Unsupervised learning and Generative models

Charles Ollion - Olivier Grisel

Outline

Unsupervised learning

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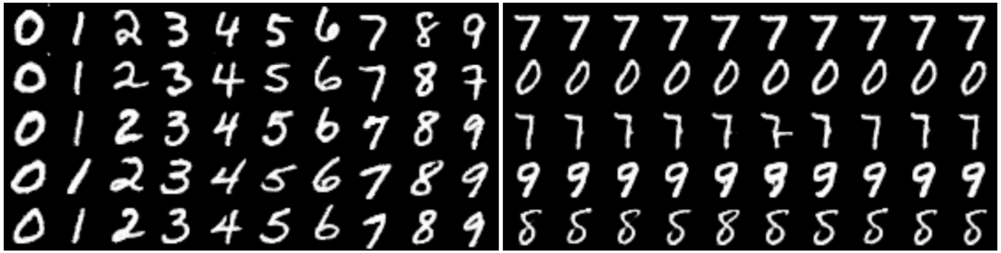
Latent space might be used to help build more efficient human labeling interfaces.

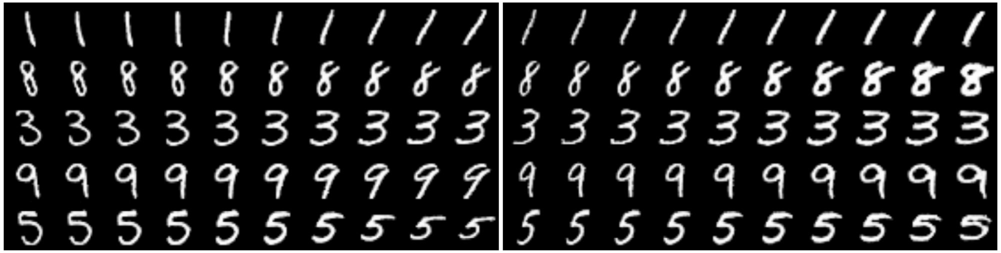
=> Goal: reduce labeling cost via active learning.

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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Use **text structure** to create supervision

- Word2Vec, BERT or GPT-1,2,3 (soon 4) language models

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Can we do the same for other domains?

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

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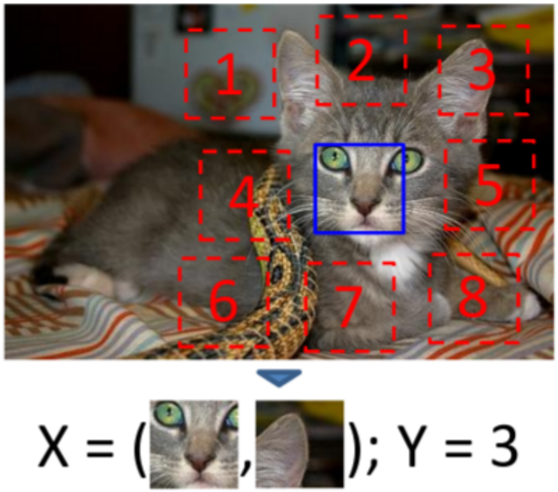
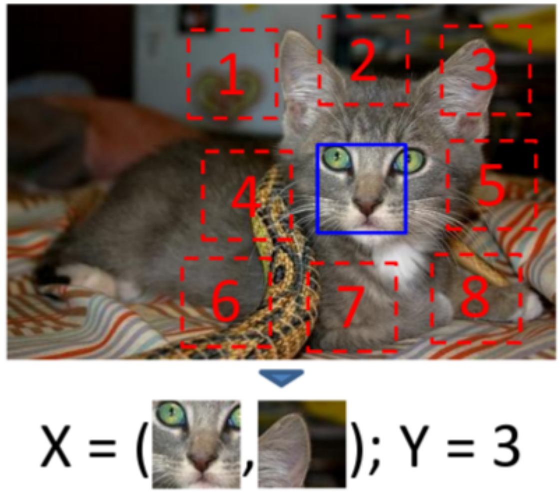
No direct **accuracy** measure: usually tested through a downstream task

Self-supervised learning



Doersch, Carl, Abhinav Gupta, and Alexei A. Efros. "Unsupervised visual representation learning by context prediction." ICCV 2015.

Self-supervised learning



- Predict patches arrangement in images: 8 class classifier
- Siamese architecture for the two patches + concat

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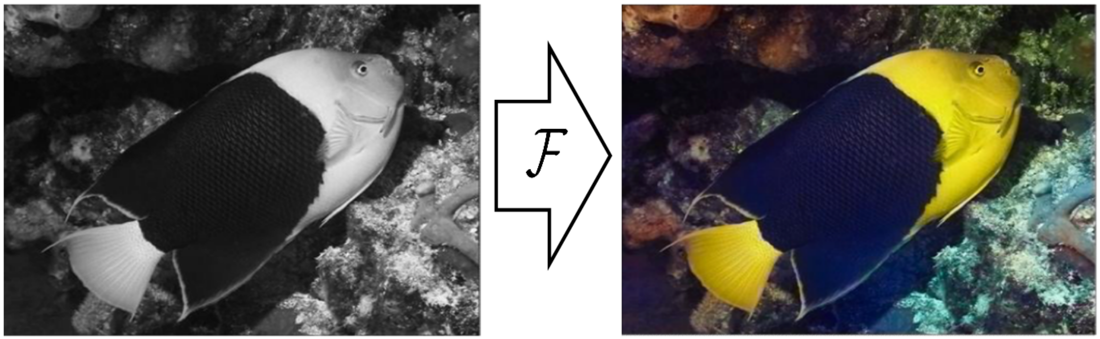
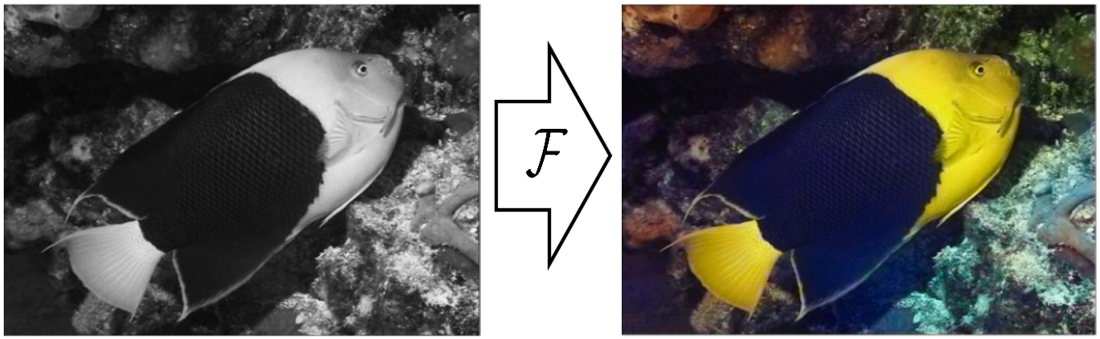


Zhang et al. "Colorful Image Colorization" ECCV 2016

Self-supervised learning



- Given RGB images, generate their grayscale version
- Train a network to predict pixels color given grayscale image

Zhang et al. "Colorful Image Colorization" ECCV 2016

Self-supervised learning

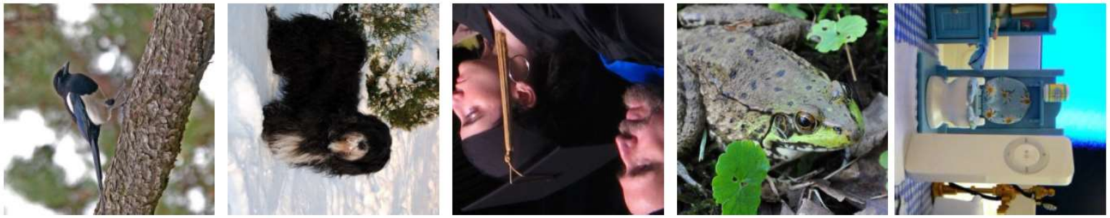
Dosovitskiy et al. "Exemplar Networks" 2014

Self-supervised learning

- Heavy augmentation of the images
- Network must predict that augmented images are similar, and another random image dissimilar

Dosovitskiy et al. "Exemplar Networks" 2014

Self-supervised learning

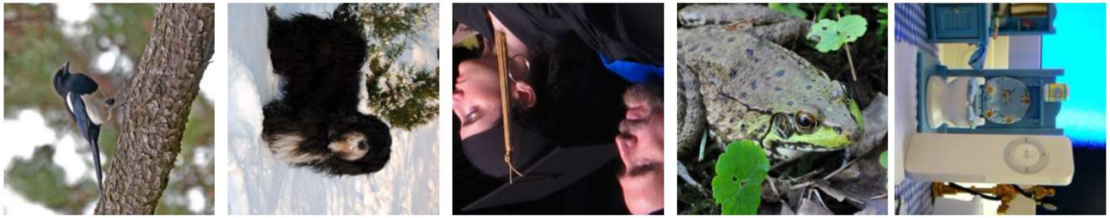


90° rotation | 270° rotation | 180° rotation | 0° rotation | 270° rotation

Figure 1: Images rotated by random multiples of 90 degrees (e.g., 0, 90, 180, or 270 degrees). The core intuition of our self-supervised feature learning approach is that if someone is not aware of the concepts of the objects depicted in the images, he cannot recognize the rotation that was applied to them.

Spyros Gidaris, Praveer Singh, Nikos Komodakis. "Unsupervised representation learning by predicting image rotations, " ICLR 2018

Self-supervised learning



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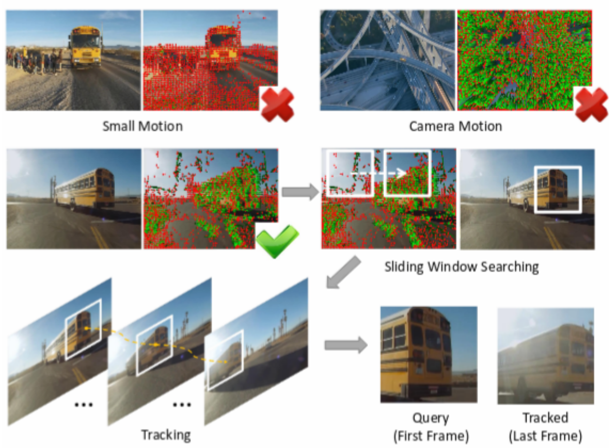
- Generate 4 versions of the image, rotated by 0°, 90°, 180°, and 270°
- Network must predict the angle

Spyros Gidaris, Praveer Singh, Nikos Komodakis. "Unsupervised representation learning by predicting image rotations, " ICLR 2018

Self-supervision from videos



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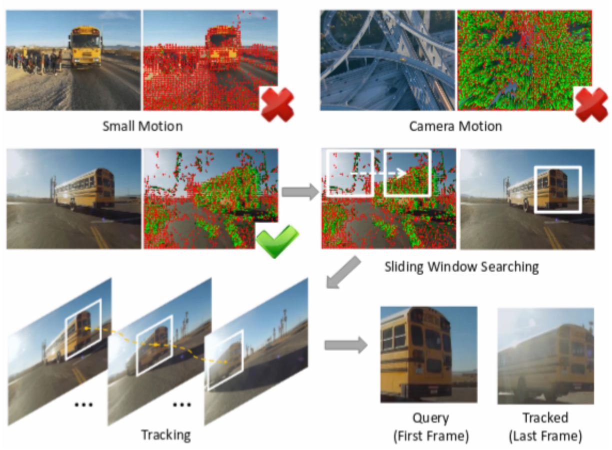

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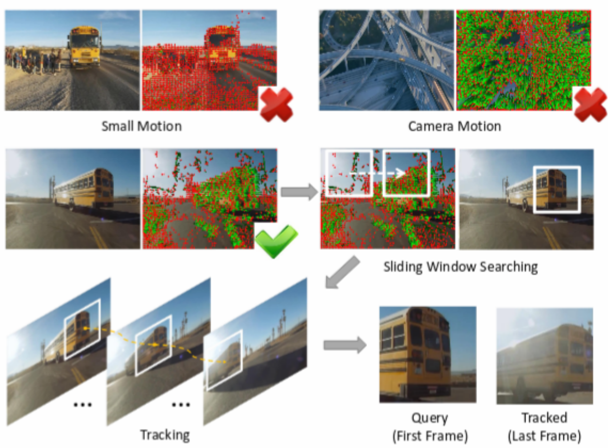

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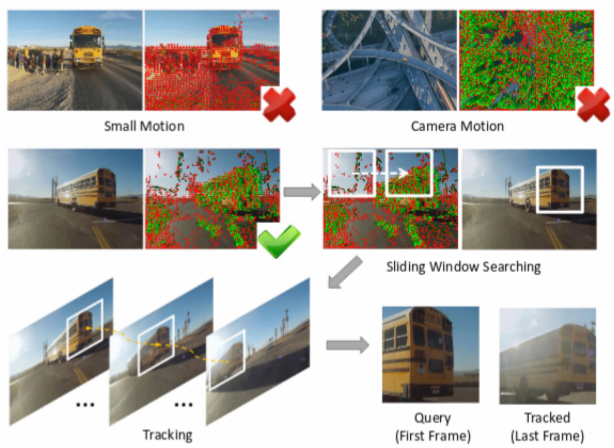
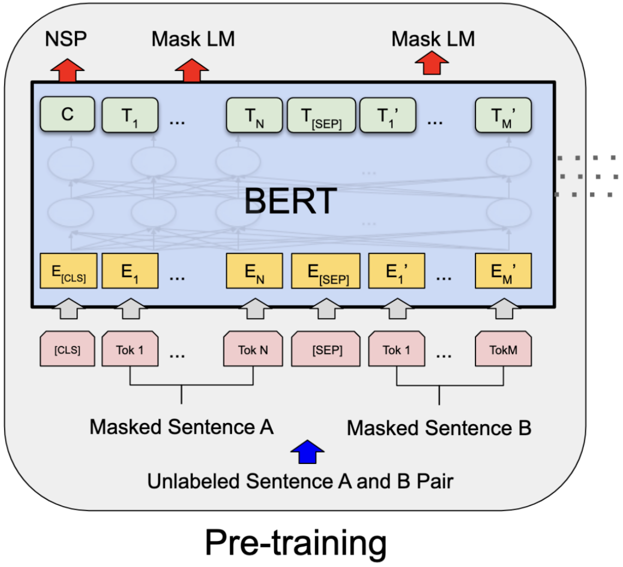


- Collect pairs of similar objects from videos
- Train a siamese net with positive pairs = similar objects detected
- Hard pairs mining: find objects with large movement

Wang, Xiaolong, and Abhinav Gupta. "Unsupervised learning of visual representations using videos." ICCV 2015.

Self-supervised learning for language



[BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding](#) Jacob Devlin, Ming-Wei Chang, Kenton Lee, Kristina Toutanova

Self-supervised learning for any modality

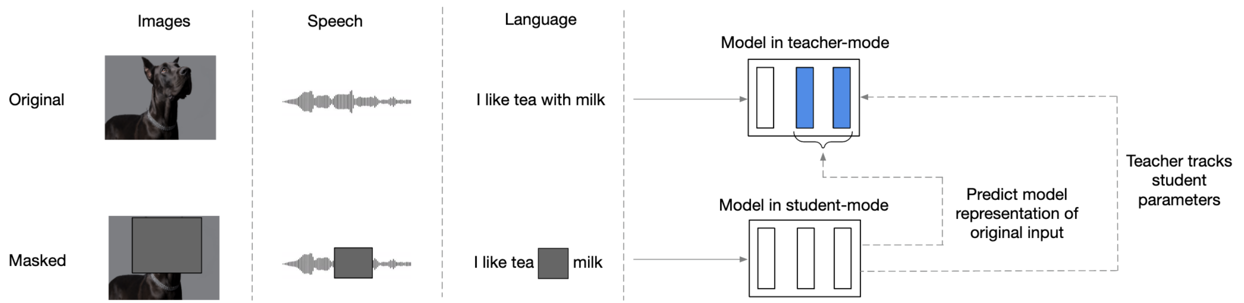
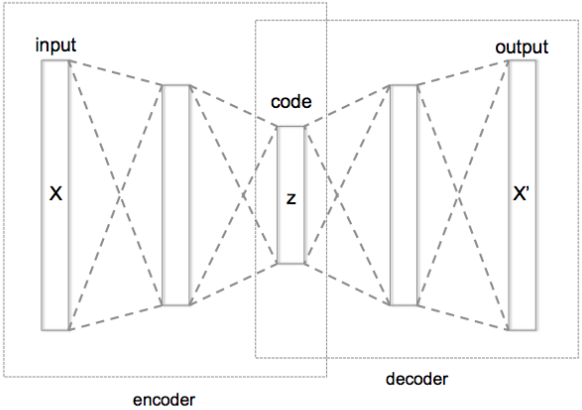


Figure 1. Illustration of how data2vec follows the same learning process for different modalities. The model first produces representations of the original input example (teacher mode) which are then regressed by the same model based on a masked version of the input. The teacher parameters are an exponentially moving average of the student weights. The student predicts the average of K network layers of the teacher (shaded in blue).

[data2vec: A General Framework for Self-supervised Learning in Speech, Vision and Language]
Alexei Baevski, Wei-Ning Hsu, Qiantong Xu, Arun Babu, Jiatao Gu, Michael Auli

Autoencoders

Autoencoder



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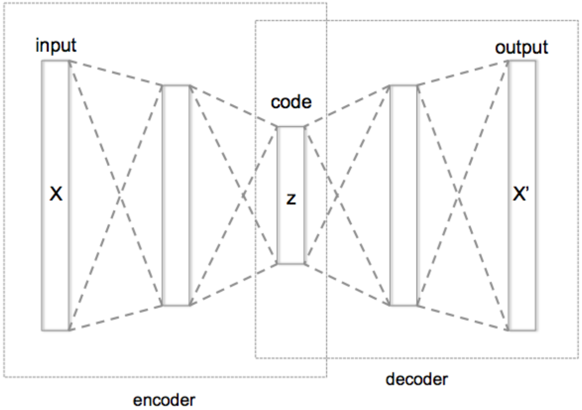

Supervision : reconstruction loss of the input, usually:

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

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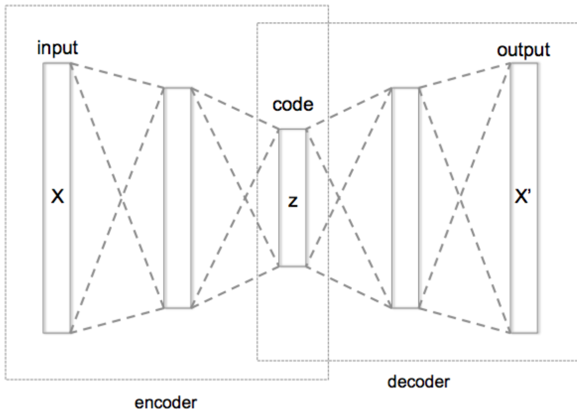

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Binary crossentropy is also used

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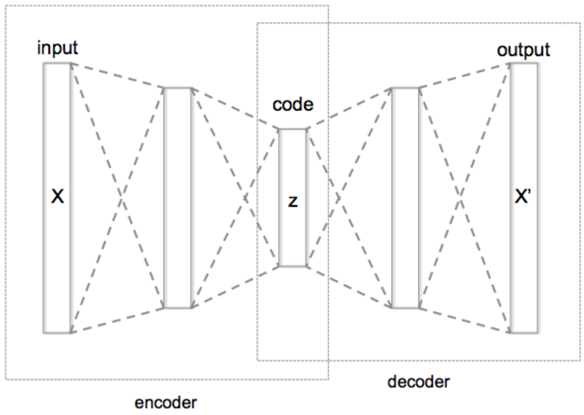

Keeping the **latent code $\mathbf{z}$** low-dimensional forces the network to learn a "smart" compression of the data, not just an identity function

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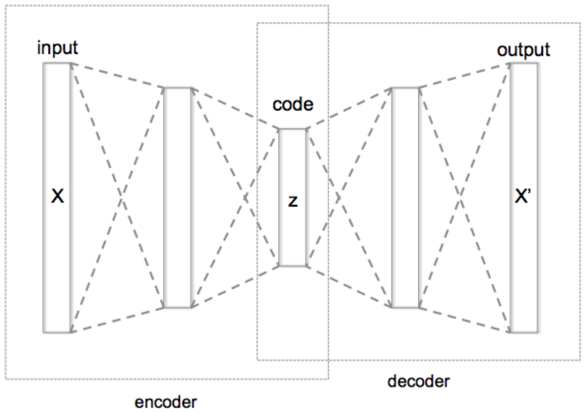

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Encoder and decoder can have arbitrary architecture (CNNs, RNNs...)

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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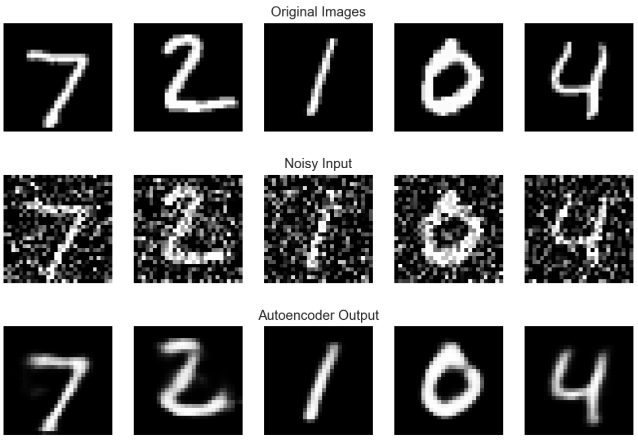
Denoising Autoencoder: train features for robustness to noise.



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)

Variational Autoencoders

Variational Autoencoders (VAE)

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

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

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- $\mathcal{L}(\theta, \phi; \mathbf{x}^{(i)})$ is a lower bound to maximize w.r.t. θ and ϕ.

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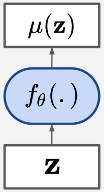
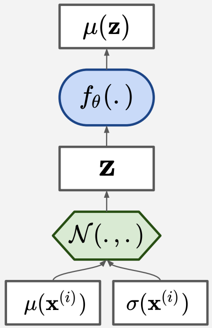
- Reparametrization trick:

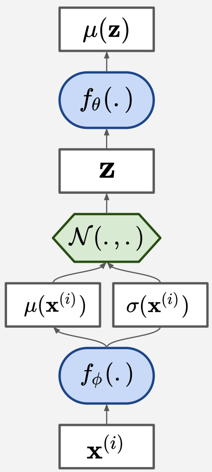
$$\mathbf{z} = \mu_\phi(\mathbf{x}^{(i)}) + \sigma_\phi(\mathbf{x}^{(i)}) \cdot \epsilon \quad \text{with} \quad \epsilon \sim \mathcal{N}(0, 1)$$



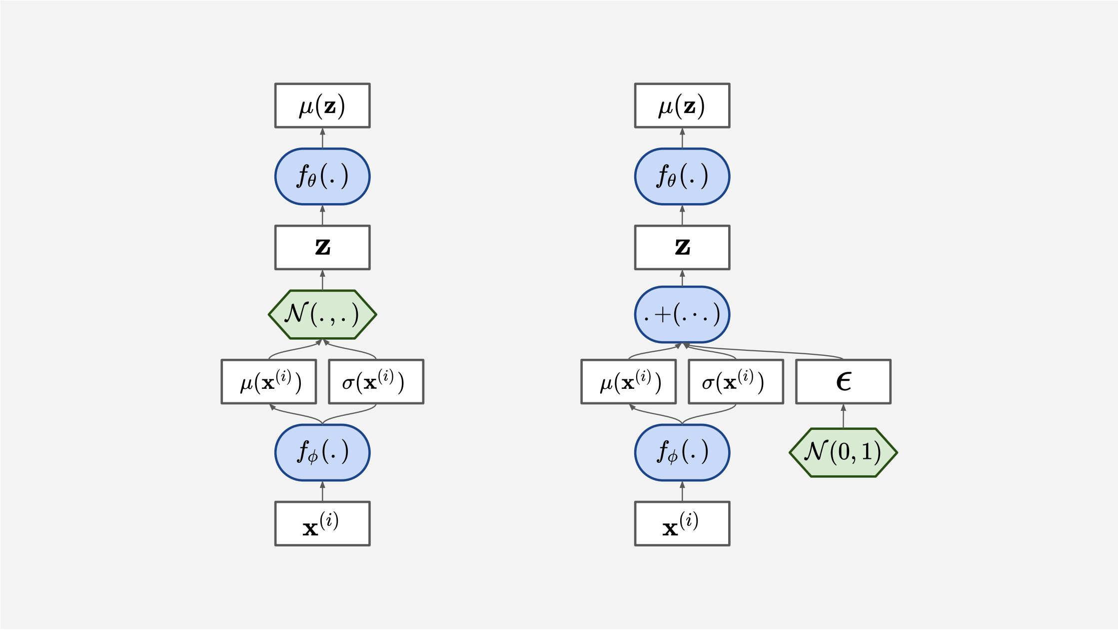
The **decoder** f_θ defines the likelihood of data.



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

Face manifold from conv/deconv variational autoencoder

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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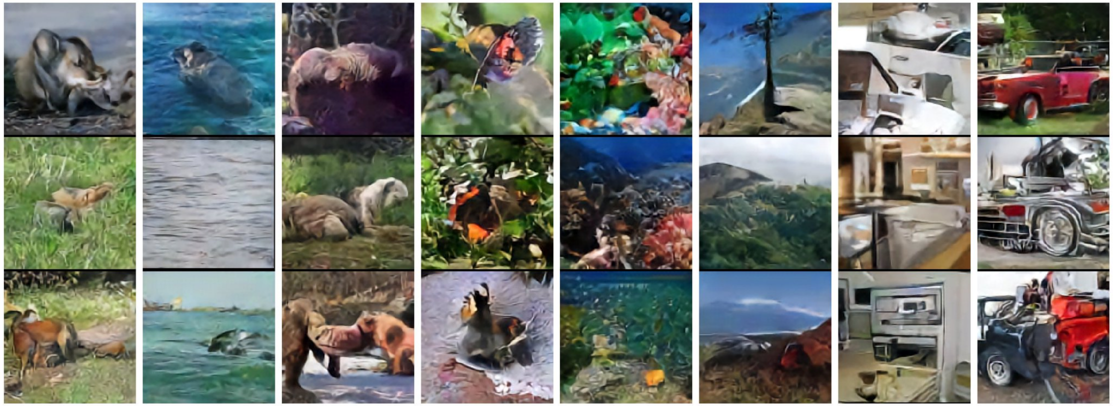
VQ-VAE

- $\mathbf{z}$ 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:

Generative Adversarial Networks

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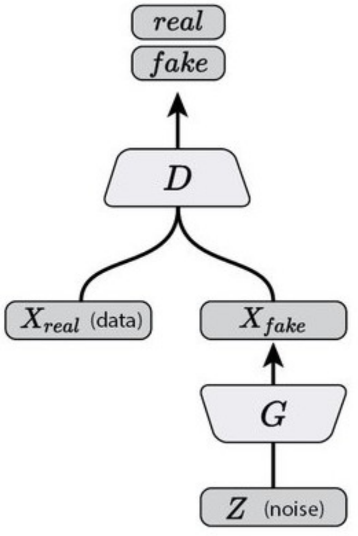

Alternate training of a **generative network** G and a **discrimininative network** D

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

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Sample real data $x \sim p_{data}$

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

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

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

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

Sample $\mathbf{z}$ and generate fake data $G(\mathbf{z})$

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

GANs

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

Sample real data $x \sim p_{data}$

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

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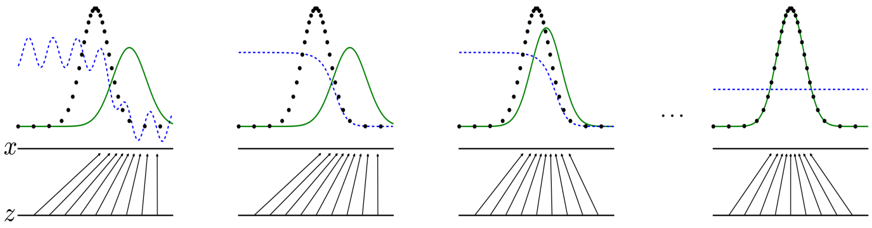
GANs

1D-example

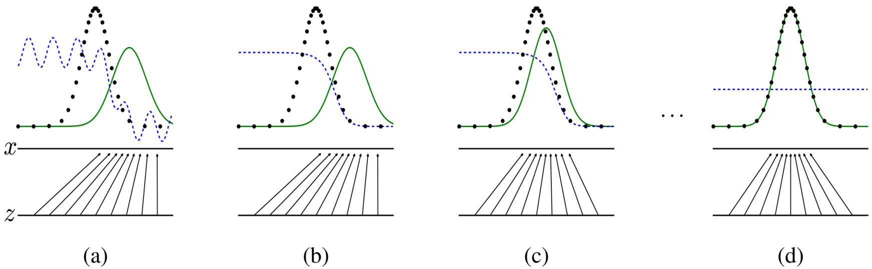


(a) (b) (c) (d)

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

GANs

1D-example



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GANs

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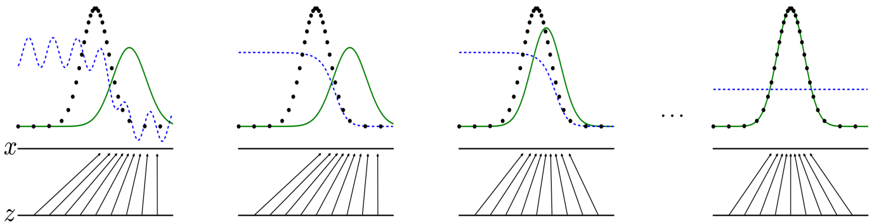
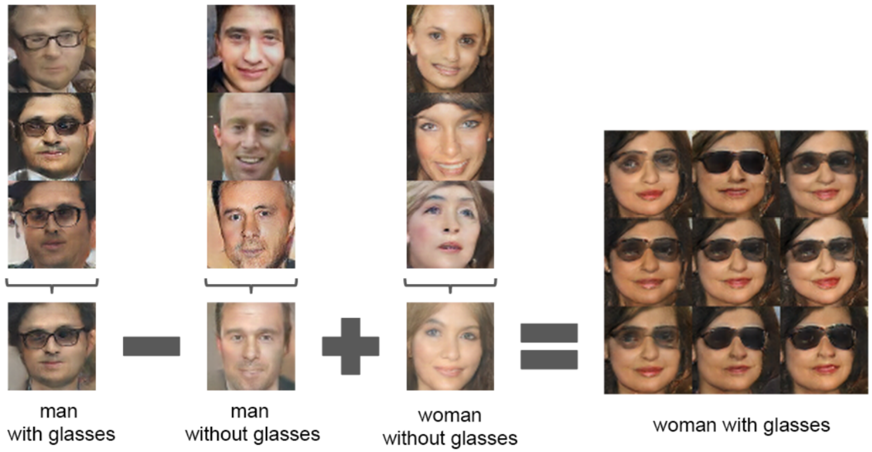


(a) (b) (c) (d)

- 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))
```

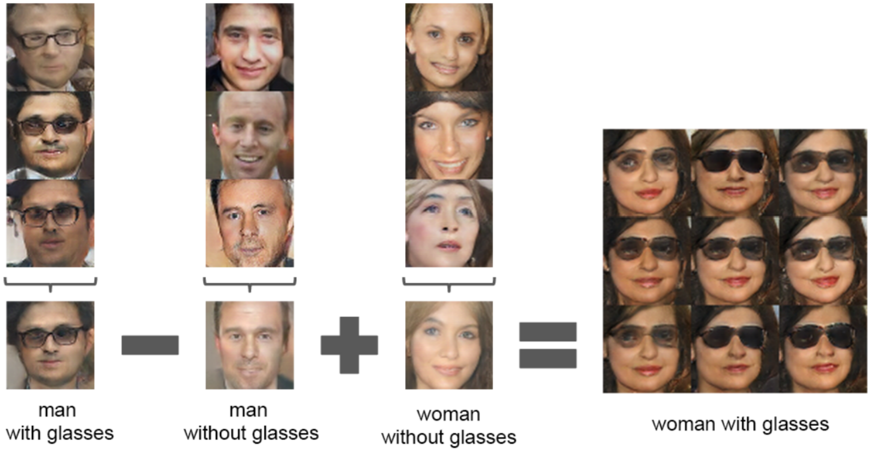
DC-GAN



- Generator generates less-blurry images than VAEs

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

DC-GAN



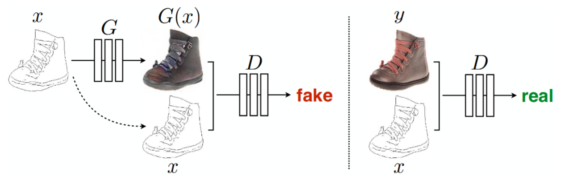
- Generator generates less-blurry images than VAEs
- Latent space has some local linar properties (vector arithmetic like with Word2Vec)

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

Style GANs

A Style-Based Generator Architecture for Generative Adversarial Networks by Tero Karras, Samuli Laine, Timo Aila, 2018, and later versions

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

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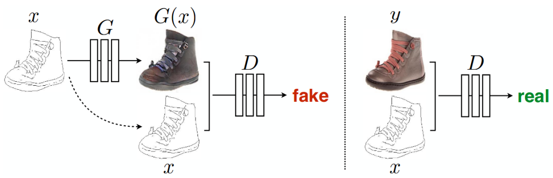

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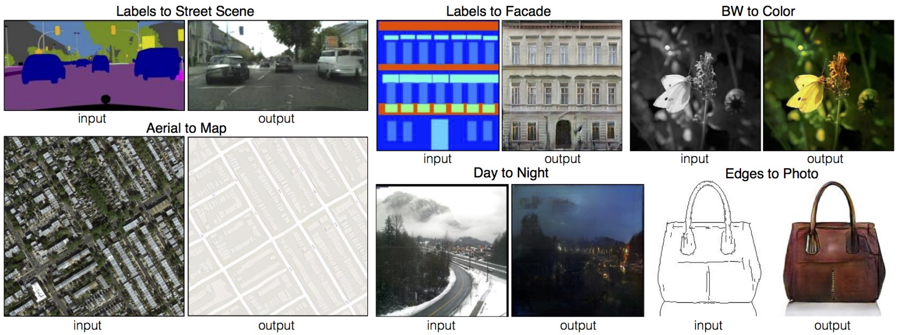

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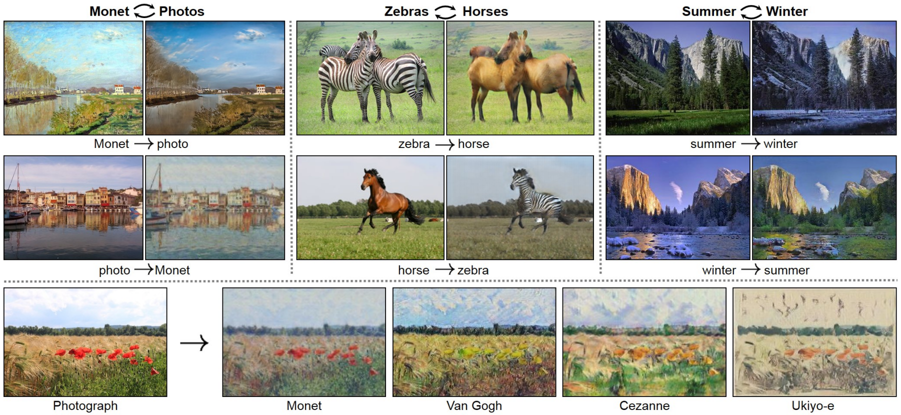
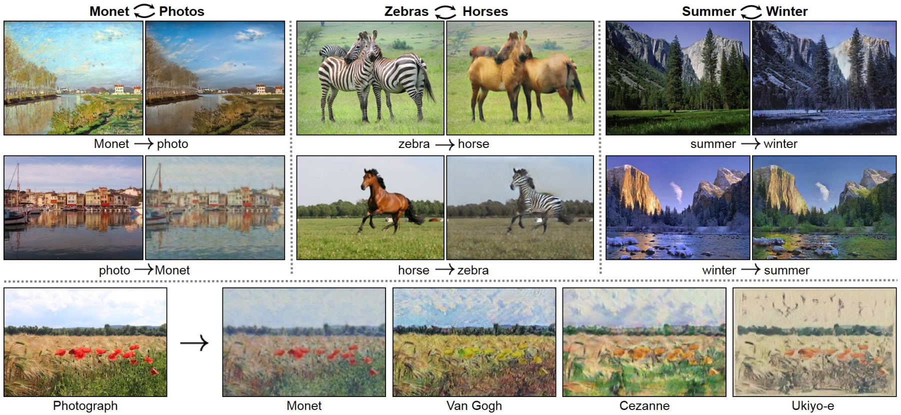
Cycle GANs



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

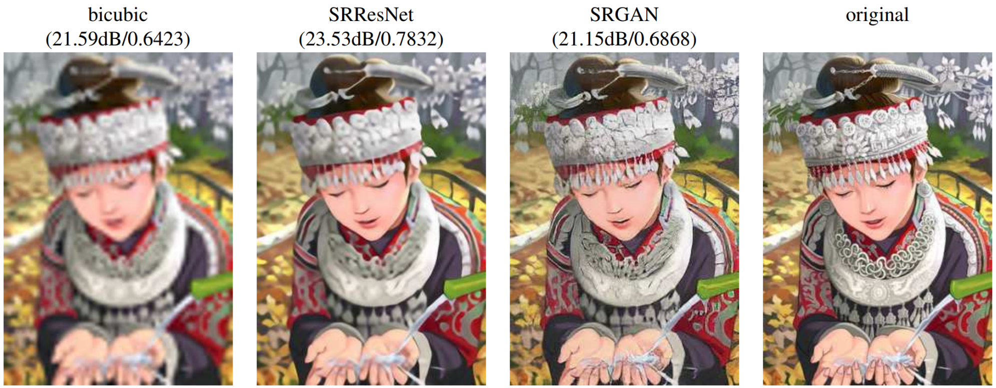
Cycle GANs



- 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

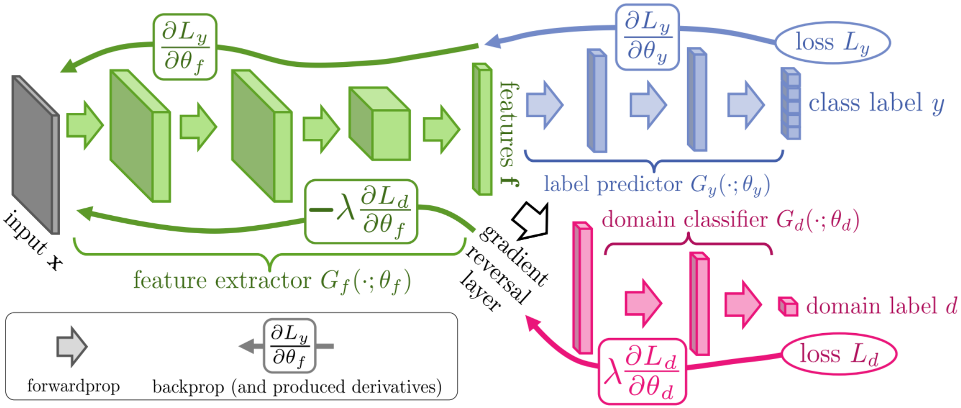
Super Resolution



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

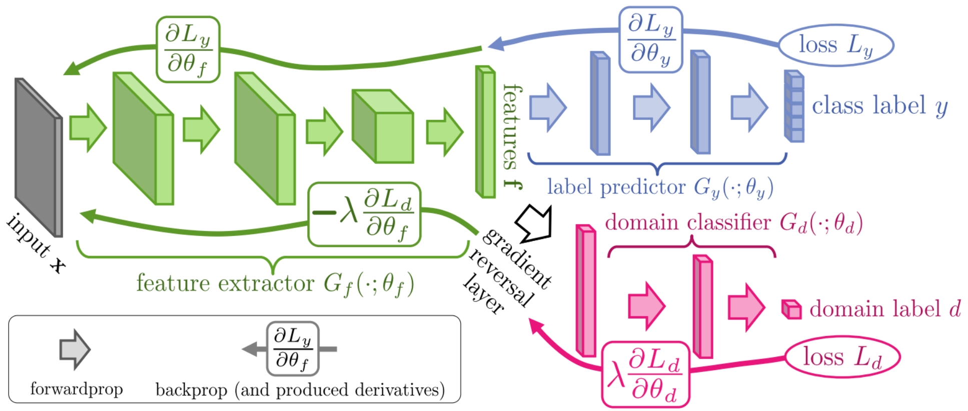
Ledig, Christian, et al. Photo-realistic single image super-resolution using a generative adversarial network. CVPR 2016.

Domain Adversarial Training



Ganin, Yaroslav, et al. Domain-adversarial training of neural networks. JMLR 2016.

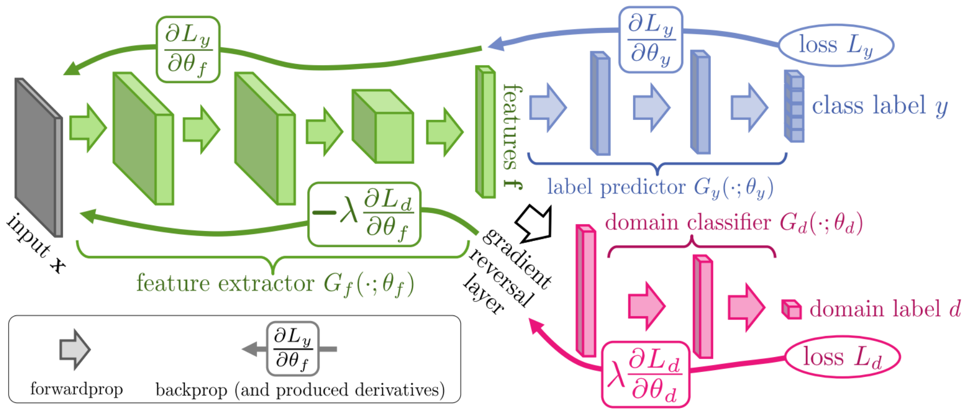
Domain Adversarial Training



- Forces the features (green) **not** to be specialised in discriminating between domains

Ganin, Yaroslav, et al. Domain-adversarial training of neural networks. JMLR 2016.

Domain Adversarial Training



- Forces the features (green) **not** to be specialised in discriminating between domains
- Easy to implement in TensorFlow / Pytorch with a `GradientReversalLayer`

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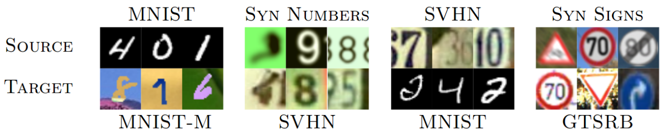
Domain Adversarial Training

- Train **labeled** source domain + **unlabeled** target domain



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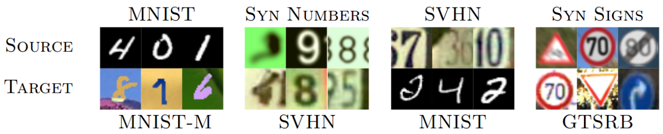
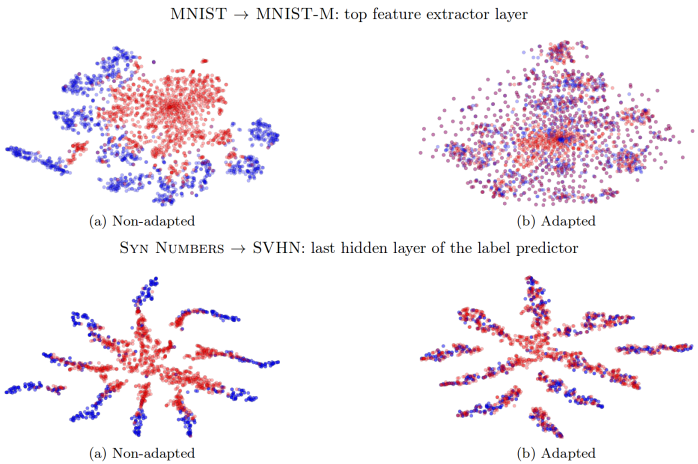
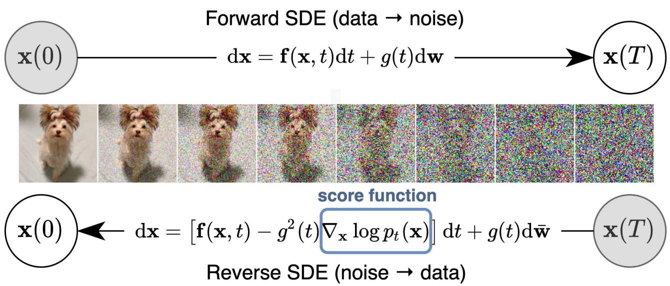


- Representation tends to be **less biased** towards the domain



Score-based matching (denoising diffusion)



Yang Song, and S. Ermon. Generative Modeling by Estimating Gradients of the Data Distribution, NeurIPS 2019.
Jonathan Ho, A. Jain, P. Abbeel, Denoising Diffusion Probabilistic Models

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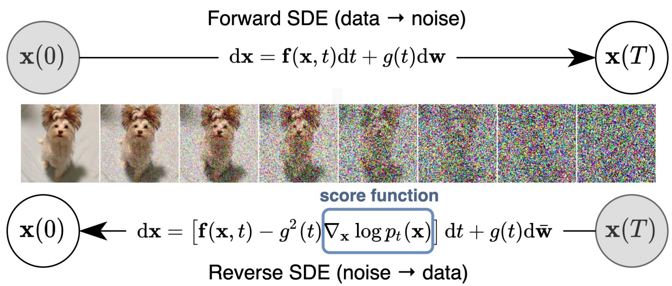
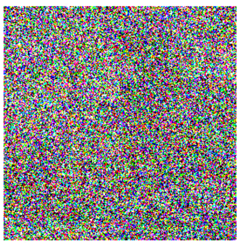
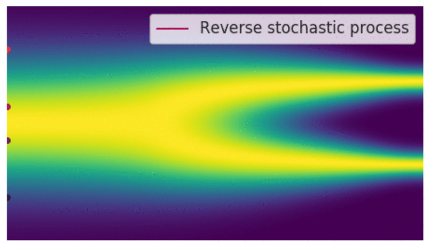


Generate images by gradually denoising random noise





Yang Song, and S. Ermon. [Generative Modeling by Estimating Gradients of the Data Distribution](), NeurIPS 2019.
Jonathan Ho, A. Jain, P. Abbeel, [Denoising Diffusion Probabilistic Models]()

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).

Takeaways

GANs

- likelihood-free generative models;
- high quality samples from high dimensional distributions;
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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...
- Score-matching / denoising diffusion models.

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.