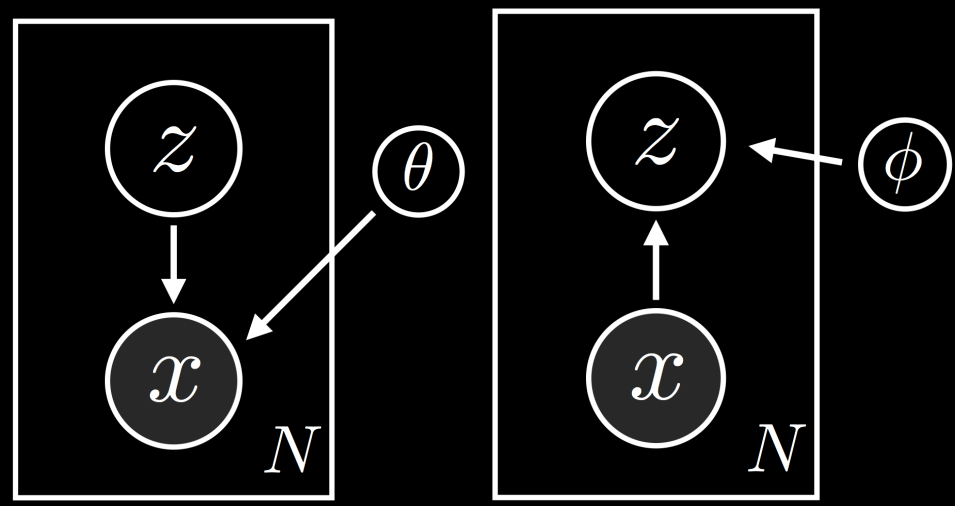


Variational Autoencoders (VAE) - KL



Variational Autoencoders (VAE) - KL

We want to find the nearest member of this family $q_\phi(\mathbf{z}|\mathbf{x})$ to the true posterior in KL terms. We want to minimise:

$$\mathrm{D}_{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})] = -\int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})}\, \mathrm{d}\mathbf{z}$$

$$= -\int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\, \mathrm{d}\mathbf{z} + \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})}\, \mathrm{d}\mathbf{z}$$

$$= -\mathcal{L}(x) + p_\theta(\mathbf{x})$$

Now we have found the gap from applying Jensen's inequality - rearrange:

$$p_\theta(\mathbf{x}) = \mathcal{L}(x) + \mathrm{D}_{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})]$$

LHS: no dep. on $q_\phi(\mathbf{z}|\mathbf{x})$, so max $\mathcal{L}(x) \rightarrow$ min $\mathrm{D}_{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})]$ wrt ϕ.

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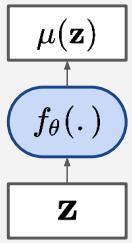
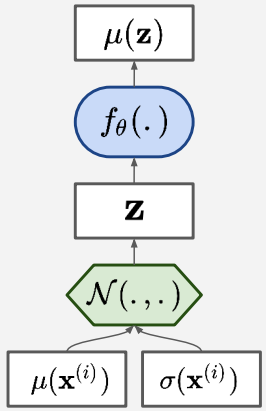
- Reparametrization trick:

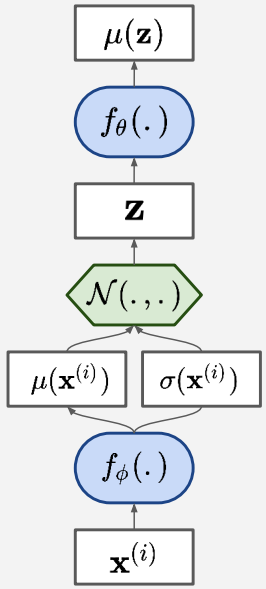
$$\mathbf{z} = \mu_\phi(\mathbf{x}^{(i)}) + \sigma_\phi(\mathbf{x}^{(i)}) \cdot \epsilon \quad \text{with} \quad \epsilon \sim \mathcal{N}(0, 1)$$



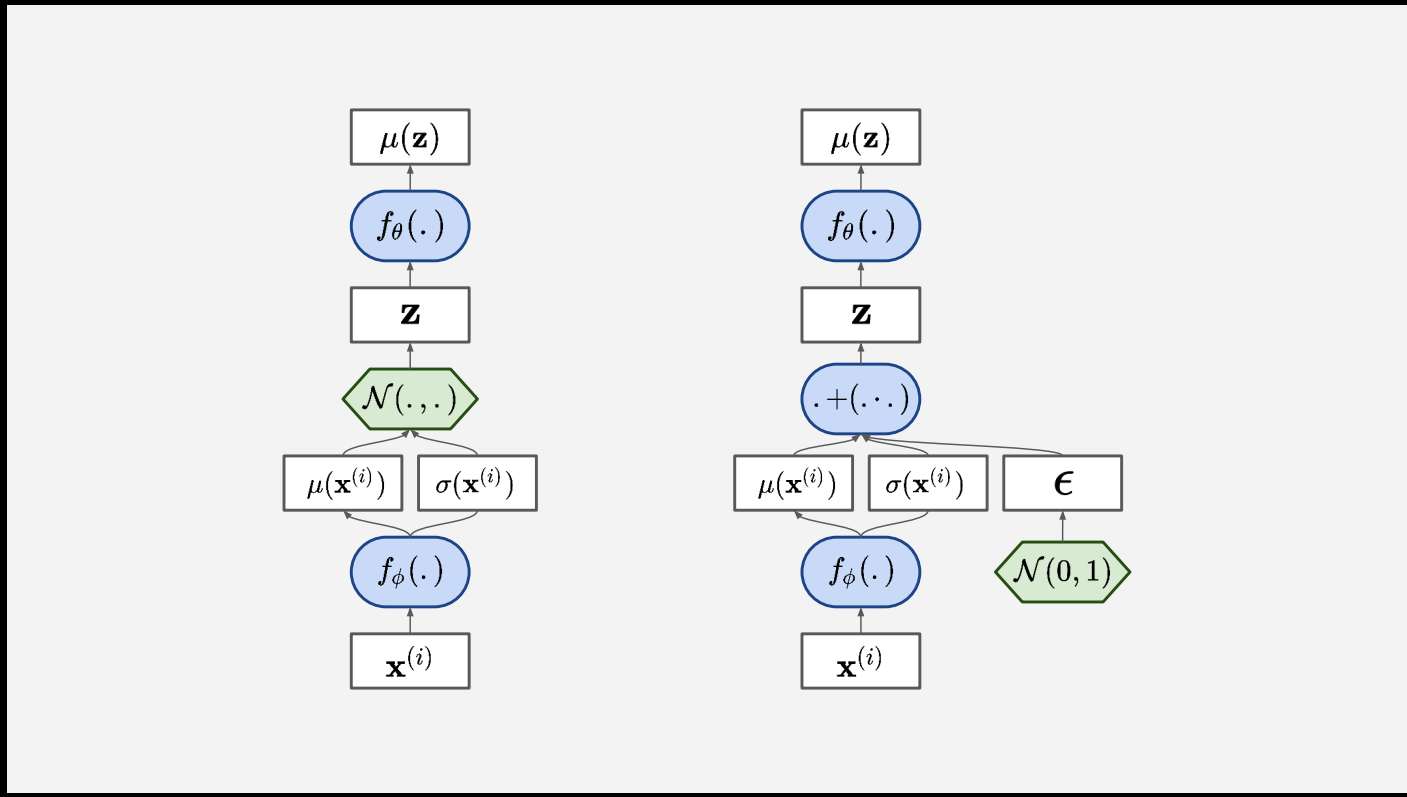
The **decoder** f_θ defines the likelihood of data.



The latent variable $\mathbf{z}$ is stochastic.



The **encoder** f_ϕ defines an approximate posterior on $\mathbf{z}$.



The reparametrization makes the objective differentiable wrt. θ & ϕ.

Conv/deconv VAEs

conv/deconv VAE trained by Alec Radford in 2015 on Labeled Faces in the Wild (LFW) dataset, 2h on single GTX 980

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Remarks

- Similar to Denoising AE but noise added to hidden layer;
- Motivated by a well-defined probablistic model of the generative process;
- Quite easy to train in practice.

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Limitations

- Is the continuous parametrization of posterior latent distribution too restrictive?
- Would a discrete latent variable make more sense?
- Gaussian parametrization of the decoder output results in blurry images.

Discrete latent variables VAE

Gumbel-Softmax / Concrete distribution VAEs

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- Trains ok but no ground breaking applications so far.

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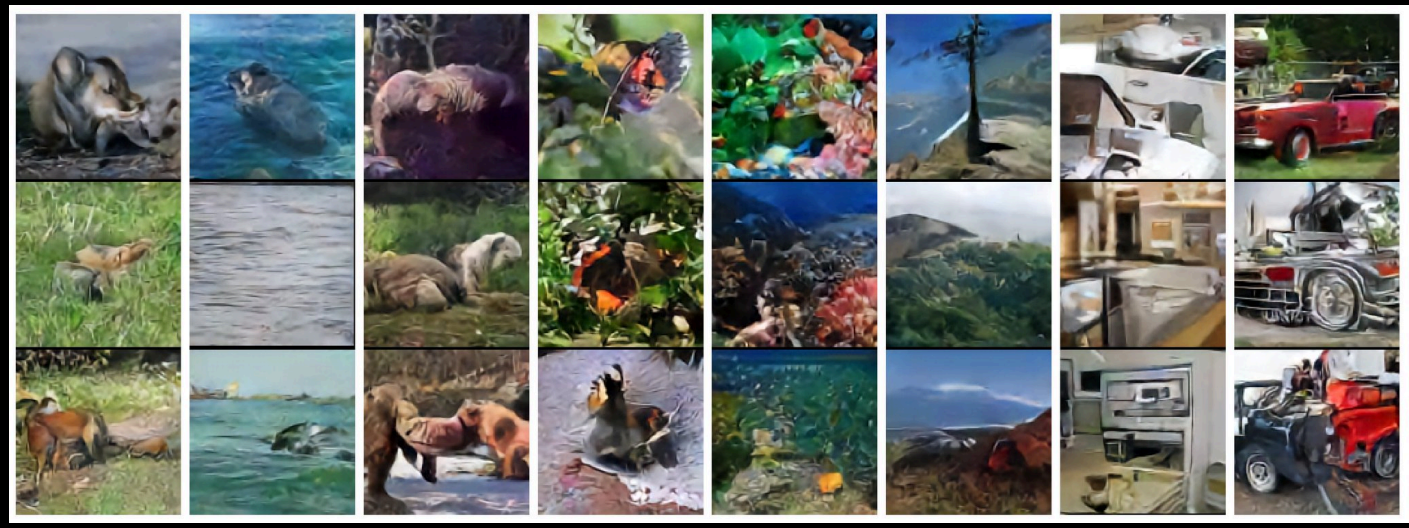
VQ-VAE

- $\mathbf{z}$ is a vector indexed in a trainable embedding matrix.
- Select $\mathbf{z}$ as embedding vector closest to encoder output.
- Approximate backprop via "gradient-copy" trick.
- Very expressive model, especially when combined with strong decoders and priors.

VQ-VAE imagenet results

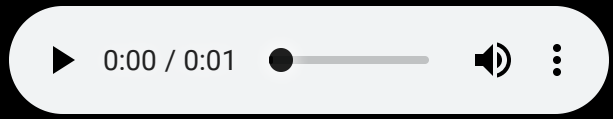


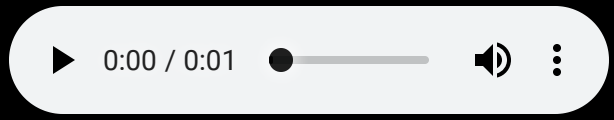
Neural Discrete Representation Learning Aaron van den Oord, Oriol Vinyals, Koray Kavukcuoglu

VQ-VAE speech results

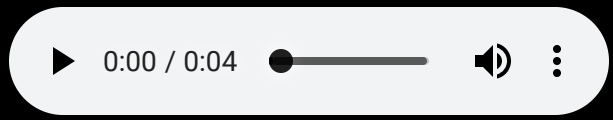
Speech synth demo: https://avdnoord.github.io/homepage/vqvae/

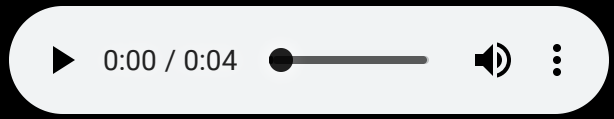
Example reconstruction:

- Original: 

- Reconstructed: 

Reconstruction conditionned on different speaker id:

- Original: 

- Reconstructed: 

Disentangled VAEs

Isolating Sources of Disentanglement in VAEs Ricky T. Q. Chen, Xuechen Li, Roger Grosse, David Duvenaud

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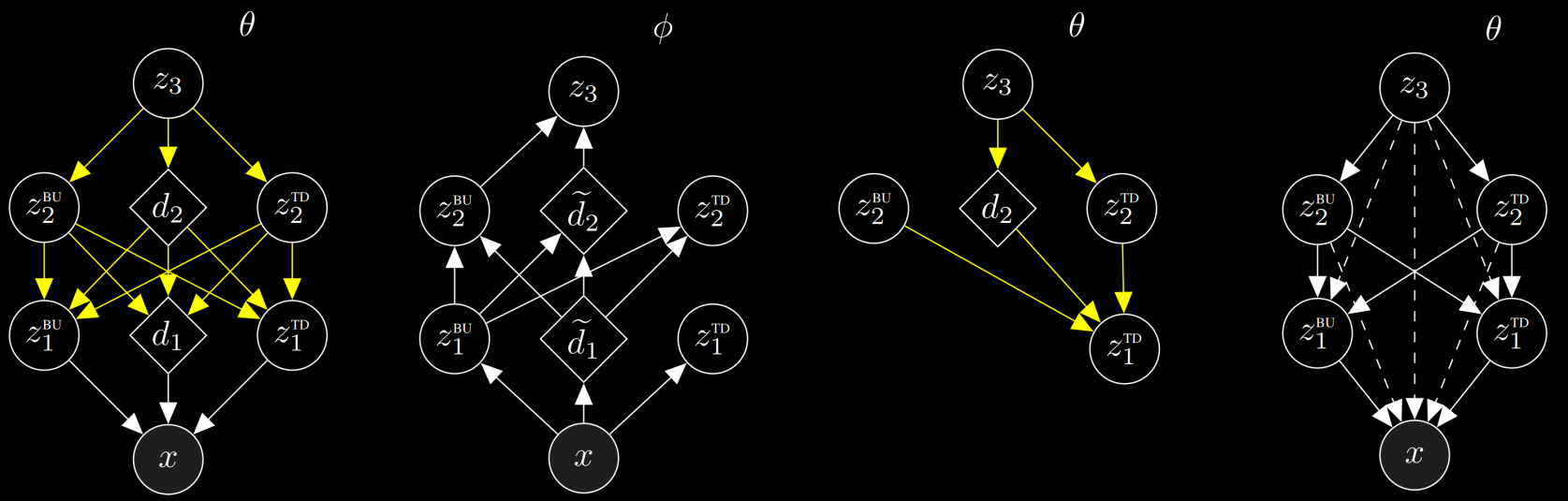
BIVA: Bidirectional-Inference VAE

Lots of changes from 'Vanilla' VAE



BIVA: Bidirectional-Inference VAE

Graphically:

- Hierarchy of $\mathbf{z}$ layers:

$$q_\phi(\mathbf{z}|x) = q_\phi(\mathbf{z}^{\text{TD}}, \mathbf{z}^{\text{BU}}|x)$$
$$= q_\phi(z_L|x, z^{\text{BU}}_{<L}) \prod_{i=1}^{L-1} q_\phi(z_i^{\text{BU}}|x, z^{\text{BU}}_{<i}) q_{\phi,\theta}(z_i^{\text{TD}}|x, z^{\text{BU}}_{\neq i}, z^{TD}_{>i})$$

$$p_\theta(x, \mathbf{z}) = p_\theta(x|\mathbf{z}) p_\theta(z_L) p_\theta(\mathbf{z}^{\text{BU}}, \mathbf{z}^{\text{TD}})$$
$$= p_\theta(x|\mathbf{z}) p_\theta(z_L) \prod_{i=1}^{L-1} p_\theta(z_i^{\text{BU}}|z_{>i}) p_\theta(z_i^{\text{TD}}|z_{>i})$$
$$\text{where} \quad z_i = [z_i^{\text{BU}}, z_i^{\text{TD}}]$$

BIVA: Bidirectional-Inference VAE

Samples:

(c) $\sigma^2 = 0.5$ (d) $\sigma^2 = 1.0$

Generative Adversarial Networks

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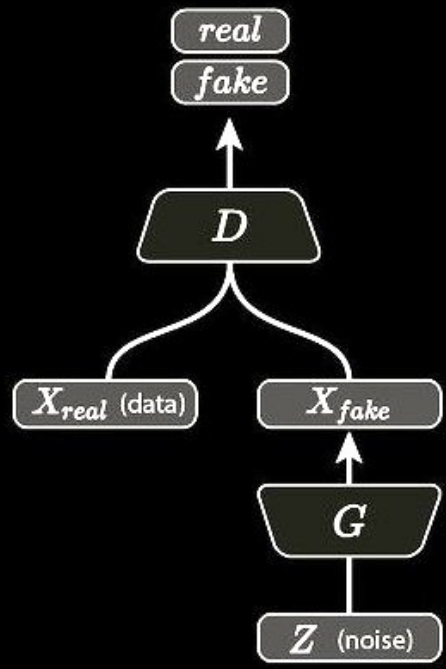

Alternate training of a **generative network** G and a **discrimininative network** D

Goodfellow, Ian, et al. Generative adversarial nets. NIPS 2014.

GANs

- D tries to find out which example are generated or real
- G tries to fool D into thinking its generated examples are real

GANs

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- G tries to fool D into thinking its generated examples are real

Sample real data $\boldsymbol{x} \sim \boldsymbol{p}_{data}$

$$\min_G \max_D V(D,G) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log D(x)] + \mathbb{E}_{z \sim p_z(z)}[\log(1 - D(G(z)))]$$

$$D(x) \in [0,1] \rightarrow 1$$

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$$D(G(z)) \in [0,1] \rightarrow 0$$

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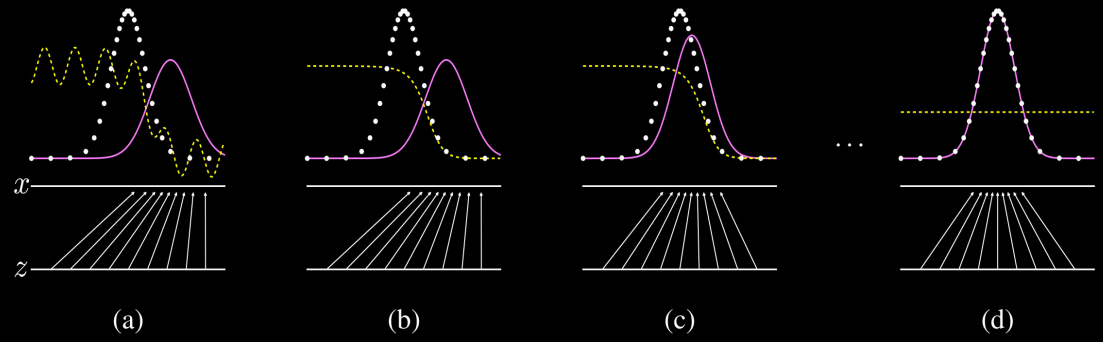
GANs

1D-example



- optimal: $D = \frac{1}{2}$, $G(\mathbf{z}) = p_{data}$

GANs

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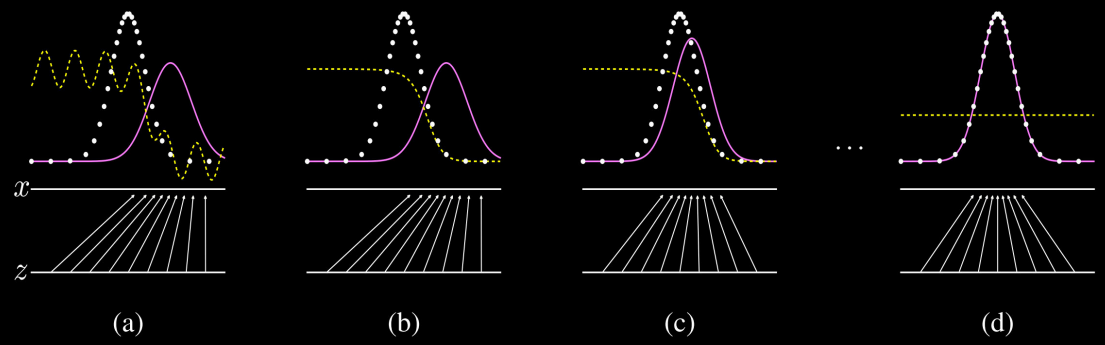

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GANs

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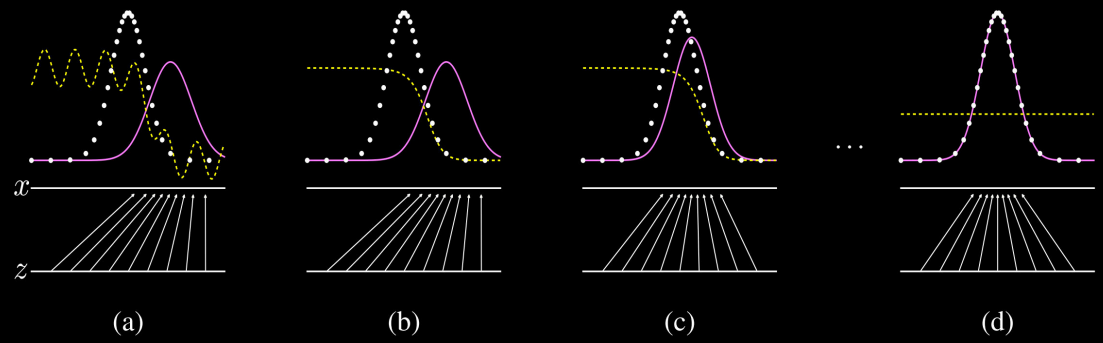
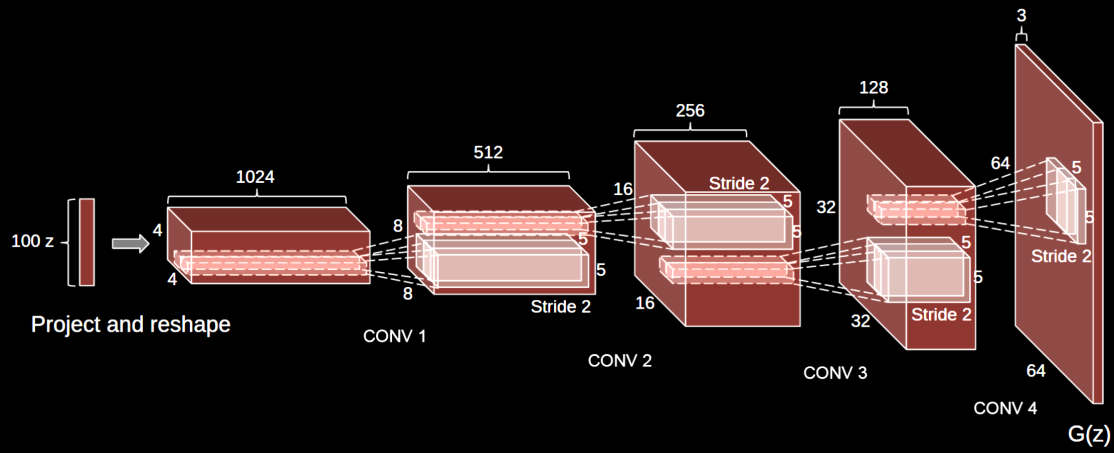


- optimal: $D = \frac{1}{2}$, $G(\mathbf{z}) = p_{data}$
- G never "sees" training data, it is solely updated from gradients coming from D
- Naive Keras implementation:

```
d_loss = K.mean(-K.log(Dx) - K.log(1 - DGz))
g_loss = K.mean(K.log(1 - DGz))
```

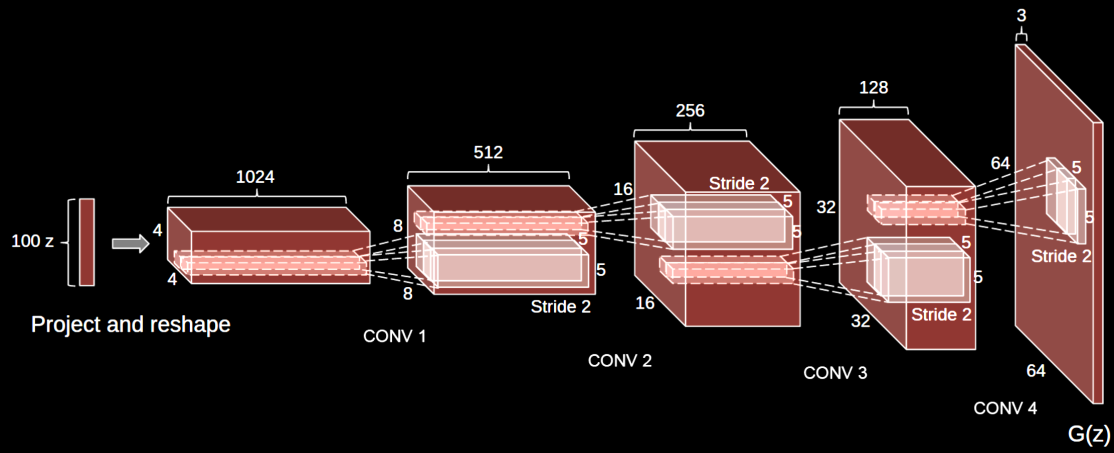
DC-GAN



- GANs training is unstable, and may suffer from **mode collapse**

Radford, Alec, Luke Metz, and Soumith Chintala. Unsupervised representation learning with deep convolutional generative adversarial networks. 2015.

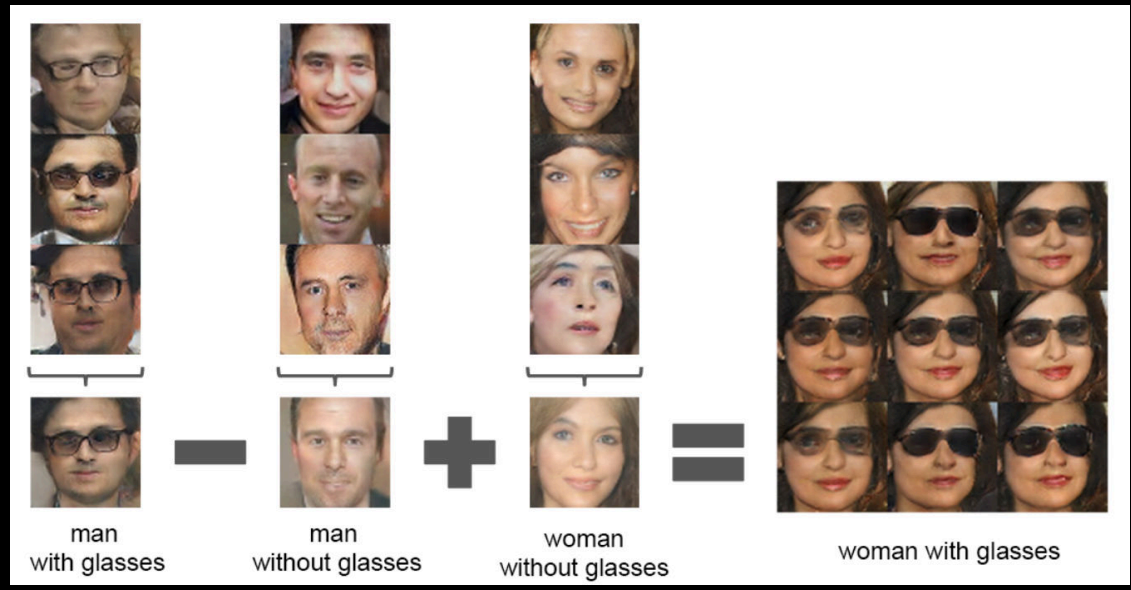
DC-GAN



- GANs training is unstable, and may suffer from **mode collapse**
- **Sensitive hyperparameters:** Use of batchnorm, strided convolutions, careful learning rates, several D updates per G updates...

Radford, Alec, Luke Metz, and Soumith Chintala. Unsupervised representation learning with deep convolutional generative adversarial networks. 2015.

DC-GAN



- Generator generates less-blurry images than VAEs

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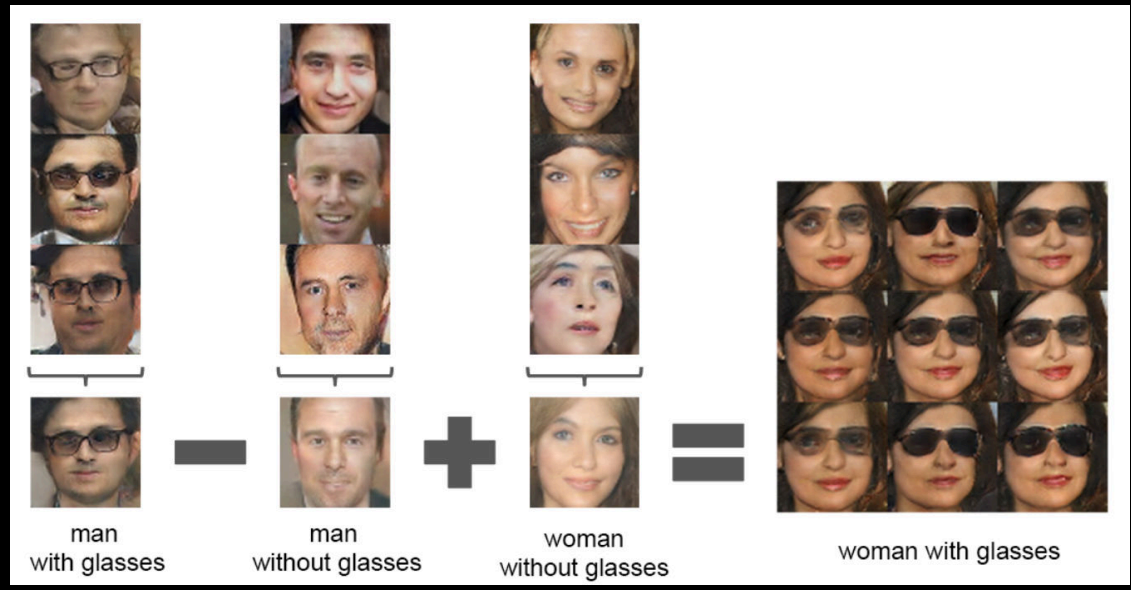
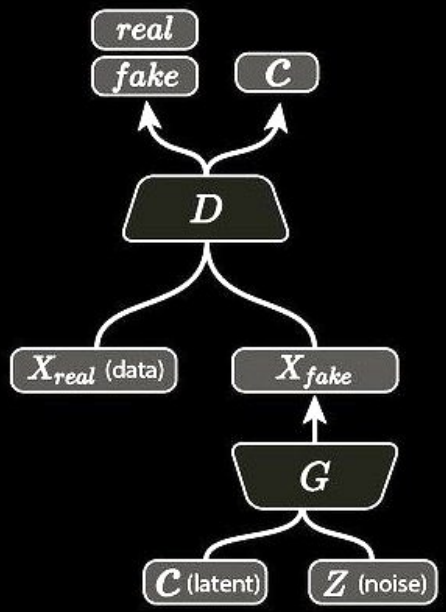


- Generator generates less-blurry images than VAEs
- Latent space has some local linar properties (vector arithmetic like with Word2Vec)

Radford, Alec, Luke Metz, and Soumith Chintala. Unsupervised representation learning with deep convolutional generative adversarial networks. 2015.

Info GAN



Chen, Xi, et al. Infogan: Interpretable representation learning by information maximizing generative adversarial nets. NIPS, 2016.

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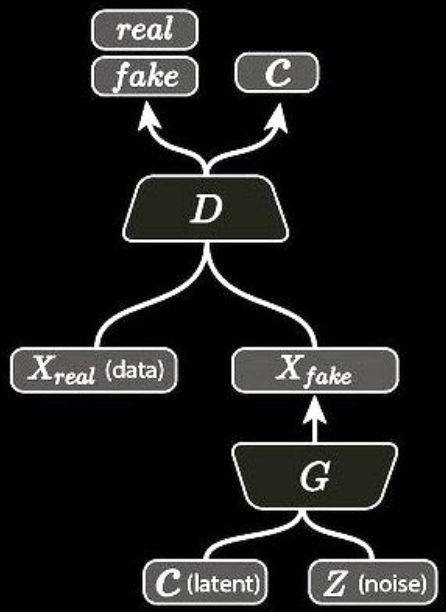

Separate noise $\mathbf{Z}$ and latent variables $\mathbf{C}$ and maximizes the mutual information between c the and the observation $G(z, c)$

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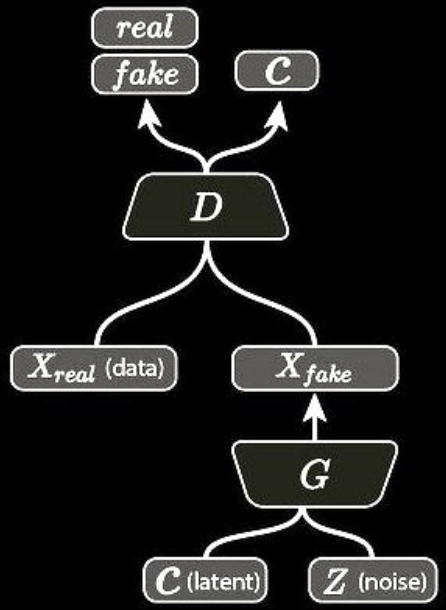

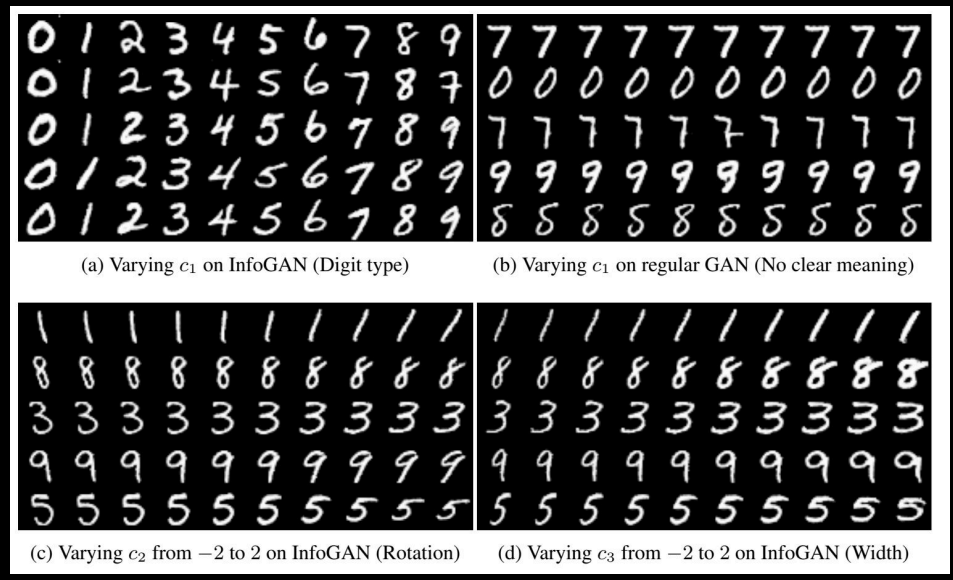

(a) Varying c_1 on InfoGAN (Digit type)

(b) Varying c_1 on regular GAN (No clear meaning)

(c) Varying c_2 from -2 to 2 on InfoGAN (Rotation)

(d) Varying c_3 from -2 to 2 on InfoGAN (Width)

Separate noise $\mathbf{Z}$ and latent variables $\mathbf{C}$ and maximizes the mutual information between c the and the observation $G(z, c)$

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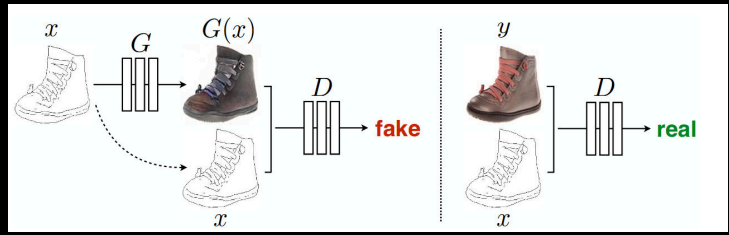
Progressive growing of GANs

All images are generated by walking through the latent space

Karras, Tero, et al. Progressive growing of gans for improved quality, stability, and variation. 2017.

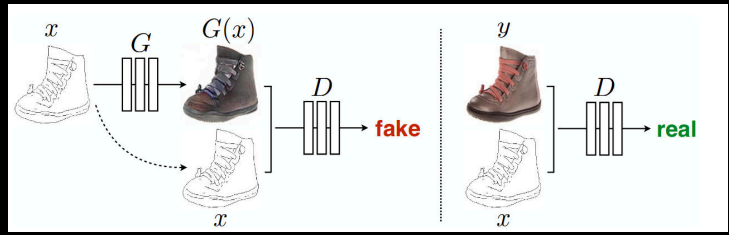
Pix2pix: Conditional GANs



The generation no longer makes use of $\mathbf{z}$, rather is conditionned by an input $\mathbf{x}$

Isola, Phillip et al. Image-to-Image Translation with Conditional Adversarial Networks, CVPR 2017

Pix2pix: Conditional GANs



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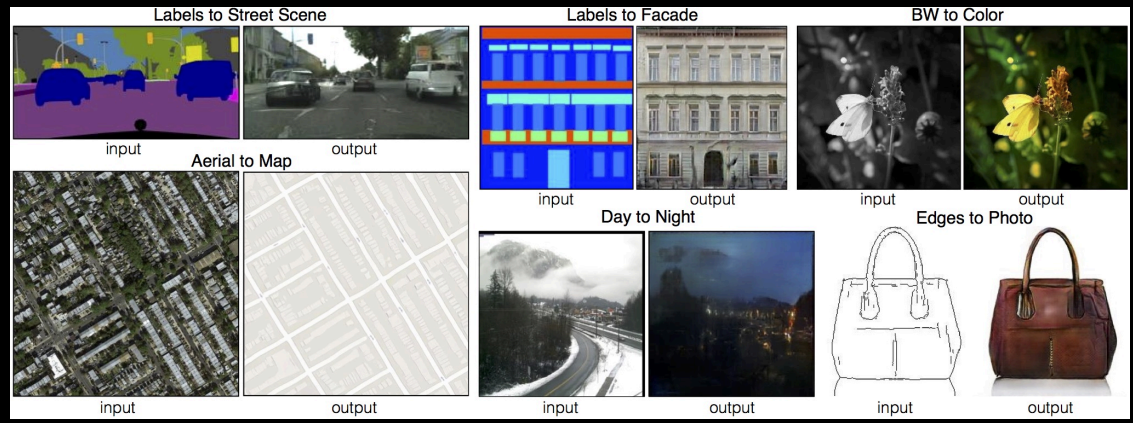

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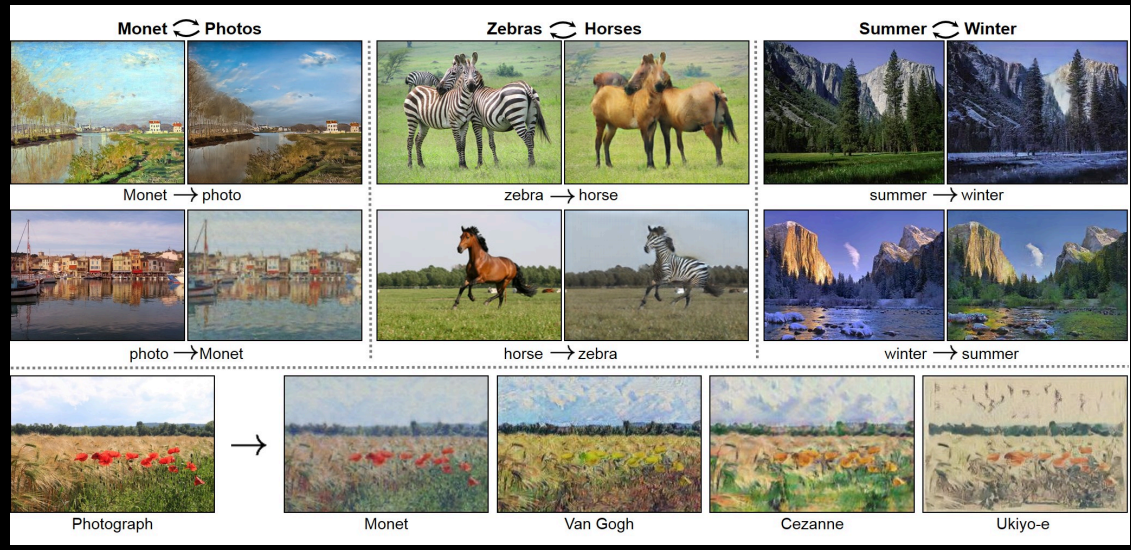
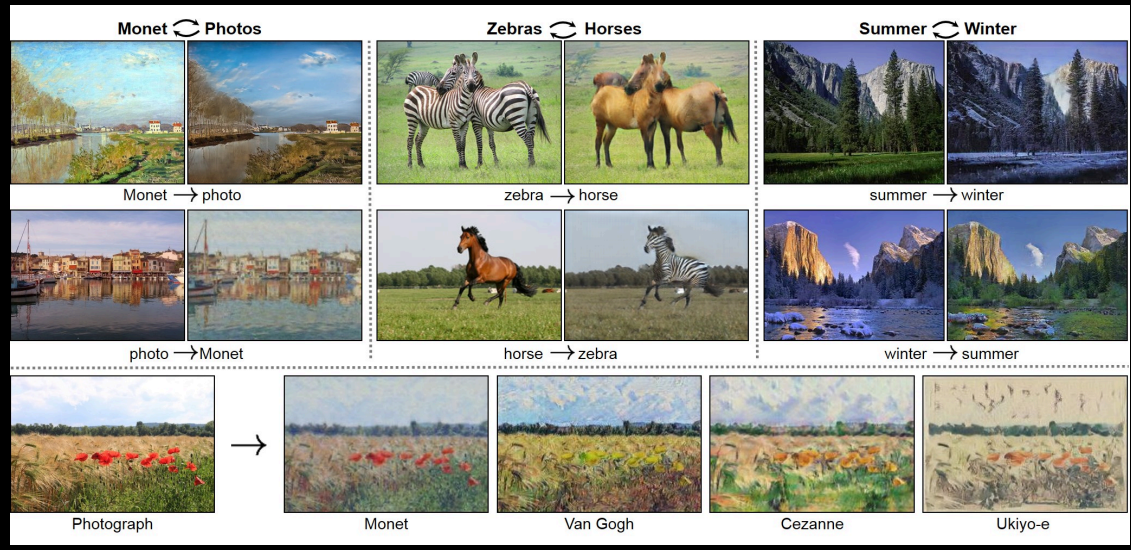
Cycle GANs



Jun-Yan Zhu et al. Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks, ICCV 2017

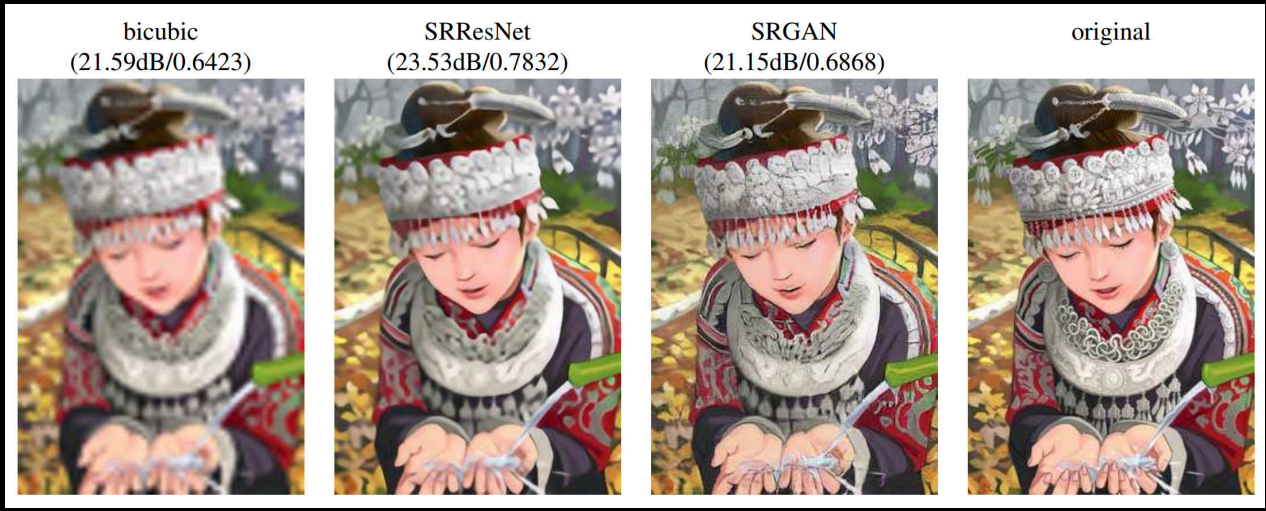
Cycle GANs



- No alignment between pairs needed, simply two different sets of images

Jun-Yan Zhu et al. Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks, ICCV 2017

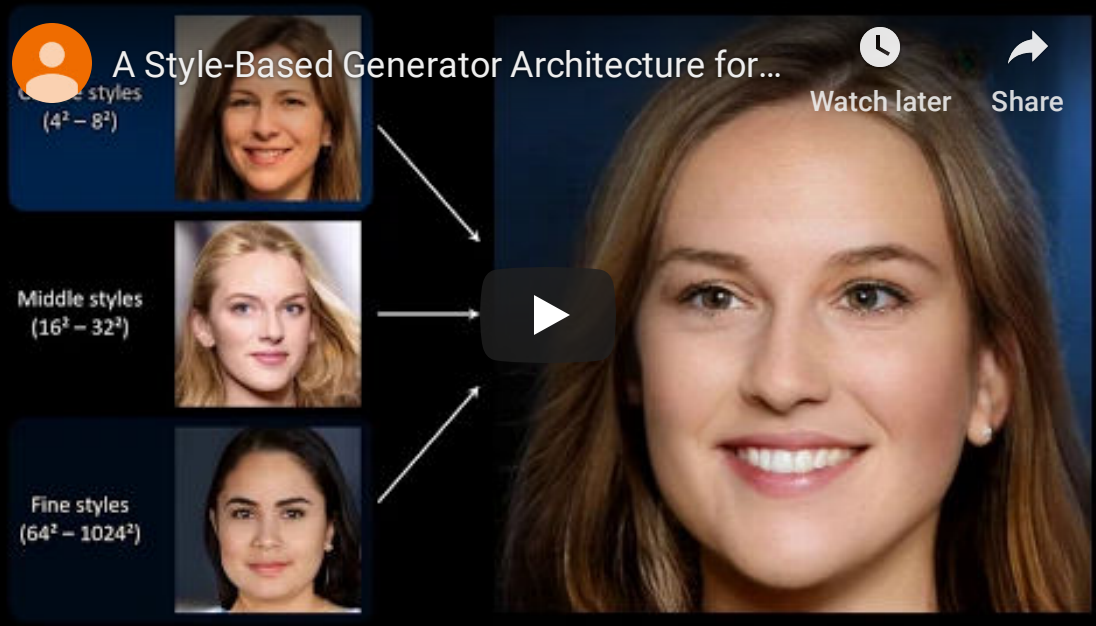
Super Resolution



"Perceptual" loss = combining pixel-wise loss mse-like loss with GAN loss

Ledig, Christian, et al. Photo-realistic single image super-resolution using a generative adversarial network. CVPR 2016.

Style GANs



A Style-Based Generator Architecture for Generative Adversarial Networks by Tero Karras, Samuli Laine, Timo Aila, 2018 (preprint)

Takeaways

(Reconstruction) Autoencoders

- have no direct probabilistic interpretation;
- are not designed to generate useful samples;
- encoder defines a useful latent representation.

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(Reconstruction) Autoencoders

- have no direct probabilistic interpretation;
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VAEs

- model explicitly (a lower bound of) the likelihood;
- high quality samples from high dimensional distributions;
- encoder defines a useful latent representation;
- optimization problem is often well-behaved.

Takeaways

GANs

- likelihood-free generative models;
- high quality samples from high dimensional distributions;
- discriminator not meant be used as encoder;
- optimization problem is trickier than for VAEs (open research).

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There exists other kinds of generative models:

- auto-regressive models: PixelCNN, WaveNet, RNN language models...
- can be used as prior and decoder for VAEs, generators for GANs.
- flow-based models: Glow, WaveGlow...

Takeaways

Adversarial training is useful beyond generative models:

- domain adaptation;
- learning representations blind to sensitive attributes;
- defend against malicious inputs (adversarial examples);
- regularization by training on adversarial examples.

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Adversarial training is useful beyond generative models:

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Quality of samples from VAE and GAN depends a lot on the architectures of sub-networks.

Thanks to

Charles Ollion and Olivier Grisel, Paris-Saclay, for the slides

Chris Holmes and Gil McVean, as always