Yes,
we GAN.

VLC = ∭ Vision Learning Control dVdLdC

Deep Generative Modelling

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Introduction

- What is generative modelling and why do we do it?
- Differentiable Generator Networks
- Variational Autoencoders
- Generative Adversarial Networks

Generative Modelling and Differentiable Generator Networks

Recap: Generative Models

- Learn models of the data: $p(\mathrm{x})$
- Learn *conditional* models of the data: $p(\mathrm{x}|\mathrm{y} = y)$
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    - The likelihood of data x is the weighted sum of the likelihood from each of the k Gaussians
    - Sampling can be achieved by sampling the categorical distribution of k weights followed by sampling a data point from the corresponding Gaussian

Why do generative modelling?

- Try to understand the processes through which the data was itself generated
    - Probabilistic latent variable models like VAEs or topic models (PLSA, LDA, ...) for text
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- Make 'new' data
  - Make 'fake' data to use to train large supervised models?
  - 'Imagine' new, but plausible, things?

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  - Generative adversarial networks - A way to train generative models by optimizing them to fool a classifier
- **Common thread in recent advances is that the loss functions are end-to-end differentiable.**

Differentiable Generator Networks: key idea

- We're interested in models that transform samples of latent variables $\boldsymbol{z}$ to
  - samples x, or,
  - distributions over samples x
- The model is a (differentiable) function $g(\boldsymbol{z}, \boldsymbol{\theta})$
  - typically g is a neural network.

Example: drawing samples from $\mathcal{N}(\mu, \Sigma)$

- Consider a simple generator network with a single affine layer that maps samples $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ to $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$:

$$\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}) \longrightarrow \boxed{g_{\boldsymbol{\theta}}(\boldsymbol{z})} \longrightarrow \boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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- Note: Exact solution is $\boldsymbol{x} = g_{\boldsymbol{\theta}}(\boldsymbol{z}) = \boldsymbol{\mu} + \boldsymbol{L}\boldsymbol{z}$ where $\boldsymbol{L}$ is the Cholesky decomposition of $\boldsymbol{\Sigma}$: $\boldsymbol{\Sigma} = \boldsymbol{L}\boldsymbol{L}^\top$, lower triangular $\boldsymbol{L}$.

Generating samples

More generally, we can think of g as providing a nonlinear change of variables that transforms a distribution over **z** into the desired distribution over **x**:

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For any *invertible, differentiable, continuous* g:

$$p_z(\boldsymbol{z}) = p_x(g(\boldsymbol{z})) \left| \det\left(\frac{\partial g}{\partial \boldsymbol{z}}\right) \right|$$

Which implicitly imposes a probability distribution over **x**:

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Note: usually use an indirect means of learning g rather than minimise $-\log(p(\boldsymbol{x}))$ directly

Generating distributions

- Rather than use g to provide a sample of $\boldsymbol{x}$ directly, we could instead use g to define a conditional distribution over x, $p(\boldsymbol{x}|\boldsymbol{z})$
    - For example, g might produce the parameters of a particular distribution - e.g.:
        - means of Bernoulli
        - mean and variance of a Gaussian

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  - For example, g might produce the parameters of a particular distribution - e.g.:
    - means of Bernoulli
    - mean and variance of a Gaussian
- The distribution over $\boldsymbol{x}$ is imposed by marginalising $\boldsymbol{z}$:$p(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}} p(\boldsymbol{x}|\boldsymbol{z})$

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- Generating distributions:
  - $+$ works for both continuous and discrete data
  - - need to specify the form of the output distribution
- Generating samples:
  - $+$ works for continuous data
    - $+$ discrete data is recently possible - we need the STargmax
  - $+$ don't need to specify the distribution in explicit form

Complexity of Generative Modelling

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- Generative modelling is more complex than classification because
  - learning requires optimizing intractable criteria
  - data does not specify both input $\boldsymbol{z}$ and output $\boldsymbol{x}$ of the generator network
  - learning procedure needs to determine how to arrange $\boldsymbol{z}$ space in a useful way and how to map $\boldsymbol{z}$ to $\boldsymbol{x}$

Variational Autoencoders

Variational Autoencoder (VAE)

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- However, VAEs map the input into a distribution.
- VAEs are a combination of neural networks (AEs) and **graphical models.**

Graphical Models (Background)

- A graphical model is a probabilistic model for which a graph expresses the conditional dependence structure between random variables.

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- Graphical models are commonly used in probability theory, statistics —particularly Bayesian statistics— and machine learning. [1]

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KL Divergence (Background)

- Kullback–Leibler divergence, $D_{\mathrm{KL}}(P \parallel Q)$: a measure of how one probability distribution Q is different from a second, reference probability distribution P. [2]

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- A simple interpretation of the divergence of P from Q is the expected excess surprise from using Q as a model when the actual distribution is P.
- While it is a distance, it is not a metric, the most familiar type of distance: it is asymmetric in the two distributions.

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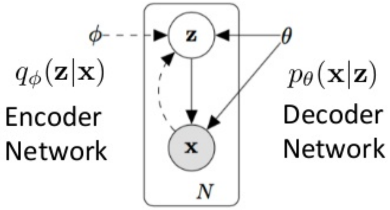
Variational Autoencoder



Minimize: $D_{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})]$

Intractable: $p_\theta(\mathbf{z}|\mathbf{x}) = \dfrac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{p_\theta(\mathbf{x})}$

[3]

[3] Auto-Encoding Variational Bayes https://arxiv.org/abs/1312.6114

The distance loss just defined is expanded as

$$\begin{aligned}
D_{KL}(q_\Phi(\mathbf{z} \mid \mathbf{x}) \parallel p_\theta(\mathbf{z} \mid \mathbf{x})) &= \int q_\Phi(\mathbf{z} \mid \mathbf{x}) \log \frac{q_\Phi(\mathbf{z} \mid \mathbf{x})}{p_\theta(\mathbf{z} \mid \mathbf{x})}\, d\mathbf{z} \\
&= \int q_\Phi(\mathbf{z} \mid \mathbf{x}) \log \frac{q_\Phi(\mathbf{z} \mid \mathbf{x}) p_\theta(\mathbf{x})}{p_\theta(\mathbf{z}, \mathbf{x})}\, d\mathbf{z} \\
&= \int q_\Phi(\mathbf{z} \mid \mathbf{x}) \left(\log(p_\theta(\mathbf{x})) + \log \frac{q_\Phi(\mathbf{z} \mid \mathbf{x})}{p_\theta(\mathbf{z}, \mathbf{x})} \right) d\mathbf{z} \\
&= \log(p_\theta(\mathbf{x})) + \int q_\Phi(\mathbf{z} \mid \mathbf{x}) \log \frac{q_\Phi(\mathbf{z} \mid \mathbf{x})}{p_\theta(\mathbf{z}, \mathbf{x})}\, d\mathbf{z} \\
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&= \log(p_\theta(\mathbf{x})) + E_{\mathbf{z} \sim q_\Phi(\mathbf{z}|\mathbf{x})}(\log \frac{q_\Phi(\mathbf{z} \mid \mathbf{x})}{p_\theta(\mathbf{z})} - \log(p_\theta(\mathbf{x} \mid \mathbf{z}))) \\
&= \log(p_\theta(\mathbf{x})) + D_{KL}(q_\Phi(\mathbf{z} \mid \mathbf{x}) \parallel p_\theta(\mathbf{z})) - E_{\mathbf{z} \sim q_\Phi(\mathbf{z}|\mathbf{x})}(\log(p_\theta(\mathbf{x} \mid \mathbf{z})))
\end{aligned}$$

At this point, it is possible to rewrite the equation as

$$\log(p_\theta(\mathbf{x})) - D_{KL}(q_\Phi(\mathbf{z} \mid \mathbf{x}) \parallel p_\theta(\mathbf{z} \mid \mathbf{x})) = E_{\mathbf{z} \sim q_\Phi(\mathbf{z}|\mathbf{x})}(\log(p_\theta(\mathbf{x} \mid \mathbf{z}))) - D_{KL}(q_\Phi(\mathbf{z} \mid \mathbf{x}) \parallel p_\theta(\mathbf{z}))$$

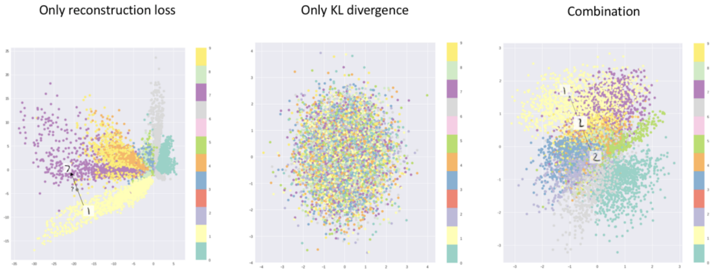
Evidence Lower Bound (ELBO) Loss

$$L_{VAE}(\theta, \phi) = -\mathbb{E}_{z \sim q_\phi(z|x)} log(p_\theta(x|z)) + D_{KL}(q_\phi(z|x)||p_\theta(z))$$

- We are trying to minimize the ELBO loss with respect to the model parameters.

Why Autoencoder?

- The reconstruction term, forces each image to be unique and spread out.

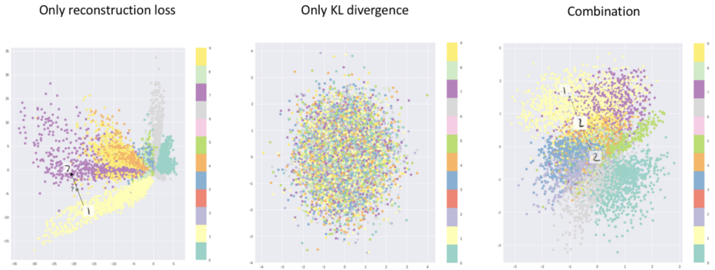


4

[4]Figure taken from https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

Why Autoencoder?

- The reconstruction term, forces each image to be unique and spread out.
- The KL term will push all the images towards the same prior.



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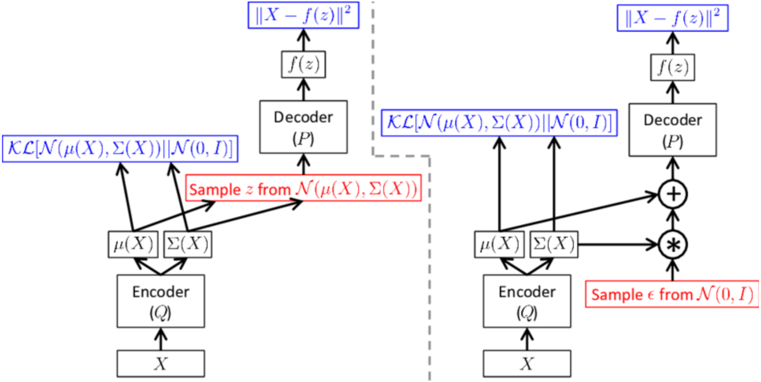
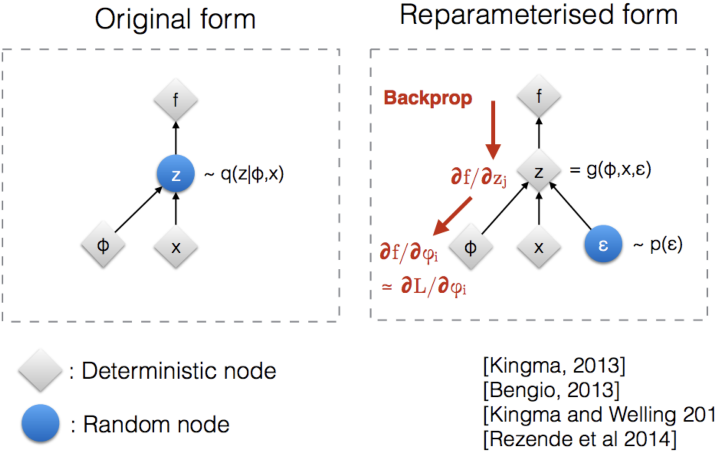


[5]

[5] Figure taken from Carl Doersch tutorial

Reparametrization Trick Visualisation



[Kingma, 2013]
[Bengio, 2013]
[Kingma and Welling 2014]
[Rezende et al 2014]

VAE Models and Performance

- VAEs can be used with any kind of data
  - the distributions and network architecture just needs to be set accordingly
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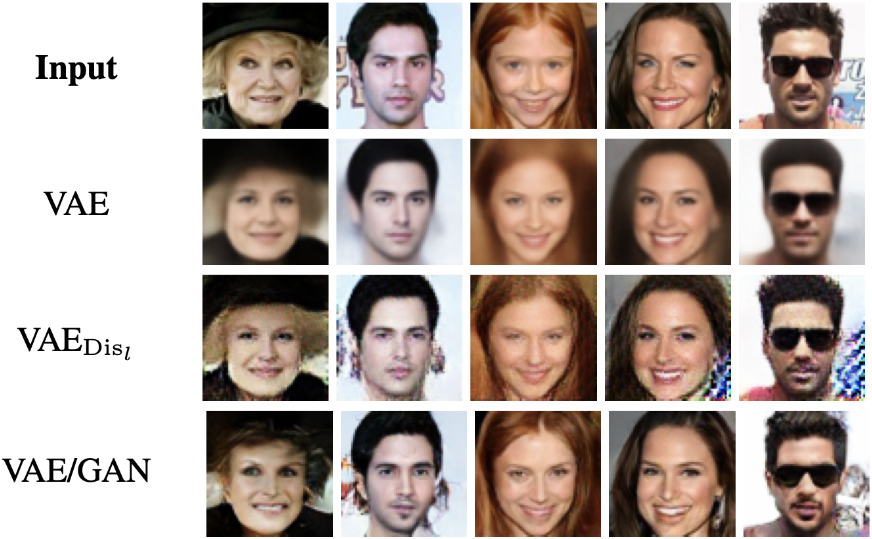
- VAEs tend to only utilise a small subset of the dimensions of $\boldsymbol{z}$

Reconstructions Example



Generative Adversarial Networks

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- Both discriminator and generator are deep networks (differentiable functions)
- LeCun quote 'GANs, the most interesting idea in the last ten years in machine learning'

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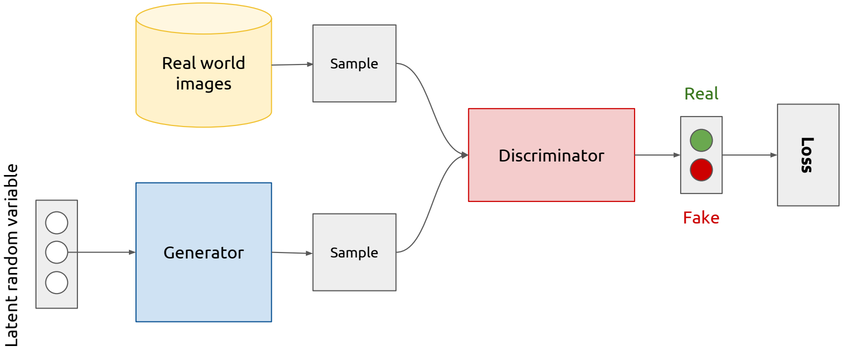
Aside: Adversarial Learning vs. Adversarial Examples

The approach of GANs is called adversarial since the two networks have *antagonistic* objectives.

This is not to be confused with *adversarial examples* in machine learning.

See these two papers for more details:
`https://arxiv.org/pdf/1412.6572.pdf`
`https://arxiv.org/pdf/1312.6199.pdf`

Generative adversarial networks (conceptual)



Picture Credit: Xavier Giro-i-Nieto

More Formally

- The **generator**

$$\boldsymbol{x} = g(\boldsymbol{z})$$

is trained so that it gets a random input $\boldsymbol{z} \in \mathbb{R}^n$ from a distribution (typically $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ or $\mathcal{U}(\mathbf{0}, \boldsymbol{I})$) and produces a sample $\boldsymbol{x} \in \mathbb{R}^d$ following the data distribution as output (ideally). Usually $n << d$.

- The **discriminator**

$$y = d(\boldsymbol{x})$$

gets a sample $\boldsymbol{x}$ as input and predicts a probability $y \in [0, 1]$ (or real-valued logit of a Bernoulli distribution) determining if it is real or fake.

More Practically

- Training a standard GAN is difficult and often results in two undesirable behaviours
  - Oscillations without convergence. No guarantee that the loss will actually decrease...
    - It has been shown that a GAN has saddle-point solution, rather than a local minima.
  - The **mode collapse** problem, when the generator models very well a small sub-population, concentrating on a few modes.
- Additionally, performance is hard to assess and often boils down to heuristic observations.

Deep Convolutional Generative Adversarial Networks (DCGANs)

- Motivates the use of GANS to learn reusable feature representations from large unlabelled datasets.
- GANs known to be unstable to train, often resulting in generators that produce "nonsensical outputs".
- Model exploration to identify architectures that result in **stable** training across datasets with higher resolution and deeper models.

Architecture Guidelines for Stable DCGAN

- Replace pooling layers with strided convolutions in the discriminator and fractional-strided (transpose) convolutions in the generator.
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- Use LeakyReLU activation in the discriminator for all layers.

Summary

- Generative modelling is a massive field with a long history
- Differentiable generators have had a profound impact in making models that work with real data at scale
- VAEs and GANs are currently the most popular approaches to training generators for spatial data
- We've only scratched the surface of generative modelling
  - Auto-regressive approaches are popular for sequences (e.g. language modelling).
    - But also for images (e.g. PixelRNN, PixelCNN)
  - typically RNN-based
  - but not necessarily - e.g. WaveNet is a convolutional auto-regressive generative model