Deep generative modelling Concepts and characteristics

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Today

- Five main modelling approaches $p(\mathbf{x}) \approx ?$
- Their concepts and characteristics
- Future research directions



Recent review

Method	Train Speed	Sample Speed	Num. Params.	Resolutio Scaling	n Free-form Jacobian	Exact Density	FID	NLL (in BPD)
Generative Adversarial Networks DCGAN [182] ProGAN [114] BigGAN [19] StyleGAN2 + ADA [115]	*****	*****	***** ***** *****	***** ***** ****	****	× × ×	37.11 15.52 14.73 2.42	
Energy Based Models IGEBM [46] Denoising Diffusion [87] DDPM++ Continuous [206] Flow Contrastive (EBM) [55] VAEBM [247]	*****	*****	***** ***** ***** *****	*****	*****	* × <>>> * *	37.9 3.17 2.20 37.30 12.19	≤ 3.75 ≈ 3.27
Variational Autoencoders Convolutional VAE [123] Variational Lossy AE [29] VQ-VAE [184], [235] VD-VAE [31]	*****	*****	***** ****** *****	*****	/ x x /	3333	106.37	$\leq 4.54 \\ \leq 2.95 \\ \leq 4.67 \\ \leq 2.87$
Autoregressive Models PixelRNN [234] Gated PixelCNN [233] PixelIQN [173] Sparse Trans. + DistAug [32], [110]	*****	***** ***** *****	***** ***** *****	******	x x x x	****	65.93 49.46 14.74	3.00 3.03 2.66
Normalizing Flows RealNVP [43] GLOW [124] FFJORD [62] Residual Flow [26]	***** ***** *****	*****	*****	*****	× × ✓	33.4.4	45.99 46.37	3.49 3.35 3.40 3.28

Bond-Taylor, Willcocks et al., "Deep Generative Modelling: A Comparative Review of VAEs, GANs, Normalizing Flows, Energy-Based and Autoregressive Models" in IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI) [1]



The data distribution P(X, Y)



Learning the data distribution

So what is it we want exactly?

- P(Y|X) discriminative model (classification)
- P(X|Y) conditional generative model
- P(X, Y) generative model

We want to learn the probability density function of our data (natures distribution)

Generative models definition

Definition: Generative models learn a joint distribution over the entire dataset with some target variable(s). They are mostly used for sampling applications or density estimation:

Sampling the model

A generative model learns to fit a model distribution over observations so we can sample novel data from the model distribution, $\mathbf{x}_{new} \sim p_{model}(\mathbf{x})$



Density estimation

Density estimation is estimating the probability of observations. Given a datapoint \mathbf{x} , what is the probability assigned by the model, $p_{model}(\mathbf{x})$?





Examples

Linguists

- What is the probability of a sentence? *P*(sentence)
 - P('the dog chased after the ball')
 - $P(\text{`printers eat avocados when sad'}) \approx 0$

Meteorologists

• What is the probability of whether it will rain? P(rain)

Artists

• What is the probability of this image being a face? P(face)

Musicians

• What is the probability this sounds like Beethoven? *P*(Beethoven)

Definition: maximum likelihood estimation

Maximum likelihood estimation (MLE) is a method for estimating the parameters of a probability distribution by maximizing a likelihood function, so that under the model the observed data is most probable

$$\begin{split} \theta^* &= \arg \max_{\theta} p_{\text{model}}(\mathbb{X}; \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^{n} p_{\text{model}}(\mathbf{x}^i; \theta) \\ &\approx \arg \max_{\theta} \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}}[\log p_{\text{model}}(\mathbf{x}; \theta)] \end{split}$$
where $\mathbb{X} = \{\mathbf{x}^1, \mathbf{x}^2, ..., \mathbf{x}^n\}$ are from $p_{\text{data}}(\mathbf{x})$





Example: cumulative distribution sampling

Given the CDF $F_X(\mathbf{x})$, the antiderivative of $f_X(\mathbf{x}) = p_{\text{model}}(\mathbf{x})$, e.g. where $F'(\mathbf{x}) = p_{\text{model}}(\mathbf{x})$

$$F_X(\mathbf{x}) = \int_{-\infty}^{\mathbf{x}} f_X(\mathbf{u}) \,\mathrm{d}\mathbf{u}$$

we can sample new data by transforming random values \mathbf{z} from the uniform distribution $\mathbf{z} \sim U$ via the inverse of the CDF $F_X^{-1}(\mathbf{z})$.





Definition: autoregressive (AR) generative models

AR models maximise the likelihood of the training data (excellent mode coverage):

$$p_{\theta}(\mathbf{x}) = p_{\theta}(x_1, ..., x_N) = \prod_{i=1}^{N} p_{\theta}(x_i | x_1, ..., x_{i-1})$$

This is slow due to the sequential nature defined by the chain rule of probability.





Definition: generative networks

The goal of generative networks is to take some simple distribution, like a normal distribution or a uniform distribution, and apply a non-linear transformation (e.g. a deep neural network) to obtain samples from $p_{\rm data}(\mathbf{x})$

In 1D, we can say $G = F_{data}^{-1}(\mathbf{x})$ and sample $\mathbf{z} \sim U$, and similarly in ND — but assuming the determinant of the Jacobian and the inverse of G are computable, which is a large restriction. Ideally we want \mathbf{z} in low dimensions



Definition: generative adversarial networks

A generative adversarial network (GAN) is a non-coorporative zero-sum game where two networks compete against each other [2].

One network $G(\mathbf{z})$ generates new samples, whereas D estimates the probability the sample was from the training data rather than G:

$$\min_{G} \max_{D} V(D, G) = \mathbb{E}_{\mathbf{x} \sim p_{\mathsf{data}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})}[\log(1 - D(G(\mathbf{z})))].$$





GAN properties

GANs benefit from differentiable data augmentation [3] for both reals and fakes, but are otherwise notoriously difficult to train:

- Non-convergence
- Diminishing gradient
- Difficult to balance
- Mode collapse (next slide)

Link to Colab example 🗹







Definition: mode collapse

This is where the generator rotates through a small subset of outputs, and the discriminator is unable to get out of the trap. Mode collapse is arguably the main limitation of GANs.



Figure from [4]. The final column shows the target data distribution and the bottom row shows a GAN rotating through the modes.



Definition: conditional GAN

GANs can be conditioned with labels y if available [5] by feeding the label information into both the generator and the discriminator:

$$\min_{G} \max_{D} V(D,G) = \mathbb{E}_{\mathbf{x},\mathbf{y} \sim p_{\mathsf{data}}(\mathbf{x})} [\log D(\mathbf{x}|\mathbf{y})] \\ + \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})} [\log(1 - D(G(\mathbf{z},\mathbf{y})|\mathbf{y}))]$$

Link to Colab example 🗹





Definition: information maximizing GANs

GANs can be trained to learn disentangled latent representations in a completely unsupervised manner. InfoGAN [6] popularised this by maximizing mutual information between the observation and a subset of the latents:

 $\min_{\boldsymbol{G},\boldsymbol{Q}} \max_{\boldsymbol{D}} V_{\mathsf{InfoGAN}}(\boldsymbol{D},\boldsymbol{G},\boldsymbol{Q}) = V(\boldsymbol{D},\boldsymbol{G}) - \lambda L_I(\boldsymbol{G},\boldsymbol{Q})$

where $L_I(G,Q)$ is a variational lower bound of the mutual information.

Link to Colab example 🗹





Definition: adversarial autoencoders

Adversarial autoencoders [7] are generative models that permit sampling.

In addition to the reconstruction loss, such $\|\mathbf{x} - \hat{\mathbf{x}}\|^2$, they use adversarial training to match the aggregated posterior of the hidden code vector \mathbf{z} of the autoencoder with an arbitrary prior distribution, such as $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.





Definition: unpaired translation (CycleGAN)

CycleGAN [8] propose an adversarial architecture that enables unpaired image translation. It has twin residual generators and two discriminators, which translate between the domains, alongside a cycle consistency loss (an L1 norm) which ensures the mapping can recover the original image.



Popular applications adversarial anomaly detection

GT

64x64

Definition: anomaly detection

Unsupervised anomaly detectors [9] learn a normal distribution over (healthy) observations. Then, when they observe something not observed in training (unhealthy/dangerous), they fail to reconstruct - detecting it as an anomaly. Region-based anomaly detectors [10] learn a distribution over inpainted (erased) regions.





Vector quantization

Vector quanitization

Imposing a discrete prior on the latents can be achieved with either variational or adversarial (non-blurry) approaches.



The Gumbel-Softmax distribution interpolates between discrete one-hot-encoded categorical distributions and continuous categorical densities.



Above: vector quantisation. **Below:** shift mode collapse to perceptually unimportant parts of the signal.



Definition: energy-based models

These are just any function that is happy when you input something that looks like data, and is not happy when you input something that doesn't look like data.

 $E(\mathbf{x}) = 0 \checkmark$ $E(\tilde{\mathbf{x}}) > 0 \checkmark$

This generic definition fits a large majority of machine learning models. For example $\mathcal{L}(E(\mathbf{x}), \mathbf{y})$ (a classifier)

Energy increases off manifold



Definition: energy-based models

GANs are also energy models. The generator G generates samples off the manifold, then the descriminator D says these should be one everywhere, whereas it says real samples should be zero everywhere.

The generator also has to get good at sampling points on the data manifold. So it has to learn to generate points in the valley regions.

Is this smooth? What does a 1-Lipschitz discriminator do to the energy landscape?

GAN energy



Definition: clustering algorithm

A cluster is a **connected-component** of a **level-set** of the **unknown PDF** over our data observations.

Traditionally:

- We don't know the PDF (the energy landscape)
- We don't necessarily know the level set
 - although 0.5 is appropriate for BCE
- This can be expensive (deep learning)

Click to watch a video that visually explains from the definition **D**

Example: clustering by its definition





Definition: softmax and softmin

Softmax and softmin functions rescale elements to be in the range [0, 1] and such that they sum to 1. So they create a probability mass function, e.g.:

$$\begin{bmatrix} 1.3\\ 7.2\\ 2.4\\ 0.5\\ 1.1 \end{bmatrix} \rightarrow \frac{e^{\mathbf{z}_i}}{\sum_{j=1}^{K} e^{\mathbf{z}_j}} \rightarrow \begin{bmatrix} 0.0027\\ 0.9858\\ 0.0081\\ 0.0012\\ 0.0022 \end{bmatrix}$$

Softmax functions are widely used (not just for EBMs) where a distribution is needed, such as the last layer of a classifier.

Challenges: energy-based models

EBMs are based on the observation that any probability density function $p(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$ can be expressed as:

$$p(\mathbf{x}) = \frac{e^{-E(\mathbf{x})}}{\int_{\tilde{\mathbf{x}} \in \mathcal{X}} e^{-E(\tilde{\mathbf{x}})}},$$

where $E(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ is the energy function. However computation of the integral is intractable [11] for most models.

Energy increases off manifold



Definition: score-based GMs

Score-based generative modeling [12] also eliminates the intractable second term (sampling from the model). For the PDF $p(\mathbf{x})$ the score function is:

$$s(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

When the score function is known, we can use Langevin dynamics to sample the model. Given a step size $\alpha > 0$, a total number of iterations T, and an initial sample x0 from any prior distribution $\pi(\mathbf{x})$, Langevin dynamics iteratively updates:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} + \alpha \nabla_{\mathbf{x}} \log p(\mathbf{x}_{t-1}) + \sqrt{2\alpha} \, \mathbf{z}_t$$

Energy increases off manifold



Diffusion probablistic modeling

Diffusion Probablistic Modeling approaches (such as DDPMs [13]) typically have a U-Net shaped architecture:

Data is gradually diffused in a forward process for T timesteps until it matches the target distribution.

The reverse process gradually removes noise starting at $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$ for T timesteps.

'Score-Based Generative Modeling through Stochastic Differential Equations' [14] has author code and PyTorch tutorials in the link.

Example: CIFAR10 samples from [13]



Diffusion-based anomaly detection



Diffusion-based anomaly detection

Like GANs, diffusion-based models work well for anomalies (great for small datasets).

- Do a partial diffusion
- Train only on healthy/normal data
- Abnormal denoising will only know how to make the data look normal
- Any error = surprise = anomalies

Our recent paper, AnoDDPM [15] (CVPR NTIRE), uses simplex noise to capture multi-scale anomalies. See also UNIT-DDPM [16] (unpaired translation).



Link to project page 🗷



Definition: flow models

Flow models restrict our function to be a chain of invertible functions, called a flow, therefore the whole function is invertible.





Recap: the determinant

The determinant of an $n \times n$ square matrix M is a scalar value that determines the factor of how much a given region of space increases or decreases by the linear transformation of M:

$$\det M = \det \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} = \sum_{j_1 j_2 \dots j_n} (-1)^{\tau(j_1 j_2 \dots j_n)} a_{1j_1} a_{2j_2} \dots a_{nj_n}$$

Watch a 3Blue1Brown's video here 🗹

PyTorch: torch.det(M), for example: torch.det(torch.eye(3,3)) returns 1.0
and torch.det(torch.tensor([[3.,2.],[0.,2.]])) returns 6.0



Definition: the change of variables theorem

Given $p_Z(\mathbf{z})$ where $\mathbf{x} = f(\mathbf{z})$ and $\mathbf{z} = f^{-1}(\mathbf{x})$ we ask what is $p_X(\mathbf{x})$?

$$p_X(\mathbf{x}) = p_Z(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\partial f^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$





Definition: normalising flows

Normalising flows $f : \mathbb{R}^n \to \mathbb{R}^n$ transform and renormalise a sample $\mathbf{z} \sim p_{\theta}(\mathbf{z})$ through a chain of bijective transformations f, where:

$$\mathbf{x} = f_{\theta}(\mathbf{z}) = f_K \circ \dots \circ f_2 \circ f_1(\mathbf{z})$$
$$\log p_{\theta}(\mathbf{x}) = \log p_{\theta}(\mathbf{z}) + \sum_{i=1}^K \log \left| \det \left(\frac{\partial f_i^{-1}}{\partial \mathbf{z}_i} \right) \right|$$





Easy to compute determinants

We have a sequence of high-dimensional bijective functions, where we need to compute the Jacobian determinants.

Computing the determinants can be expensive, so most of the literature focuses on restricting the function f^{-1} to those with easy-to-compute Jacobian determinants.

This is done by ensuring the Jacobian matrix of the functions is triangular.

Definition: triangular Jacobian

If the Jacobian is lower triangular:



then the determinant is simply the product of its diagonals.

Normalising flows normalising flow layers



Description	Function	Log-Determinant
Additive Coupling [17]	$\mathbf{y}^{(1:d)} = \mathbf{x}^{(1:d)} \mathbf{y}^{(d+1:D)} = \mathbf{x}^{(d+1:D)} + f(\mathbf{x}^{(1:d)})$	0
Planar [18]	$\mathbf{y} = \mathbf{x} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b)$ With $\mathbf{w} \in \mathbb{R}^D$, $\mathbf{u} \in \mathbb{R}^D$, $\mathbf{b} \in \mathbb{R}$	$\ln 1 + \mathbf{u}^T h'(\mathbf{w}^T \mathbf{z} + b)\mathbf{w} $
Affine Coupling [19]	$\mathbf{y}^{(1:d)} = \mathbf{x}^{(1:d)}$ $\mathbf{y}^{(d+1:D)} = \mathbf{x}^{(d+1:D)} \oplus f_{(\mathbf{x}^{(1:d)}) + f_{(\mathbf{x}^{(1:d)})}}$	$\sum_{1}^{d} \ln f_{\sigma}(x^{(i)}) $
Batch Normalization [19]	$\mathbf{y} = \frac{\mathbf{x} - \hat{\mu}}{\sqrt{\hat{\sigma}^2 + \epsilon}}$	$-\frac{1}{2}\sum_{i}\ln\left(\tilde{\sigma}_{i}^{2}+\epsilon\right)$
1x1 Convolution [20]	With $h \times w \times c$ tensor $\mathbf{x} \& c \times c$ tensor \mathbf{W} $\forall i, j : \mathbf{y}_{i,j} = \mathbf{W} \mathbf{x}_{i,j}$	$h\cdot w\cdot \ln \det \mathbf{W} $
i-ResNet [21]	$\begin{aligned} \mathbf{y} &= \mathbf{x} + f(\mathbf{x}) \\ \text{where } \left\ f \right\ _L < 1 \end{aligned}$	$ tr(\ln(\mathbf{I} + \nabla_{\mathbf{x}} f)) = \\ \sum_{k=1}^{\infty} (-1)^{k+1} \frac{tr((\nabla_{\mathbf{x}} f)^k)}{k} $
Emerging Convolutions [22]	$ \begin{array}{ll} \mathbf{k} = \mathbf{w}_1 \odot \mathbf{m}_1, \qquad \mathbf{g} = \mathbf{w}_2 \odot \mathbf{m}_2 \\ \mathbf{y} = \mathbf{k} \star_l \left(\mathbf{g} \star_l \mathbf{x} \right) \end{array} $	$\sum_{c} \ln \left \mathbf{k}_{c,c,m_y,m_x} \mathbf{g}_{c,c,m_y,m_x} \right ^{32/48}$



Definition: variational autoencoders

Variational autoencoders are generative models, as they impose a prior over the latent space $p(\mathbf{z})$, typically $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, I)$ which can be sampled from.

$$\mathbf{z} \sim E(\mathbf{x}) = q(\mathbf{z}|\mathbf{x}), \quad \hat{\mathbf{x}} \sim D(\mathbf{z}) = p(\mathbf{x}|\mathbf{z})$$

The VAE loss is the negated expected log-likelihood (the reconstruction error) and the prior regularization term:

$$\mathcal{L}_{\text{VAE}} = -\mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} \right] = \mathcal{L}_{\text{recon}}^{\text{pixel}} + \mathcal{L}_{\text{prior}}$$

where

$$\mathcal{L}_{\text{recon}}^{\text{pixel}} = -\mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}|\mathbf{z})]$$
$$\mathcal{L}_{\text{prior}} = D_{\text{KL}}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}))$$



Definition: ELBO

VAEs therefore have three components:

- 1. the decoder $p_{\theta}(\mathbf{x}|\mathbf{z})$
- 2. the *approximate posterior* (encoder) $q_{\phi}(\mathbf{z}|\mathbf{x})$
- 3. the prior distribution $p_{\theta}(\mathbf{z})$

They are trained with the reparameterisation trick to maximise the evidence lower bound (ELBO):

 $\log p_{\theta}(\mathbf{x}) \geq \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{z}) - D_{\mathsf{KL}}[q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\theta}(\mathbf{z})]$

Read [23] for detail on the theory (where the figure is from) and [24] for a state-of-the-art method that stacks VAEs hierarchically (Very Deep VAEs).





Definition: implicit representations

Consider data $\Phi \colon \mathbb{R}^m \to \mathbb{R}^n$, like a single image, as a function of coordinates $\mathbf{c} \in \mathbb{R}^m$. The aim is to learn a neural approximation of Φ that satisfies an implicit equation:

$$R(\mathbf{c}, \Phi, \nabla_{\Phi}, \nabla_{\Phi}^2, \dots) = 0, \quad \Phi \colon \mathbf{c} \mapsto \Phi(\mathbf{c}).$$

Equations with this structure arise in a myriad of fields, namely 3D modelling, image, video, and audio representation.

Example: implicit network





Definition: SIREN

SInusoidal REpresentation Networks (SIREN) are a simple implicit representation network with fully connected layers, but use sin (with clever initialisation to scale it appropriately) as their choice of non-linearity [25].

sin is periodic, so it allows to capture patterns over all of the coordinate space (it's translation invariant, like convolutions).

Example: SIREN (implicit network)



Link to project page 🗹



Definition: NeRF

Neural Radiance Fields (NeRF) are similar to SIRENs, but instead of representing an image, they represent a single 3D scene [26].

They map from pixel positions (x, y, z) and a viewing direction (θ, ϕ) to a colour and density value σ integrated via a ray on F_{θ} .



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Definition: gradient origin networks

Gradient origin networks (GON) treat the derivative of the decoder as an encoder [27]. This allows us to compute the latents:

 $\mathbf{z} = -\nabla_{\mathbf{z}_0} \mathcal{L}(\mathbf{x}, F(\mathbf{z}_0))$

which are then jointly optimised, giving the GON objective:

 $G_{\mathbf{x}} = \mathcal{L}(\mathbf{x}, F(-\nabla_{\mathbf{z}_0} \mathcal{L}(\mathbf{x}, F(\mathbf{z}_0))))).$

Link to project page 🗹

Example: implicit GON





Summary

$$p(\mathbf{x}) = \prod_{i=1}^{N} p(x_i | x_1, ..., x_{i-1})$$

$$p(\mathbf{x}) \approx \frac{e^{-E(\mathbf{x})}}{\int_{\tilde{\mathbf{x}} \in \mathcal{X}} e^{-E(\tilde{\mathbf{x}})}} \text{ e.g. } \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

$$\log p(\mathbf{x}) \ge \mathcal{L}_{\text{recon}}^{\text{pixel}} - D_{\text{KL}} \left[q_{\phi}(\mathbf{z} | \mathbf{x}) | | p(\mathbf{z}) \right]$$

$$\log p(\mathbf{x}) \ne \log D(\mathbf{x}) \quad \text{(in GAN)}$$

$$p(\mathbf{x}) = p_Z(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\partial f^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

Our hybrids "Unleashing transformers" [28] 🖸 (ECCV22) or "Megapixel image generation" (new) [29].





Our hybrid [29] 2 seconds generation, 2 days training, single GTX 1080Ti







Contributions

- State-of-the-art = hybrids
- Some applications only need partial diffusion (AnoDDPM, UNIT-DDPM)
- Start of non-hybrid generative implicit networks (GONs)—we need new interpolated modelling theory please (more like [30])

Tips, tricks and the future

- Eventually move discriminative modelling tasks to generative modelling
- Measuring progress sucks (not just quality/performance)
- For vision state-of-the-art:
 - Intentionally mode collapse parts of signal you don't care about
 - Model with good coverage + quality (AR,EBM) the remaining signal

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