Deep learning

Deep Generative Models

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Table of contents

Introduction

Supervised learning

1. In supervised setting, we have a dataset $S = \{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}$.
2. Discriminative models estimate the conditional distribution $P(y|x)$.
   - Linear regression, logistic regression, generalized linear models
   - Standard Neural Networks, CNN, RNN...
   - Decision trees, boosting, random forests, kernel methods, KNN, ...
3. Generative models estimate the joint distribution $P(x, y)$.
   - Naive Bayes
   - Linear/quadratic discriminant analysis
4. Generating new data requires to model the joint distribution $P(x, y)$.

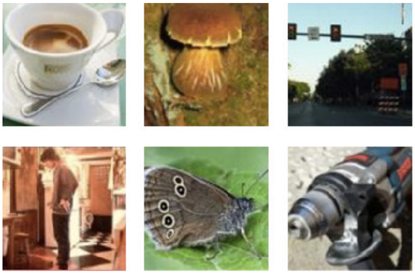
1. In unsupervised setting, we have a dataset $S = \{x_1, x_2, \ldots, x_m\}$.
2. We have no target output, thus nothing to predict nor discriminate.
3. In unsupervised setting, we have different goals:
   - Descriptive analysis: detect structure, correlations in the data set using descriptive/graphical tools or using more involved methods (PCA for example)
   - Clustering: create "homogeneous" groups of observations (usually spending 90% of the allocated time to properly define "homogeneous")
   - Estimating the distribution of observations: detect suspect data/behaviour, detect changes in the data set if the data are collected through time
   - Generating new data: closely related to the previous point.

Why Generative Models?

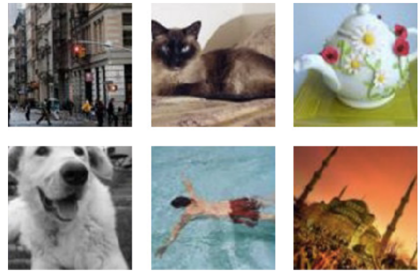
1. We have seen discriminative models
   - Given an image x, predict label y
   - Estimates $P(y|x)$
2. Discriminative models have several key limitations
   - Can't model $P(x)$, i.e. the probability of seeing a certain image
   - Thus, can't sample from $P(x)$, i.e. can't generate new images
3. Generative models (in general) cope with all of the above problems
   - Can model $P(x)$
   - Can generate x such as new images
4. Generate new data by sampling from the learned distribution.
5. Evaluate the likelihood of data observed at test time.
6. Find the conditional relationship between variables, eg learning the distribution $p(x_2|x_1)$ allows us to build discriminative classification or regression models.
7. Score algorithms by using complexity measures like entropy, mutual information, and moments of the distribution.

Generative Models

1. Given training data, generate new samples from same distribution[1],



Train from $x \sim p_{data}(x)$



Generate from $x \sim p_{model}(x)$

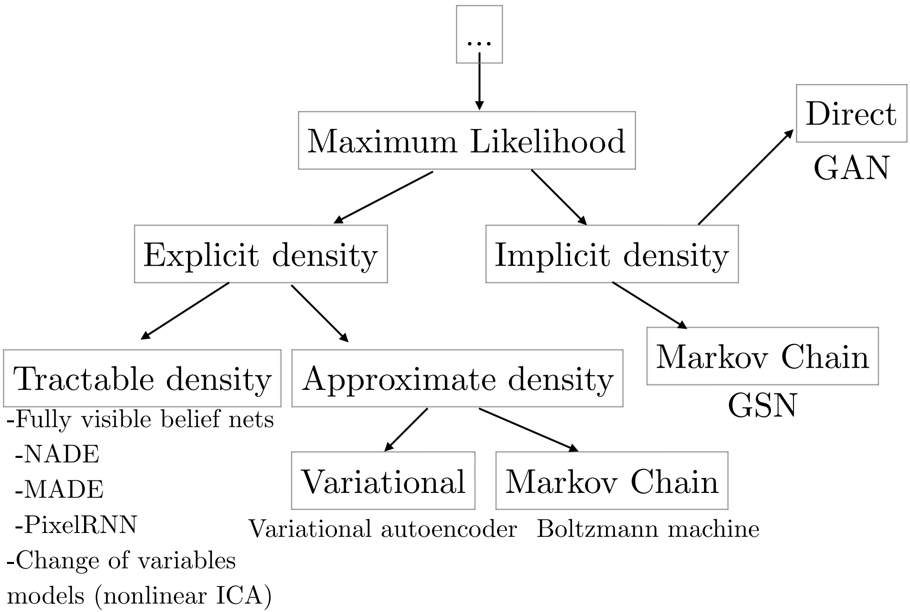
Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

2. Several flavors
   - Explicit density estimation: explicitly define and solve for $p_{model}(x)$
   - Implicit density estimation: learn model that can sample from $p_{model}(x)$ w/o explicitly defining it

[1] Taken from Fei-Fei Li et al. slides and Tutorial on Generative Adversarial Networks, 2017.

1. The following images were generated from a generative model (Karras et al. 2018).

Taxonomy of Generative Models



Different approaches for building generative models

1. Without using latent variables
    - Parametric density estimation
    - Non parametric density estimation
2. With using latent variables
    - Mixture models
    - Deep generative models

Introduction

Generative models without using latent variables

1. We assume $x_1, x_2, \ldots, x_m$ are IID random variables distributed as $p(x;\theta)$, hence we have

$$p(x;\theta) \quad = \quad p(x_1, x_2, \ldots, x_m; \theta_i) = \prod_{k=1}^{m} p(x_k;\theta)$$

2. $p(x;\theta)$ is a function of θ and is known as likelihood function.
3. The maximum likelihood (ML) method estimates θ so that the likelihood function takes its maximum value, that is,

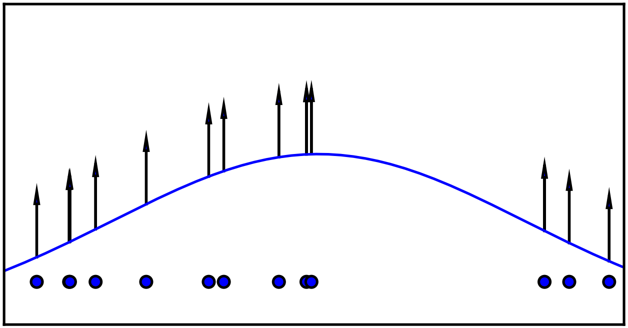
$$\hat{\theta}_{ML} \quad = \quad \underset{\theta}{argmax} \prod_{k=1}^{m} p(x_k;\theta)$$

4. To obtain $\hat{\theta}_{ML}$ that maximizing the likelihood function, we must have

$$\frac{\partial \prod_{k=1}^{m} p(x_k;\theta)}{\partial \theta} \quad = \quad 0$$

1. It is more convenient to work with the logarithm of the likelihood function than with the likelihood function itself. Hence,

$$\mathcal{L}(\theta) = \ln \prod_{k=1}^{m} p(x_k;\theta) = \sum_{k=1}^{m} \ln p(x_k;\theta)$$



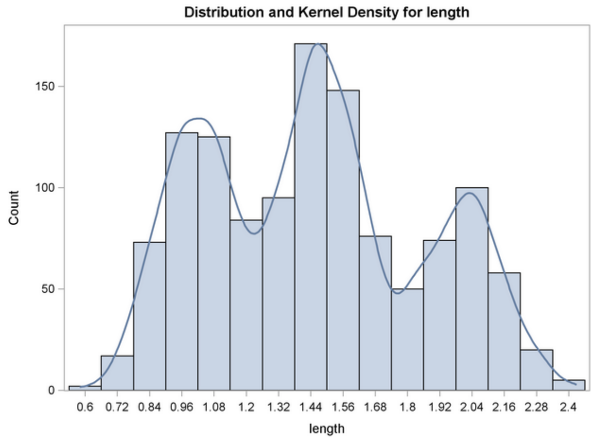
$$\hat{\theta}_{ML} = \underset{\theta}{argmax} \mathcal{L}(\theta)$$

Nonparametric methods for density estimation

1. Parametric forms do not always fit the densities encountered in practice.
2. Most of parametric densities are unimodal, whereas many practical problems have multi-modal densities.
3. Non-parametric methods can be used with arbitrary distributions without assumption of knowing the forms of the underlying densities.
4. In nonparametric estimation, we assume that similar inputs have similar outputs.
5. This is a reasonable assumption because the world is smooth and functions, whether they are densities, discriminants, or regression functions, change slowly.
6. Some approaches for nonparametric density estimation
   - Histogram
   - Parzen window
   - Kernel density estimator
   - Nearest neighbors

1. Divide the space into a set of regular intervals of the form

$$I_j = (x_0 + jh, x_0 + (j+1)h], \qquad \text{for } j \in \{\ldots, -1, 0, 1, \ldots\}.$$



2. In each interval, the density is constant and is proportional to the number of observations falling into this interval.

1. Naive estimator, addresses the choice of bin locations, thus the origin is eliminated.
2. For bin width h, bin denoted by $\mathcal{R}(x)$ is interval $\left[x - \frac{h}{2}, x + \frac{h}{2}\right)$ and the estimate is

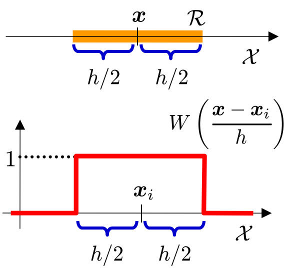
$$\hat{p}(x) = \frac{|\mathcal{R}(x)|}{mh}$$

3. The estimator can also be written as

$$\hat{p}(x) = \frac{1}{mh} \sum_{k=1}^{m} w\left(\frac{x - x_k}{h}\right)$$

w is weight function as

$$w(u) = \begin{cases} 1 & \text{if } |u| \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$



1. To get a smooth estimate, a smooth weight function (kernel function) is used.

$$\hat{p}(x) = \frac{1}{mh}\sum_{i=1}^{m} w\left(\frac{x-x_i}{h}\right)$$

   $w(.)$ is some kernel function and h is the smoothing parameter.

2. Gaussian kernel function with mean 0 and variance 1 is usually used.

$$w(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

3. Function $w(.)$ determines shape of influences and h determines window width.

4. The kernel estimator can be generalized to $D-$dimensional data.

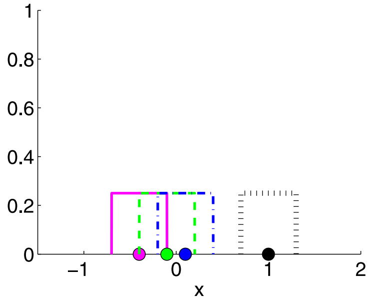
$$\hat{p}(x) = \frac{1}{mh^D}\sum_{k=1}^{m} w\left(\frac{x-x_k}{h}\right)$$

$$w(u) = \left(\frac{1}{\sqrt{2\pi}}\right)^D \exp\left(-\frac{||u||^2}{2}\right)$$

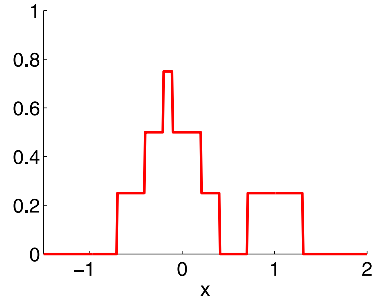
5. The total number of data points lying in this window (cube) equals to (drive it.)

$$k = \sum_{i=1}^{m} w\left(\frac{x-x_i}{h}\right)$$

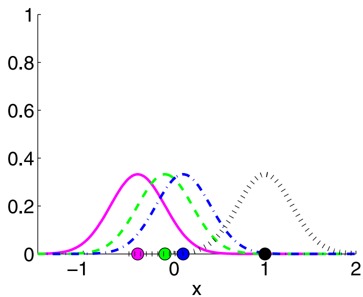
Kernel density estimator



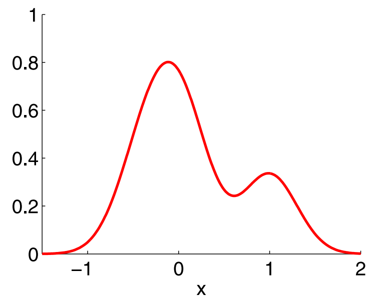
(a) Each Parzen window function



(b) Parzen window estimator



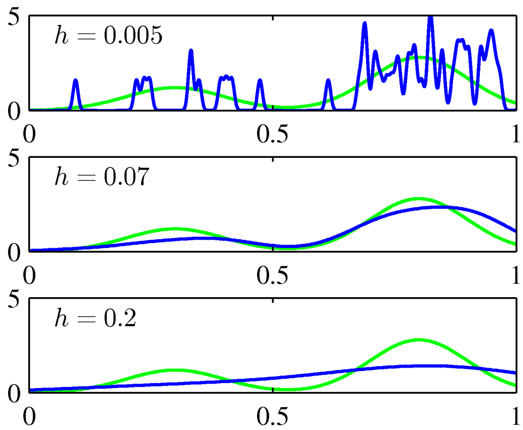
(a) Each Gaussian kernel function



(b) Kernel density estimator

Kernel density estimator

1. A difficulty with KDE is that the parameter h is fixed for all kernels.
2. Large value of h may lead to over-smoothing.
3. Reducing value of h may lead to noisy estimates.
4. The optimal choice of h may be dependent on location within the data space.



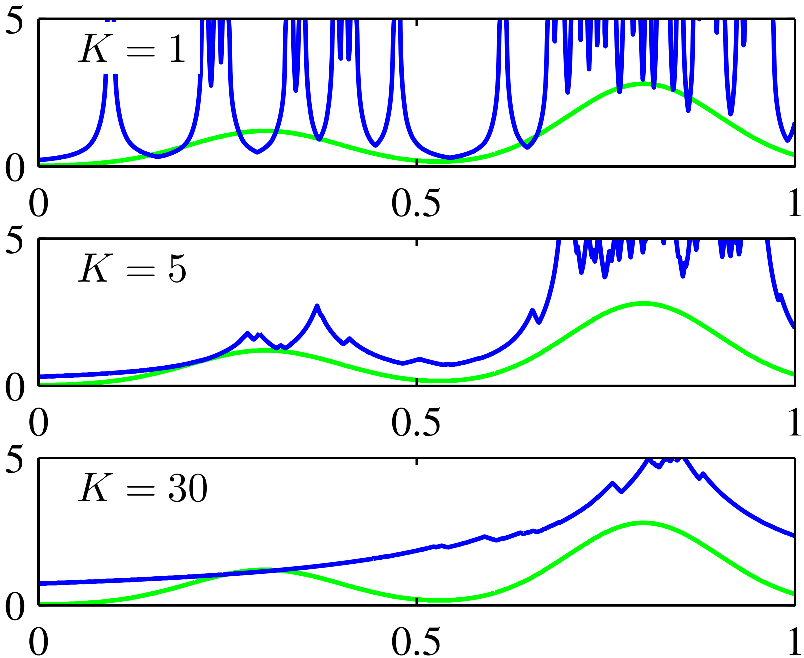
1. Instead of fixing h and determining the value of k from the data, we fix the value of k and use the data to find an appropriate value of h.
2. To do this, we consider a small sphere centered on the point x at which we wish to estimate the density $p(x)$ and allow the radius of the sphere to grow until it contains precisely k data points (Why?).

$$\hat{p}(x) = \frac{k}{mV}$$

   V is the volume of the resulting sphere.
3. Value of k determines the degree of smoothing and there is an optimum choice for k that is neither too large nor too small.
4. Note that: The model produced by k nearest neighborhood is not a true density model because the integral over all space diverges.

Theorem

It can be shown that both the K-NN and the kernel density estimators converge to the true probability density in the limit $N \to \infty$ provided V shrinks suitably with N, and K grows with N (Duda, Hart, and Stork 2001).



5
$K = 1$
0
0
0.5
1
5
$K = 5$
0
0
0.5
1
5
$K = 30$
0
0
0.5
1

Introduction

Generative models using latent variables

Mixture models for density estimation

1. An alternative way to model an unknown density function $p(x)$ is via linear combination of M density functions in the form of

$$p(x) = \sum_{k=1}^{M} \pi_k p(x|k)$$

where

$$\sum_{k=1}^{M} \pi_k = 1$$

$$\int_x p(x|k) dx = 1$$

2. This modeling implicitly assumes that each point x may be drawn from any M model distributions with probability π_k (for $k = 1, 2, \ldots, M$).

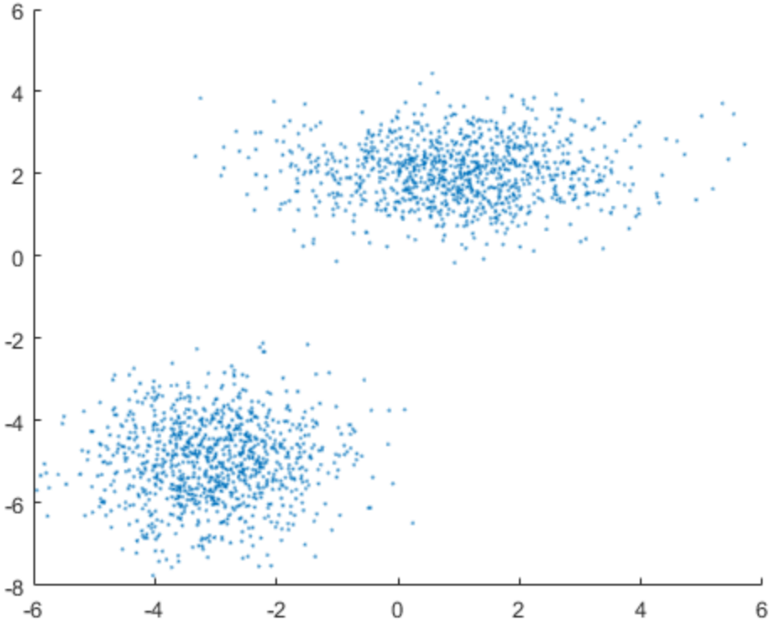
Mixture models for density estimation

1. It can be shown that this modeling can approximate closely any continuous density function for a sufficient number of mixtures M and appropriate model parameters.
2. First, we select a set of density components $p(x|k)$ in the parametric form $p(x|k, \theta)$.

$$p(x; \theta) = \sum_{k=1}^{M} \pi_k p(x|\theta_k)$$

3. Then, we compute parameters $\theta_1, \theta_2, \ldots, \theta_M$ and $\pi_1, \pi_2, \ldots, \pi_M$ based on training data.
4. The parameter set is defined as $\boldsymbol{\theta} = \{\pi_1, \pi_2, \ldots, \pi_M, \theta_1, \theta_2, \ldots, \theta_M\}$ and $\sum_i \pi_1 = 1$.
5. In order to find parameters, we use EM algorithm.

Gaussian Mixture models



Deep generative models

1. We assume that dataset $S = \{x_1, x_2, \dots, x_m\}$ are samples from distribution $p(x)$.
2. Goal of any generative model is to approximate $p(x)$ given access to the dataset S.
3. If we can learn a good generative model, we can use it for inference.
4. We usually have three fundamental inference queries for evaluating a generative model.
   - Density estimation: Given a point x, what is the probability assigned by the model, i.e., $p(x; \theta)$?
   - Sampling: How can we generate new data from the model distribution, i.e., $x_{new} \sim p(x; \theta)$?
   - Unsupervised representation learning: How can we learn meaningful feature representations for a point x?

Deep generative models

Latent variable models

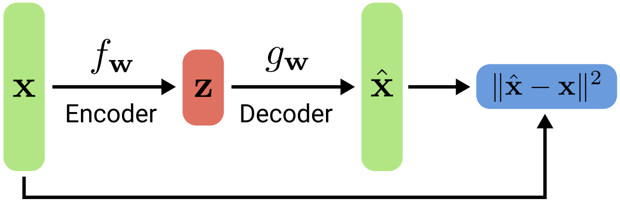
Latent variable models[2]

1. These models map between observation space $\mathbf{x} \in \mathbb{R}^D$ and latent space $\mathbf{z} \in \mathbb{R}^Q$:

   Encoder $f_\mathbf{w} = \mathbf{x} \mapsto \mathbf{z}$

   Dncoder $g_\mathbf{w} = \mathbf{z} \mapsto \mathbf{x}$

2. Each latent variable gets associated with each data point in the training set.
3. The latent vectors are smaller than the observations $(Q < D) \Rightarrow$ compression.
4. Models are linear or non-linear, deterministic or stochastic, with/without encoder.



[2]This slide taken from slides of Prof. Geiger

Generative latent variable models[3]

1. These models often consider a simple Bayesian model

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) d\mathbf{z} = \hat{\mathbb{E}}_{\mathbf{z}\sim p(\mathbf{z})} [p(\mathbf{x}|\mathbf{z})]$$

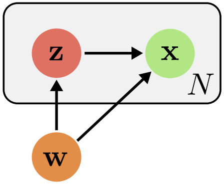
   - $p(\mathbf{z})$ is the prior over the latent variable $\mathbf{z} \in \mathbb{R}^Q$.
   - $p(\mathbf{x}|\mathbf{z})$ is the likelihood (= decoder that transforms $\mathbf{z}$ into a distribution over $\mathbf{x}$).
   - $p(\mathbf{x})$ is the marginal over the joint distribution $p(\mathbf{x}, \mathbf{z})$.

2. The goal is to maximize $p(\mathbf{x})$ for dataset S by learning the two models $p(\mathbf{z})$ and $p(\mathbf{x}|\mathbf{z})$ such that latent variables $\mathbf{z}$ best capture the latent structure of data.

[3] This slide taken from slides of Prof. Geiger

Generative latent variable models[4]

1. These models are represented using graphical model in plate notation.

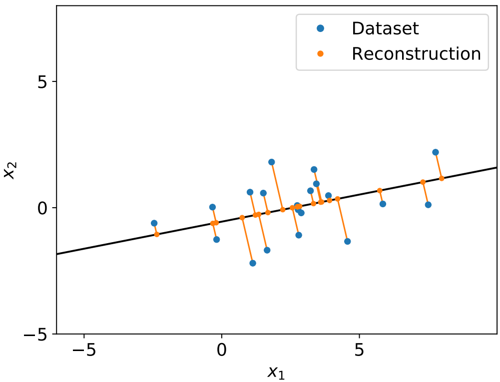


- Variables inside plates are replicated (we have N data points to explain).
- Each data point $\mathbf{x}$ is associated with a latent variable $\mathbf{z}$.
- We use a single $\mathbf{w}$ to refer to all model parameters and parameters are global (exist only once).

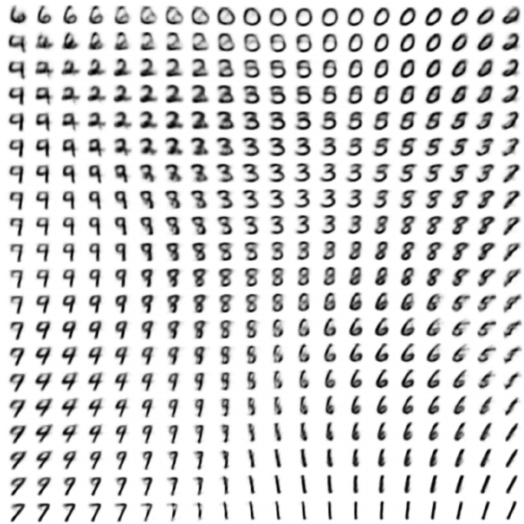
[4] This slide taken from slides of Prof. Geiger

Generative latent variable models(Kingma and Welling 2014)

1D Manifold in 2D Space



Learned MNIST manifold



Deep generative models

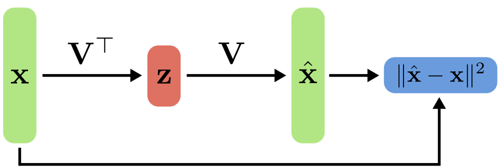
Principal component analysis

Principal component analysis (PCA)[5]

1. Let
   - $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)^\top \in \mathbb{R}^{N \times D}$ be a dataset of samples $\mathbf{x}_i \in \mathbb{R}^D$,
   - $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)^\top \in \mathbb{R}^{N \times Q}$ be the corresponding latent variables $\mathbf{z}_i \in \mathbb{R}^Q$.
2. The goal of PCA is to learn a linear bidirectional mapping $\mathcal{X} \longleftrightarrow \mathcal{Z}$ such that as much information of $\mathcal{X}$ as possible is retained in $\mathcal{Z}$.
3. Let the following linear mapping maps data from latent to observation space.

$$\hat{\mathbf{x}}_i = \bar{\mathbf{x}} + \sum_{j=1}^{Q} z_{ij} \mathbf{v}_j$$

   where $\bar{\mathbf{x}}$ is data mean and $\mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_Q)$ is an orthonormal basis.



4. The goal is to minimize the L_2 reconstruction loss wrt. $\mathbf{Z}$ and $\mathbf{V}$.

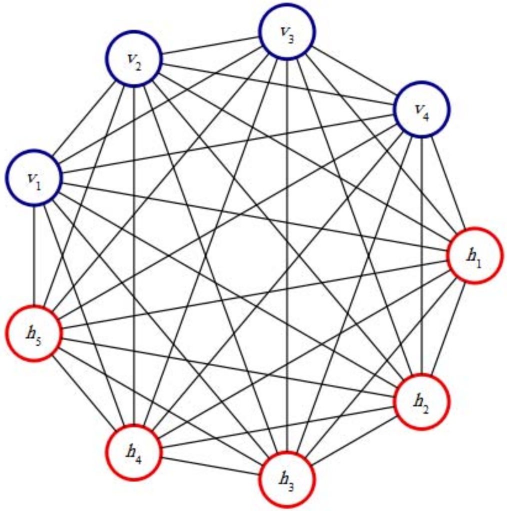
$$\mathcal{L}(\mathbf{Z}, \mathbf{V}) = \sum_{i=1}^{N} \|\hat{\mathbf{x}}_i - \mathbf{x}_i\|^2$$

[5] This slide taken from slides of Prof. Geiger

Deep generative models

Boltzmann Machine

1. BMs are fully connected networks of binary units.
2. BM is an undirected symmetric network of binary units that are divided into visible and hidden units.



1. BMs are theoretically capable of learning any given distribution.
2. The network sets the strengths of the connections between the units to capture the correlations between them to build a generative network capable of producing new examples of the same distribution.
3. Since all variables in a BM are not directly observed, it gives us a handle to control the sampling of new examples.
4. The model can take in an incomplete example and use it to output the complete version.

1. BM is a network with an energy defined for the overall network.
2. For a BM with only observed units, the energy is defined as

$$E(\mathbf{x}) = -\sum_{ij} w_{ij} x_i x_j - \sum_{i=1} b_i x_i$$
$$= -\mathbf{x}^\top \mathbf{W}\mathbf{x} - \mathbf{b}^\top \mathbf{x}$$
$$H(\mathbf{x}) = -E(\mathbf{x})$$

Alternatively, happiness is used to avoid multiple minus signs.

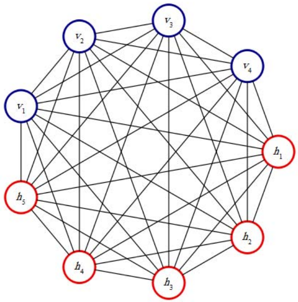
- $\mathbf{x} = (x_1, x_2, \dots, x_d) \in \{0,1\}^d$ is the input vector.
- $\mathbf{W} = (w_{ij})$ is the weight matrix
- $\mathbf{b} = (b_1, b_2, \dots, b_d) \in \{0,1\}^d$ is the bias vector.

3. The joint probability distribution defined as

$$p_{\text{model}}(\mathbf{x}) = \frac{\exp(-E(\mathbf{x}))}{Z}$$

Z is Partition function that ensures $\sum_x p_{\text{model}}(x) = 1$.

1. BM becomes more powerful when not all the variables are observed.
2. The latent variables can act similarly to hidden units in a MLP.



3. By decomposing units into two subsets: visible $\mathbf{v}$ and hidden units $\mathbf{h}$, we obtain.

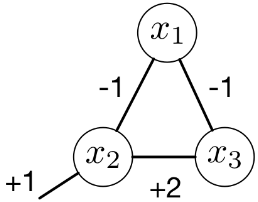
$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{v}^\top \mathbf{R}\mathbf{v} - \mathbf{v}^\top \mathbf{W}\mathbf{h} - \mathbf{h}^\top \mathbf{S}\mathbf{h} - \mathbf{b}^\top \mathbf{v} - \mathbf{c}^\top \mathbf{h}$$

4. The joint probability distribution defined as

$$p_{\text{model}}(\mathbf{v}, \mathbf{h}) = \frac{\exp\left(-E(\mathbf{v}, \mathbf{h})\right)}{Z}$$

Z is Partition function that ensures $\sum_x p_{\text{model}}(x) = 1$.

Example:

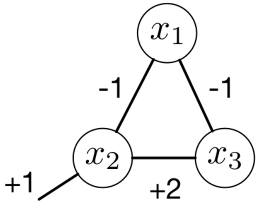


x_1	x_2	x_3	$w_{12}x_1x_2$	$w_{13}x_1x_3$	$w_{23}x_2x_3$	b_2x_2	$H(\mathbf{x})$	$\exp(H(\mathbf{x}))$	$p(\mathbf{x})$
-1	-1	-1	-1	-1	2	-1	-1	0.368	0.0021
-1	-1	1	-1	1	-2	-1	-3	0.050	0.0003
-1	1	-1	1	-1	-2	1	-3	0.368	0.0021
-1	1	1	1	1	2	1	5	148.413	0.8608
1	-1	-1	1	1	2	-1	3	20.086	0.1165
1	-1	1	1	-1	-2	-1	-3	0.050	0.0003
1	1	-1	-1	1	-2	1	-1	0.368	0.0021
1	1	1	-1	-1	2	1	1	2.718	0.0158

$$\mathcal{Z} = 172.420$$

Figure: Roger Grosse

Marginal probabilities:



$$p(x_1 = 1) = \frac{1}{\mathcal{Z}} \sum_{\mathbf{x}:x_1=1} \exp(H(\mathbf{x}))$$
$$= \frac{20.086 + 0.050 + 0.368 + 2.718}{172.420}$$
$$= 0.135$$

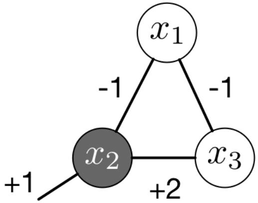
x_1	x_2	x_3	$w_{12}x_1x_2$	$w_{13}x_1x_3$	$w_{23}x_2x_3$	b_2x_2	$H(\mathbf{x})$	$\exp(H(\mathbf{x}))$	$p(\mathbf{x})$
-1	-1	-1	-1	-1	2	-1	-1	0.368	0.0021
-1	-1	1	-1	1	-2	-1	-3	0.050	0.0003
-1	1	-1	1	-1	-2	1	-3	0.368	0.0021
-1	1	1	1	1	2	1	5	148.413	0.8608
1	-1	-1	1	1	2	-1	3	20.086	0.1165
1	-1	1	1	-1	-2	-1	-3	0.050	0.0003
1	1	-1	-1	1	-2	1	-1	0.368	0.0021
1	1	1	-1	-1	2	1	1	2.718	0.0158

$$\mathcal{Z} = 172.420$$

Figure: Roger Grosse

Conditional probabilities:

$$p(x_1 = 1 \mid x_2 = -1) = \frac{\sum_{\mathbf{x}:x_1=1,x_2=-1} \exp(H(\mathbf{x}))}{\sum_{\mathbf{x}:x_2=-1} \exp(H(\mathbf{x}))}$$
$$= \frac{20.086 + 0.050}{0.368 + 0.050 + 20.086 + 0.050}$$
$$= 0.980$$



x_1	x_2	x_3	$w_{12}x_1x_2$	$w_{13}x_1x_3$	$w_{23}x_2x_3$	b_2x_2	$H(\mathbf{x})$	$\exp(H(\mathbf{x}))$	$p(\mathbf{x})$
-1	-1	-1	-1	-1	2	-1	-1	0.368	0.0021
-1	-1	1	-1	1	-2	-1	-3	0.050	0.0003
-1	1	-1	1	-1	-2	1	-3	0.368	0.0021
-1	1	1	1	1	2	1	5	148.413	0.8608
1	-1	-1	1	1	2	-1	3	20.086	0.1165
1	-1	1	1	-1	-2	-1	-3	0.050	0.0003
1	1	-1	-1	1	-2	1	-1	0.368	0.0021
1	1	1	-1	-1	2	1	1	2.718	0.0158

Figure: Roger Grosse

Boltzmann Machine Learning

1. Learning algorithms for BMs are usually based on maximum likelihood.
2. All BMs have an intractable partition function, so the maximum likelihood gradient must be approximated.
3. An interesting property of BMs is that the update for a particular w_{ij} depends only on the statistics of x_i and x_j.

1. A BM admits the following likelihood for points $x^{(1)}, \dots, x^{(n)}$.

$$\mathcal{L}(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}) = \prod_{i=1}^{n} p(\mathbf{x}^{(i)})$$

2. We will work with the log-likelihood instead of the true likelihood.

$$\begin{aligned}
\log \mathcal{L}(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}) &= \sum_{k=1}^{n} \log \frac{\exp\left(H(\mathbf{x}^{(k)})\right)}{Z} \\
&= \sum_{k=1}^{n} \left[\log\left(\exp\left(H(\mathbf{x}^{(k)})\right)\right) - \log Z\right] \\
&= \sum_{k=1}^{n} \left[H(\mathbf{x}^{(k)}) - \log Z\right]
\end{aligned}$$

3. The aim is to maximize $\mathbb{E}_{x \sim p_{\text{data}}}\left[\mathcal{L}(\mathbf{x})\right]$

$$\mathop{\mathbb{E}}_{\mathbf{x} \sim p_{\text{data}}}\left[\mathcal{L}(\mathbf{x})\right] = \sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \mathcal{L}(\mathbf{x}^{(k)})$$

1. Now, deriving the gradient with respect to the weights ($\nabla_{w_{i,j}} \log \mathcal{L}$)

$$\nabla_{w_{i,j}} \left[\sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \left(H(\mathbf{x}^{(k)}) - \log Z \right) \right] = \sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \nabla_{w_{i,j}} H(\mathbf{x}^{(k)}) - \sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \nabla_{w_{i,j}} \log Z$$

2. The first term equals to

$$\begin{aligned}
\sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \nabla_{w_{i,j}} H(\mathbf{x}^{(k)}) &= \sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) \nabla_{w_{i,j}} \left[\sum_{i \neq j} w_{i,j} x_i^{(k)} x_j^{(k)} \right. \\
&\quad \left. + \sum_{i} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) b_i x_i^{(k)} \right] \\
&= \sum_{k=1}^{n} p_{\text{data}}(\mathbf{x} = \mathbf{x}^{(k)}) x_i^{(k)} x_j^{(k)} \\
&= \mathop{\mathbb{E}}_{\mathbf{x} \sim p_{\text{data}}} [x_i x_j]
\end{aligned}$$

1. The second term equals to

$$\begin{aligned}
\nabla_{w_{i,j}} \log Z &= \nabla_{w_{i,j}} \log \sum_{\mathbf{x}} \exp\left(H(\mathbf{x})\right) \\
&= \frac{1}{\sum_{\mathbf{x}} \exp\left(H(\mathbf{x})\right)} \nabla_{w_{i,j}} \sum_{\mathbf{x}} \exp\left(H(\mathbf{x})\right) \\
&= \frac{1}{Z} \nabla_{w_{i,j}} \sum_{\mathbf{x}} \exp\left(H(\mathbf{x})\right) \\
&= \frac{1}{Z} \sum_{\mathbf{x}} \exp\left(H(\mathbf{x})\right) \nabla_{w_{i,j}} H(\mathbf{x}) \\
&= \sum_{\mathbf{x}} \frac{\exp\left(H(\mathbf{x})\right)}{Z} \nabla_{w_{i,j}} H(\mathbf{x}) \\
&= \sum_{\mathbf{x}} p_{\text{model}}(\mathbf{x}) \nabla_{w_{i,j}} H(\mathbf{x}) \\
&= \sum_{\mathbf{x}} p_{\text{model}}(\mathbf{x}) [x_i x_j] \\
&= \mathop{\mathbb{E}}_{\mathbf{x} \sim p_{\text{model}}} [x_i x_j]
\end{aligned}$$

1. By combining the above equations, the gradient w.r.t weights becomes

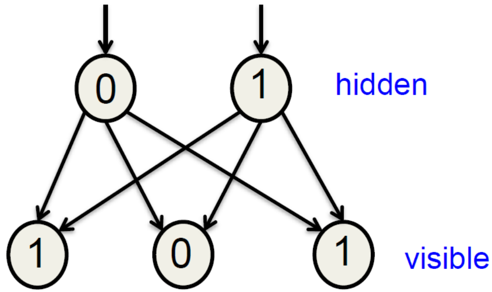
$$\nabla_{w_{i,j}} \log \mathcal{L} = \mathop{\mathbb{E}}_{\mathbf{x}\sim p_{\text{data}}} [x_i x_j] - \mathop{\mathbb{E}}_{\mathbf{x}\sim p_{\text{model}}} [x_i x_j]$$

2. By combining the above equations, the gradient w.r.t biases becomes

$$\nabla_{b_i} \log \mathcal{L} = \mathop{\mathbb{E}}_{\mathbf{x}\sim p_{\text{data}}} [x_i] - \mathop{\mathbb{E}}_{\mathbf{x}\sim p_{\text{model}}} [x_i]$$

Generating a sample by Boltzmann Machine

1. In BM, we generate in two steps:
   - Pick the hidden states from $p(\mathbf{h})$.
   - Pick the visible states from $p(\mathbf{v}|\mathbf{h})$.



2. The probability of generating a visible vector, $\mathbf{v}$, is computed by summing over all possible hidden states.

$$p(\mathbf{v}) = \sum_{\mathbf{h}} p(\mathbf{h})p(\mathbf{v}|\mathbf{h})$$

1. Given an ordered set of variable, $x_1, \ldots, x_d$, and a starting configuration $x^0 = (x_1^0, \ldots, x_d^0)$,

Gibbs sampling uses the following procedure

- Repeat until convergence for $t = 1, 2, \ldots,$
  - Set $\mathbf{x} \leftarrow \mathbf{x}^{t-1}$.
  - For each variable x_i in the order we fixed:
    1) Sample $x_i' \sim p(x_i \mid \mathbf{x}_{-i})$.
    2) Update $\mathbf{x} \leftarrow (x_1, \ldots, x_i', \ldots, x_d)$.
  - Set $\mathbf{x}^t \leftarrow \mathbf{x}$.

We use $\mathbf{x}_{-i}$ to denote all variables in $\mathbf{x}$ except x_i.

2. It is often very easy to performing each sampling step, since we only need to condition x_i on other variables.
3. Note that when we update x_i, we immediately use its new value for sampling other variables x_j.

Gibbs sampling (example)

1. Let $d = 3$, we need to define

$$
\begin{aligned}
x_0' &\sim p(x_0|x_1, x_2)\\
x_1' &\sim p(x_1|x_0', x_2)\\
x_2' &\sim p(x_2|x_0', x_1')
\end{aligned}
$$

2. Each dimension is binary, the above 3 models must necessarily return the probability of observing a 1.
3. Note that when we update x_i, we immediately use its new value for sampling other variables x_j.

Gibbs sampling

1. We drive $p(x_i|\mathbf{x}_{-i})$ using probability of axioms and discarding bias terms

$$
\begin{aligned}
p(x_i = 1|\mathbf{x}_{-i}) &= \frac{p(x_i = 1, \mathbf{x}_{-i})}{p(x_i = 1, \mathbf{x}_{-i}) + p(x_i = 0, \mathbf{x}_{-i})} \\
&= \frac{\exp\left[\sum_{i \neq j} w_{ij} x_j\right]}{1 + \exp\left[\sum_{i \neq j} w_{ij} x_j\right]} \\
&= \frac{1}{1 + \exp\left[-\sum_{j \neq i} w_{ij} x_j\right]} \\
&= \sigma\left(\sum_{j \neq i} w_{i,j} x_j\right)
\end{aligned}
$$

Gibbs sampling (example)

1. We drive $p(x_0|x_1, x_2)$ using probability of axioms

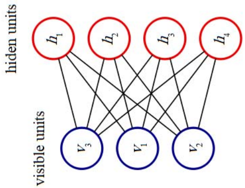
$$
\begin{aligned}
p(x_0 = 1|x_1, x_2) &= \frac{p(x_0 = 1, x_1, x_2)}{p(x_1, x_2)} = \frac{p(x_0 = 1, x_1, x_2)}{\sum_{x_0 \in \{0,1\}} p(x_0, x_1, x_2)} \\
&= \frac{p(x_0 = 1, x_1, x_2)}{p(x_0 = 0, x_1, x_2) + p(x_0 = 1, x_1, x_2)} \\
&= \frac{1}{1 + \frac{p(x_0=0, x_1, x_2)}{p(x_0=1, x_1, x_2)}} = \frac{1}{1 + \frac{\exp\left(H(x_0=0, x_1, x_2)\right))}{\exp\left(H(x_0=1, x_1, x_2)\right))}} \\
&= \frac{1}{1 + \exp\left(H(x_0 = 0, x_1, x_2) - H(x_0 = 1, x_1, x_2)\right)} \\
&= \frac{1}{1 + \exp\left(\sum_{i \neq j} w_{ij} x_i x_j + \sum_i b_i x_i - \left(\sum_{i \neq j} w_{ij} x_i x_j + \sum_i b_i x_i\right)\right)} \\
&= \frac{1}{1 + \exp\left(-\sum_{j \neq i = 0} w_{ij} x_j - b_i\right)} \\
&= \sigma\left(\sum_{j \neq i = 0} w_{i,j} x_j + b_i\right)
\end{aligned}
$$

Deep generative models

Restricted Boltzmann Machine

Restricted Boltzmann Machine (RBM)

1. The tractability of the joint distribution is one of the biggest drawbacks of BMs.
2. RBMs are a special type of BMs with two layers: One visible and one hidden layer.



3. The connections in an RBM are undirected and the graph is a bipartite graph.
4. By the Markov property, $p(\mathbf{h}|\mathbf{v})$ and $p(\mathbf{v}|\mathbf{h})$ both factorize (Show later).

$$p(\mathbf{h}|\mathbf{v}) = \prod_i p(h_i|\mathbf{v})$$

$$p(\mathbf{v}|\mathbf{h}) = \prod_j p(v_j|\mathbf{h})$$

5. There is no need for variational Bayes and Gibbs sampling can be implemented efficiently by alternating between hidden and visible levels, known as block Gibbs sampling.
6. The marginal distributions $p(\mathbf{v})$ and $p(\mathbf{h})$ do not factorize (Show it).

Restricted Boltzmann Machine (RBM)

1. This bipartite architecture allows us to have more control over the joint distribution.
2. RBMs are a powerful replacement for fully connected BMs when building a deep architecture because of the independence of units within the same layer, which allows for more freedom and flexibility.
3. The latent variables can act similarly to hidden units in a MLP.
4. RBMs can be trained using the techniques of maximum likelihood.
5. Sampling from an RBM can be done using Gibbs sampling method or any other Markov Chain Monte Carlo (MCMC) method.

1. Hidden units are conditionally independent given the visible units and vice versa.

$$p(v_i = 1|\mathbf{h}) = \sigma\left(\sum_j w_{ij} h_j + b_i\right)$$
$$p(h_j = 1|\mathbf{v}) = \sigma\left(\sum_i w_{ij} v_i + c_j\right)$$

2. Given visible $\mathbf{v}$, we can sample each h independently.
3. Given hidden $\mathbf{h}$, we can sample each v_j independently.

1. The energy of the joint state $\{\mathbf{v}, \mathbf{h}\}$ is defined as follows:

$$E(v, h; \theta) = -\mathbf{v}^\top \mathbf{W}\mathbf{h} - \mathbf{b}^\top \mathbf{v} - \mathbf{a}^\top \mathbf{h}$$

   where $\theta = \{\mathbf{W}, \mathbf{b}, \mathbf{a}\}$ are the model parameters. W_{ij} represents the symmetric interaction term between visible variable i and hidden variable j, and b_i and a_j are bias terms.

2. The joint distribution equals to

$$p(\mathbf{v}, \mathbf{h}; \theta) = \frac{1}{Z(\theta)} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right)$$
$$Z(\theta) = \sum_{\mathbf{v}} \sum_{\mathbf{h}} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right)$$

1. The model assigns the following probability to a visible vector $\mathbf{v}$

$$p(\mathbf{v};\theta) = \sum_{\mathbf{h}} p(\mathbf{v},\mathbf{h};\theta)$$

2. The hidden variables can be explicitly marginalized out

$$\begin{aligned}
p(\mathbf{v};\theta) &= \frac{1}{Z(\theta)} \sum_{\mathbf{h}} \exp\left(-E(\mathbf{v},\mathbf{h};\theta)\right) \\
&= \frac{1}{Z(\theta)} \sum_{\mathbf{h}} \exp\left(\mathbf{v}^\top \mathbf{W}\mathbf{h} + \mathbf{b}^\top \mathbf{v} + \mathbf{a}^\top \mathbf{h}\right) \\
&= \frac{1}{Z(\theta)} \exp(\mathbf{b}^\top \mathbf{v}) \prod_{j=1}^{F} \sum_{h_j \in \{0,1\}} exp\left(a_j h_j + \sum_i W_{ij} v_i h_j\right) \\
&= \frac{1}{Z(\theta)} \exp(\mathbf{b}^\top \mathbf{v}) \prod_{j=1}^{F} \left(1 + exp\left(a_j + \sum_i W_{ij} v_i\right)\right)
\end{aligned}$$

1. Bipartite graph structure of RBM has the following property.
2. Conditionals $p(\mathbf{h}|\mathbf{v})$ and $p(\mathbf{v}|\mathbf{h})$ are factorized and easy computed.

$$\begin{aligned} p(\mathbf{h}|\mathbf{v}) &= \frac{p(\mathbf{h},\mathbf{v})}{p(\mathbf{v})} = \frac{1}{p(\mathbf{v})}\frac{1}{Z}\exp\left(\mathbf{b}^\top\mathbf{v} + \mathbf{c}^\top\mathbf{h} + \mathbf{v}^\top\mathbf{W}\mathbf{h}\right) \\ &= \frac{1}{Z'}\exp\left(\mathbf{c}^\top\mathbf{h} + \mathbf{v}^\top\mathbf{W}\mathbf{h}\right) \\ &= \frac{1}{Z'}\exp\left(\sum_j c_j h_j + \sum_j \mathbf{v}^\top\mathbf{W}_{:j}h_j\right) \\ &= \frac{1}{Z'}\prod_j \exp\left(c_j h_j + \mathbf{v}^\top\mathbf{W}_{:j}h_j\right) \end{aligned}$$

3. Normalizing the distributions over individual binary h

$$\begin{aligned} p(h_j = 1|\mathbf{v}) &= \frac{\tilde{p}(h_j = 1|\mathbf{v})}{\tilde{p}(h_j = 0|\mathbf{v}) + \tilde{p}(h_j = 1|\mathbf{v})} \\ &= \frac{\exp\left(c_j + \mathbf{v}^\top\mathbf{W}_{:j}\right)}{\exp(0) + \exp\left(c_j + \mathbf{v}^\top\mathbf{W}_{:j}\right)} = \sigma\left(c_j + \mathbf{v}^\top\mathbf{W}_{:j}\right) \end{aligned}$$

4. Similarly

$$p(v_i = 1|\mathbf{h}) = \sigma\left(c_i + \mathbf{W}_{i:}\mathbf{h}\right)$$

Restricted Boltzmann Machine Training (Contrastive Divergence)

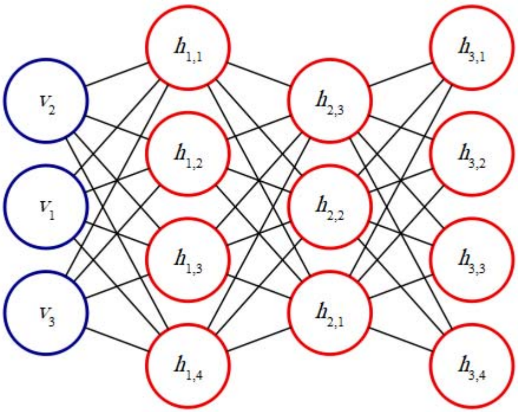
1. **Initialize Model Parameters**
   - Initialize weights, visible biases, and hidden biases randomly.
2. **Compute Probabilities of Hidden Units**
   - Given a training example, compute the probabilities of hidden units being activated.
3. **Sample hidden Configuration**
   - Sample a binary hidden unit configuration based on the computed probabilities.
4. **Reconstruction Visible Units**
   - Given sampled hidden configuration, compute probabilities of visible units being activated.
5. **Update Model Parameters**
   - Update weights based on difference between outer products of original training and reconstructed samples.
   - The goal is to make model more likely to generate training examples and less likely to generate samples that do not resemble the training data.
6. **Repeat Steps for Multiple Iterations**
   - Iterate through steps 2-5 for multiple training examples and/or epochs to refine model parameters.

Deep generative models

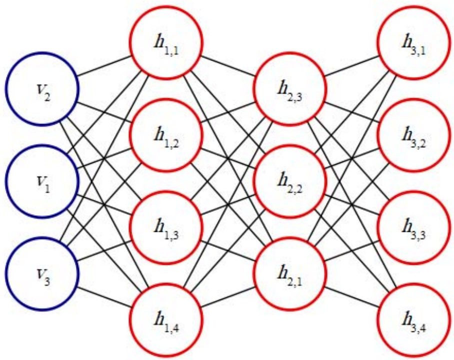
Deep Boltzmann Machine

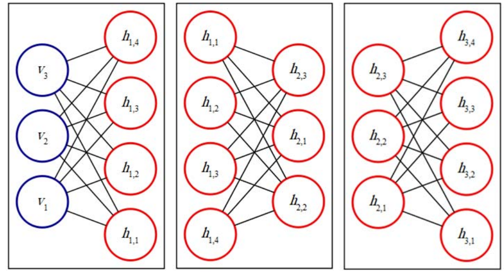
Deep Boltzmann Machine (DBM)

1. DBM is an undirected deep network of several hidden layers (Salakhutdinov and Larochelle 2010).
2. Every unit is connected to every unit from the adjacent layers.
3. There are no connections between units of the same layer.



1. DBMs can also be viewed as a group of RBMs stacked together.

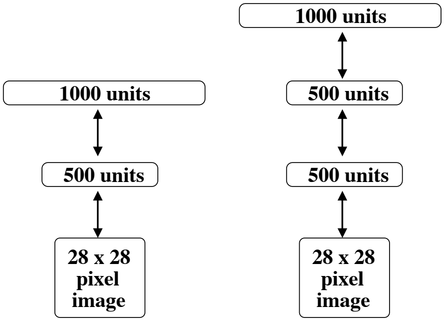




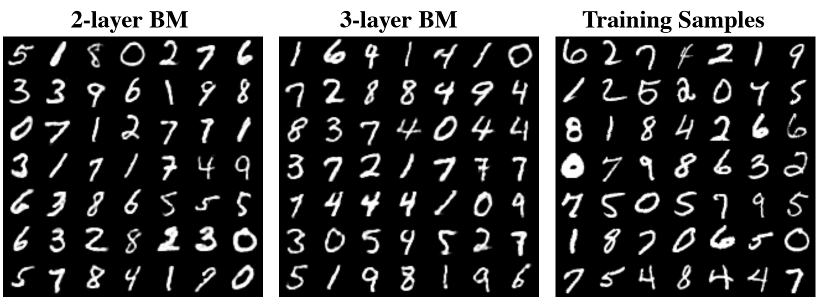
2. Training of DBMs is often done in two stages:
   - A pre-training stage where every RBM is trained independently.
   - a fine tuning stage where the network is trained at once using backpropagation.

Deep Boltzmann Machine (DBM)

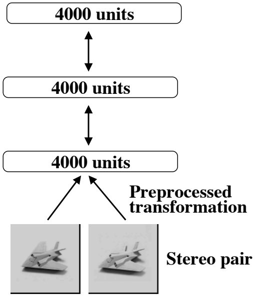
1. Considering two architectures for MNIST dataset.



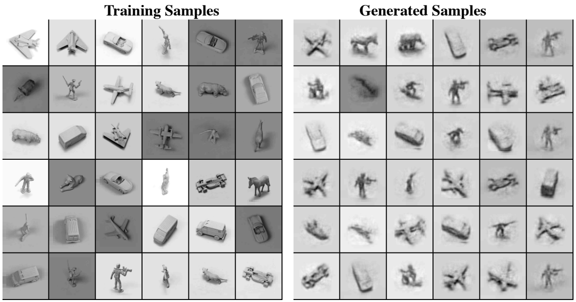
2. The results using Gibbs sampling.



1. Considering the following architecture for NORB dataset.



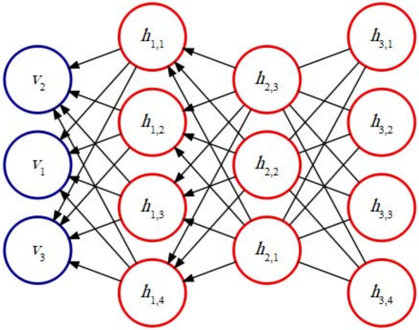
2. The results using Gibbs sampling.



Deep generative models

Deep Belief Networks

1. DBN is a hybrid PGM involving both directed and undirected connections.
2. Deep belief networks consisting of many hidden layers.
3. Connections between top two layers are undirected
4. Connections between all other layers is directed, pointing towards data.



$$p(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \ldots, \mathbf{h}^{(k)}) = p(\mathbf{v}|\mathbf{h}^{(1)})p(\mathbf{h}^{(1)}|\mathbf{h}^{(2)}) \ldots p(\mathbf{h}^{(k-2)}|\mathbf{h}^{(k-1)})p(\mathbf{h}^{(k-1)}, \mathbf{h}^{(k)})$$

5. $p(\mathbf{h}^{(k-1)}, \mathbf{h}^{(k)})$ (the marginal distribution over the top two layers) is an RBM.

1. A DBN with k hidden layers has k weight matrices $\mathbf{W}^{(1)}, \dots, \mathbf{W}^{(k)}$.
2. It contains $k+1$ bias vectors $\mathbf{b}^{(0)}, \dots, \mathbf{b}^{(1)}$, where $\mathbf{b}^{(0)}$ is bias vector for visible layer.
3. Probability distribution represented by DBN is

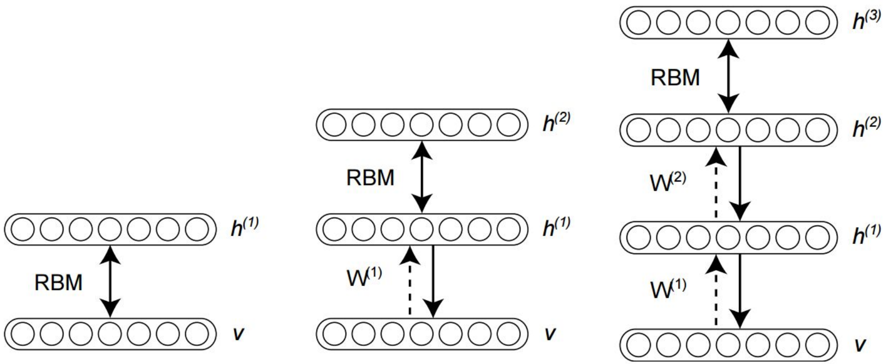
$$p(\mathbf{h}^{(k-1)}, \mathbf{h}^{(k)}) \propto \exp\left[\mathbf{b}^{(k)\top}\mathbf{h}^{(k-1)} + \mathbf{b}^{(k-1)\top}\mathbf{h}^{(k)} + \mathbf{h}^{(k-1)\top}\mathbf{W}^{(k)}\mathbf{h}^{(k)}\right]$$

$$p(h_i^{(j)} = 1|\mathbf{h}^{(j+1)}) = \sigma\left(b_i^{(j)} + \mathbf{W}_{:i}^{(j+1)}\mathbf{h}^{(j+1)}\right)$$

$$p(v_i = 1|\mathbf{h}^{(1)}) = \sigma\left(b_i^{(0)} + \mathbf{W}_{:i}^{(1)}\mathbf{h}^{(1)}\right)$$

4. For generating a sample from a DBN, do
   - Use several Gibbs sampling steps from top two hidden layers.
   - Use a single pass of ancestral sampling through rest of model.

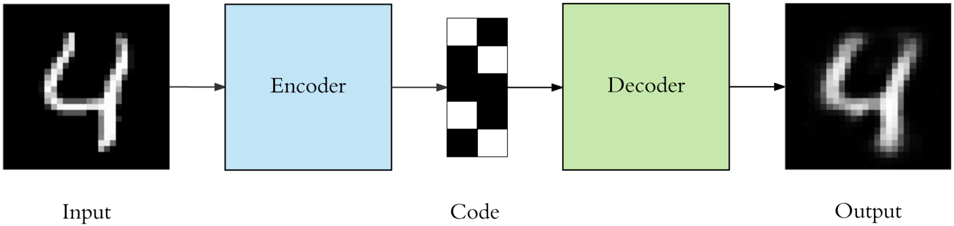
1. Deep belief networks training



(a) Stage 1 (b) Stage 2 (c) Stage 3

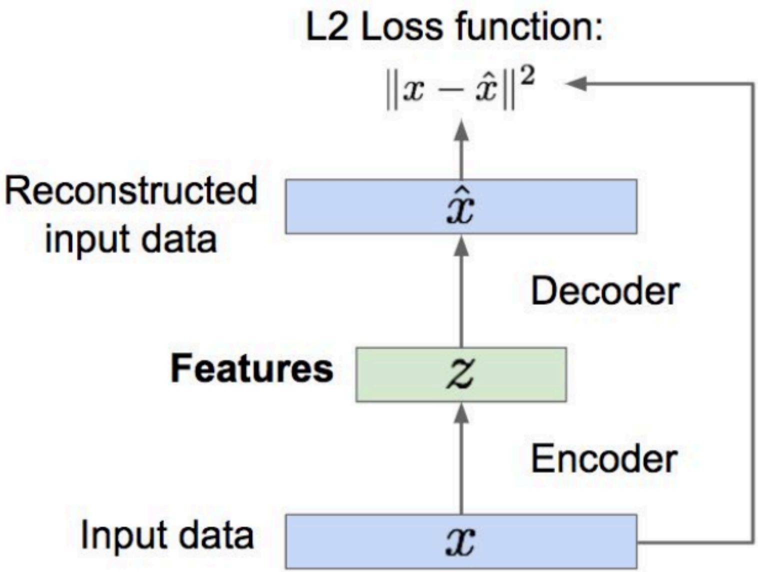
Autoencoder models

1. An autoencoder consists of 3 components: encoder, code and decoder.

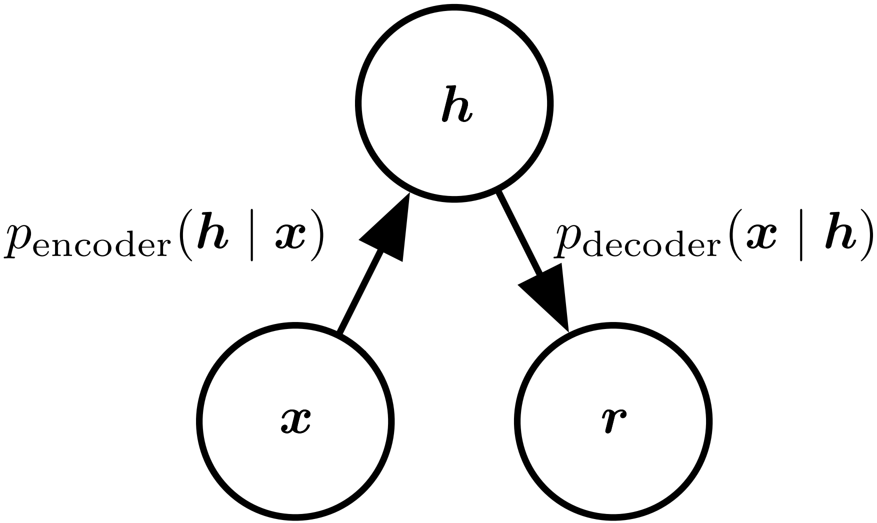


2. The encoder compresses the input and produces the code, the decoder then reconstructs the input only using this code.

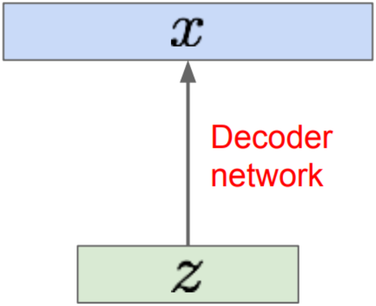
1. We don't use labels but the Autoencoder is trained in supervised manner.



1. The Autoencoder has the following probabilistic model.

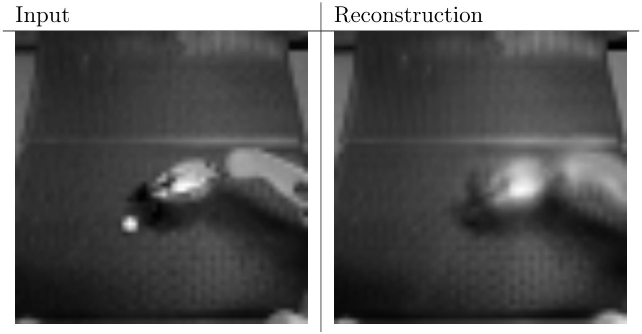


1. Can we generate new sample from an auto encoder?
2. Suppose training data is generated from latent representation z.
3. x is an input sample, z is latent factors used to generate x.



4. How generate a new sample?
   - Sample from some prior $p(z)$.
   - Obtain $p(x|z)$.

1. A sample generated from an Autoencoder.



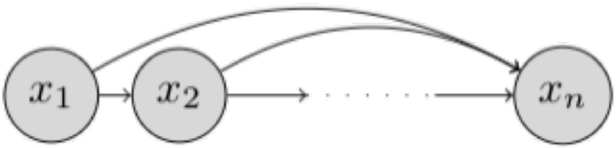
2. MSE can ignore small but task-relevant features.
3. The ping pong ball vanishes because it is not large enough to significantly affect the MSE.
4. Unfortunately, the autoencoder has limited capacity, and the training with MSE did not identify the relevant features.
5. We want to sample from complex, high-dimensional training distribution. No direct way to do this! How do it?

Autoregressive models

1. We assume we have a dataset $S = \{x_1, x_2, \ldots, x_m\}$ of n-dimensional points.
2. For simplicity, we assume points are binary, i.e., $x \in \{0, 1\}^n$.
3. Using chain rule, we can factorize the joint distribution as

$$p(x) = p(x_1, x_2, \ldots, x_n) = \prod_{i=1}^{n} p(x_i | x_1, x_2, \ldots, x_{i-1}) = \prod_{i=1}^{n} p(x_i | \mathbf{x}_{<i})$$

   where $\mathbf{x}_{<i} = [x_1, x_2, \ldots, x_{i-1}]$ denotes a vector of random variables with index less than i.
4. The chain rule factorization can be expressed graphically as a Bayesian network.



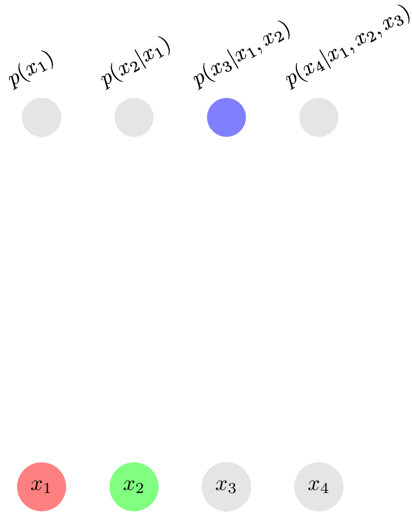
1. The autoregressive constraint is a way to model sequential data.
2. The factorization contains n factors and some of these factors contain many parameters ($O(2^n)$ in total).
3. It is infeasible to learn such an exponential number of parameters.
4. AR models use (deep) neural network to parameterize these factors $p(x_i|x_{<i})$.
5. We assume the conditional distributions $p(x_i|x_{<i})$ correspond to Bernoulli random variables and learn a function that maps the proceeding random variables $x_1, x_2, \ldots, x_{i-1}$ to the mean of this distribution as

$$p_{\theta_i}(x_i|x_{<i}) = Bern(f_i(x_1, x_2, \ldots, x_{i-1}))$$

   where θ_i denotes the set of parameters used to specify the mean function $f_i : \{0, 1\}^{i-1} \mapsto [0, 1]$.
6. The number of parameters of an autoregressive generative model equals to $\sum_{i=1}^{n} |\theta_i|$.
7. Tractable exact likelihood computations.
8. No complex integral over latent variables in likelihood.
9. Slow sequential sampling process.
10. Cannot rely on latent variables.

Autoregressive models

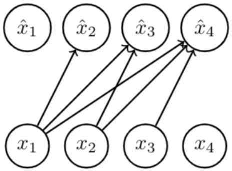
1. The nth output should only be connected to the previous $n-1$ inputs.
2. For example, when computing $p(x_4|x_3, x_2, x_1)$ the only inputs that we should consider are x_1, x_2, x_3 because these are the only variables given to us while computing the conditional probability.



1. In the simplest case, we can specify the function as a linear combination of the input elements followed by a sigmoid non-linearity (to restrict the output to lie between 0 and 1).
2. This gives us the formulation of a fully-visible sigmoid belief network (FVSBN).

$$f_i(x_1, x_2, \ldots, x_{i-1}) = \sigma\left(a_0^i + \sum_{j=1}^{i-1} a_j^i x_j\right)$$

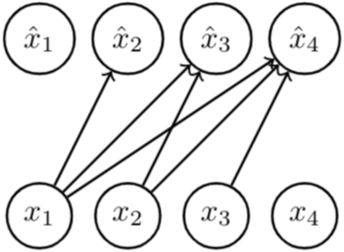
   where σ is sigmoid function and $\theta_i = \{a_0^i, \ldots, a_{i-1}^i\}$.
3. At the output layer we want to predict n conditional probability distributions.
4. At the input layer we are given the n input variables.



5. The conditional variables $x_i|x_1, \ldots, x_{i-1}$ are Bernoulli with parameters

$$\hat{x}_i = p(x_i = 1|x_1, \ldots, x_{i-1}; \theta_i) = \sigma\left(a_0^i + \sum_{j=1}^{i-1} a_j^i x_j\right)$$

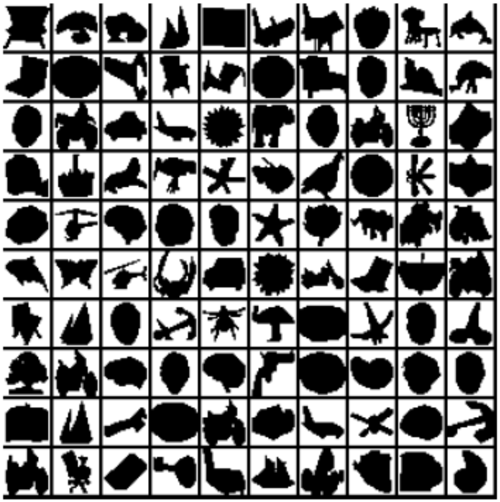
1. How to evaluate $p(x_1, \ldots, x_{900})$?
2. Multiply all the conditionals factors.
3. How to sample from $p(x_1, \ldots, x_{900})$?
   - Sample $\bar{x}_1 \sim p(x_1)$.
   - Sample $\bar{x}_2 \sim p(x_2 | x_1 = \bar{x}_1)$.
   - Sample $\bar{x}_3 \sim p(x_3 | x_1 = \bar{x}_1, x_2 = \bar{x}_2)$.
4. How many parameters? $1 + 2 + 3 + \ldots + n \approx \frac{n^2}{2}$

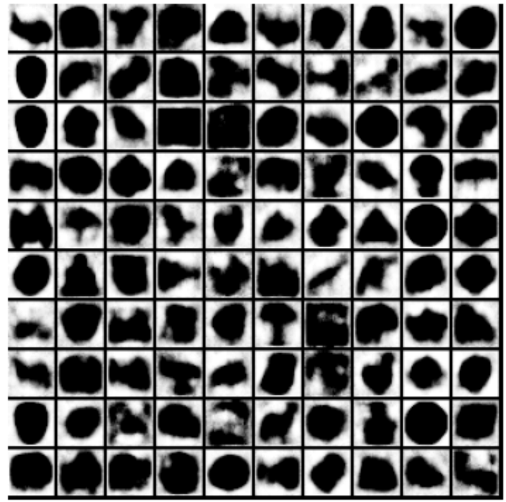


5. This model is called Fully Visible Sigmoid Belief Network (FVSBN).

FVSBN results (Gan et al. 2015)

1. Left: Training (Caltech 101 Silhouettes) Right: Samples from the model





Autoregressive models

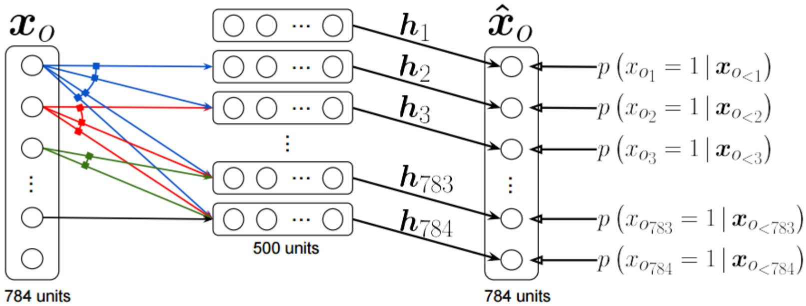
Neural Autoregressive Density Estimator

1. To increase the expressiveness of an autoregressive generative model, we can use more flexible parameterizations for the mean function such as MLP instead of logistic regression.
2. For example, consider the case of a neural network with one hidden layer.
3. The mean function for variable i can be expressed as

$$\mathbf{h}_i = \sigma(A_i \mathbf{x}_{<i} + \mathbf{c}_i)$$
$$f_i(x_1, x_2, \ldots, x_{i-1}) = \sigma\left((\boldsymbol{\alpha}^{(i)}\mathbf{h}_i + b_i\right)$$

   where $\mathbf{h}_i \in \mathbb{R}^d$ is hidden layer activations of MLP.

4. Hence, we have the following architecture



1. To improve model, use a neural network with one hidden layer instead of logistic regression.

$$\mathbf{h}_i = \sigma(A_i \mathbf{x}_{<\mathbf{i}} + \mathbf{c}_i)$$
$$\hat{x}_i = p(x_i = 1 | x_1, \ldots, x_{i-1}; \boldsymbol{\theta}^i) = \sigma(\boldsymbol{\alpha}^{(i)} \mathbf{h}_i + b_i)$$

where $\mathbf{h}_i \in \mathbb{R}^d$ denotes the hidden layer activations for the MLP.

2. **If parameter sharing was not used, the total number of parameters is $O(n^2 d)$.**
3. NADE provides an alternate MLP-based parameterization that is more statistically and computationally efficient than the given approach (Larochelle and Murray 2011).
4. **NADE shares parameters A and c across the functions used for evaluating the conditionals**.
5. The hidden layer activations are specified as

$$\mathbf{h}_i = \sigma(A_{., <i} \mathbf{x}_{<\mathbf{i}} + \mathbf{c})$$
$$\hat{x}_i = p(x_i = 1 | x_1, \ldots, x_{i-1}; \boldsymbol{\theta}^i) = \sigma(\boldsymbol{\alpha}^{(i)} \mathbf{h}_i + b_i)$$

Neural Autoregressive Density Estimator (NADE)

1. Sharing parameters has two benefits:
   - The total number of parameters gets reduced from $O(n^2 d)$ to $O(nd)$.
   - The hidden unit activations can be evaluated in $O(nd)$ time via the following recursive strategy:

$$\mathbf{h}_i = \sigma(\mathbf{a}_i)$$
$$\mathbf{a}_{i+1} = \mathbf{a}_i + A[., i]x_i$$

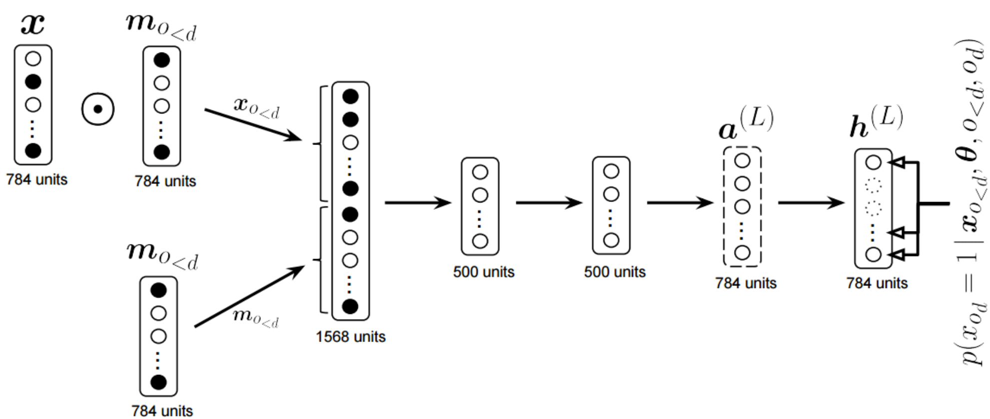
     with the base case given by $\mathbf{a}_1 = \mathbf{c}$.

2. Training of NADE is done by minimizing the average negative log-likelihood of the parameters given the training set:

$$-\frac{1}{T}\sum_{i=1}^{T} \log p(x_i)$$

1. Samples from NADE trained on a binary version of MNIST.

1. The input to the network (DeepNADE) is the concatenation of the masked data and the mask itself (Uria, Côté, et al. 2016).
2. This allows the network to identify cases when input data is truly zero from cases when input data is zero because of the mask.
3. NADE also explored other autoencoder architectures such as convolutional neural networks
4. DeepNade with two hidden layers



1. The RNADE algorithm extends NADE to learn generative models over real-valued data (Uria, Murray, and Larochelle 2013).
2. For real-valued variables, the conditionals are modeled via a continuous distribution such as mixture of K Gaussian.
3. Instead of learning a mean function, we know learn the means $\mu_{i,1}, \mu_{i,2}, \ldots, \mu_{i,K}$, variances $\sigma_{i,1}, \sigma_{i,2}, \ldots, \sigma_{i,K}$, and probability of sampling from each mixture $\pi_{i,1}, \pi_{i,K}, \ldots, \pi_{i,K}$ of the K Gaussian for every conditional.

$$p(x_i|x_{<i}) = \sum_{j=1}^{K} \pi_{ij} \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$$

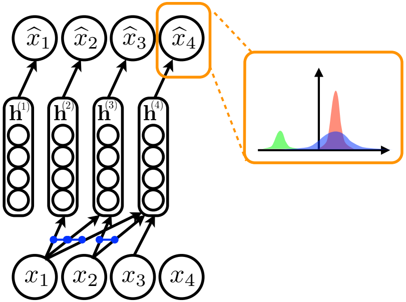
1. Output of the network are parameters of a mixture model for $p(x_k|x_{<k})$
2. Means are $\mu_{i,k} = b^{\mu_i}_{i,k} + \boldsymbol{\alpha}^{\mu_i}_{i,k} h_i$
3. Standard deviations are

$$\sigma_{i,k} = \exp\left(b^{\sigma_i}_{i,k} + \boldsymbol{\alpha}^{\sigma_i}_{i,k} h_i\right)$$

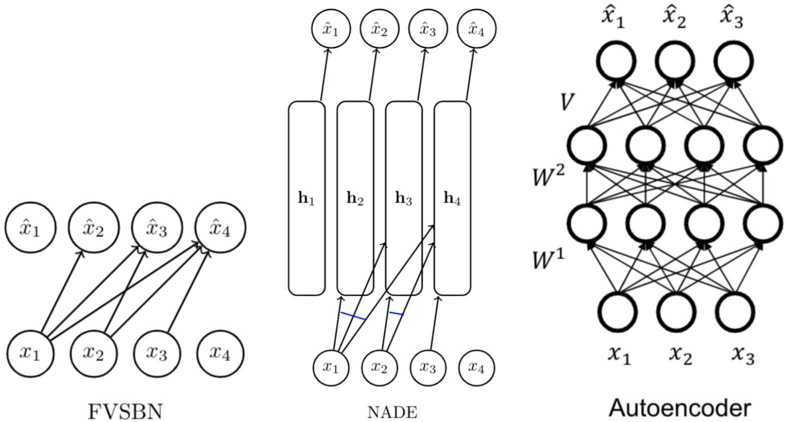
4. Mixing weights are

$$\pi_{i,k} = softmax\left(b^{\pi_i}_{i,k} + \boldsymbol{\alpha}^{\pi_i}_{i,k} h_i\right)$$

5. Please study DocNADE.

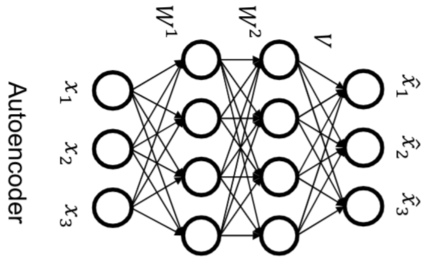


1. Considering the following models.



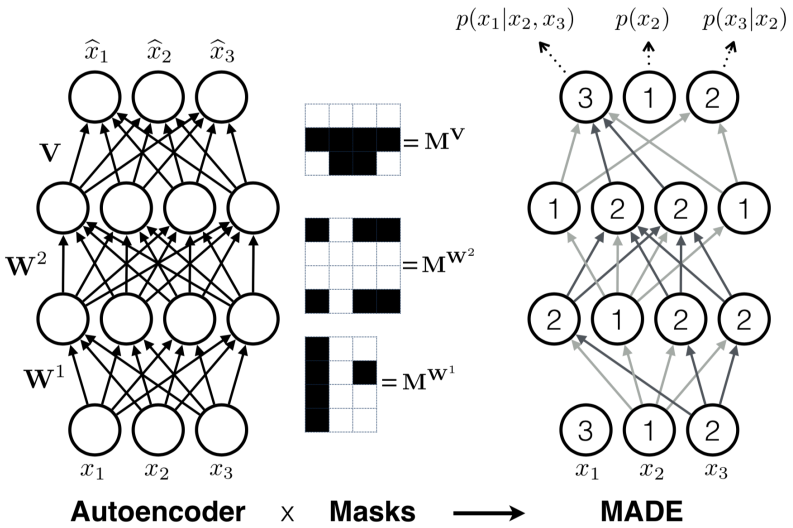
2. FVSBN and NADE look similar to an autoencoder.
3. An encoder computing hidden.
4. A decoder computing densities.
5. A loss function, which is likelihood.

1. An autoencoder is not a generative model: it does not define a distribution over x for sampling new data points.



2. Can we get a generative model from an autoencoder?
3. We need to make sure it corresponds to a valid Bayesian Network, i.e., we need an ordering. If the ordering is 1, 2, 3, then
   - $\hat{x}_1$ cannot depend on any input x.
   - $\hat{x}_2$ can only depend on x_1.
4. We can use a single neural network to produce all the parameters.

1. MADE is an autoencoder that preserves autoregressive property (Germain et al. 2015).



1. MADE is a specially designed architecture to enforce the autoregressive property in the autoencoder efficiently.
2. MADE removes the contribution of certain hidden units by using mask matrices so that each input dimension is reconstructed only from previous dimensions in a given ordering in a single pass.
3. In a multilayer fully-connected neural network, say, we have L hidden layers with weight matrices $\mathbf{W}^1, \ldots, \mathbf{W}^L$ and an output layer with weight matrix V. The output $\hat{x}$ has dimensions $\hat{x}_i = p(x_i | x_{1:i-1})$
4. Without any mask, we have

$$
\begin{aligned}
\mathbf{h}^0 &= \mathbf{x} \\
\mathbf{h}^l &= \text{activation}^l(\mathbf{W}^l \mathbf{h}^{l-1} + \mathbf{b}^l) \\
\hat{\mathbf{x}} &= \sigma(\mathbf{V}\mathbf{h}^L + \mathbf{c})
\end{aligned}
$$

1. Without any mask, we have

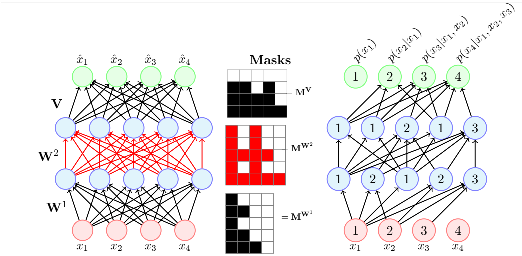
$$\begin{aligned}\mathbf{h}^0 &= \mathbf{x} \\ \mathbf{h}^l &= \text{activation}^l(\mathbf{W}^l\mathbf{h}^{l-1} + \mathbf{b}^l) \\ \hat{\mathbf{x}} &= \sigma(\mathbf{V}\mathbf{h}^L + \mathbf{c})\end{aligned}$$

2. To zero out some connections between layers, we can simply element-wise multiply every weight matrix by a binary mask matrix.

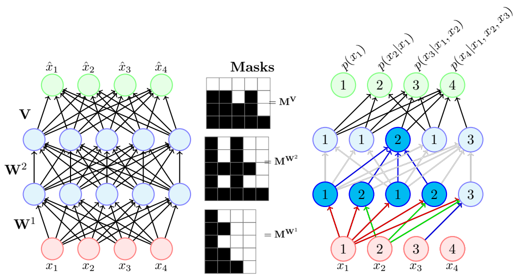
$$\begin{aligned}\mathbf{h}^l &= \text{activation}^l((\mathbf{W}^l \odot \mathbf{M}^{\mathbf{W}^l})\mathbf{h}^{l-1} + \mathbf{b}^l) \\ \hat{\mathbf{x}} &= \sigma((\mathbf{V} \odot \mathbf{M}^{\mathbf{V}})\mathbf{h}^L + \mathbf{c})\end{aligned}$$

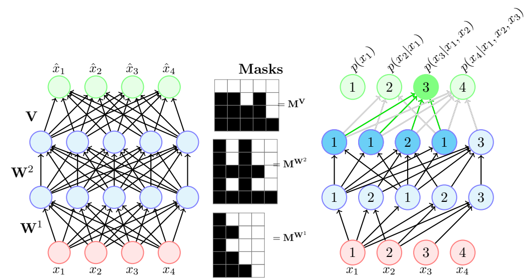
3. Mask matrix is constructed by a labeling process.

Masked Autoencoder for Distribution Estimation (MADE)

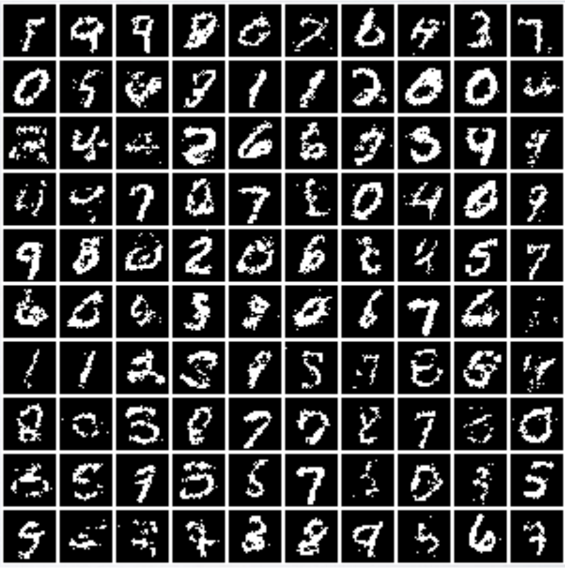


$$
\begin{bmatrix}
W^2_{11} & W^2_{12} & W^2_{13} & W^2_{14} & W^2_{15} \\
W^2_{21} & W^2_{22} & W^2_{23} & W^2_{24} & W^2_{25} \\
W^2_{31} & W^2_{32} & W^2_{33} & W^2_{34} & W^2_{35} \\
W^2_{41} & W^2_{42} & W^2_{43} & W^2_{44} & W^2_{45} \\
W^2_{51} & W^2_{52} & W^2_{53} & W^2_{54} & W^2_{55}
\end{bmatrix}
\odot
\begin{bmatrix}
1 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 \\
1 & 1 & 1 & 1 & 1
\end{bmatrix}
$$





1. The results of MADE on MNIST.



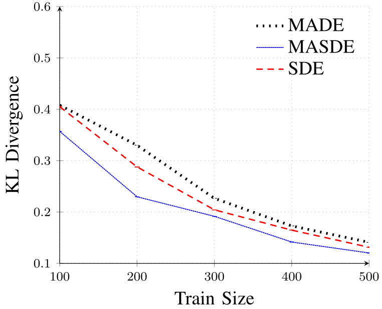
1. We know the structure (Markov random field) of the data (Khajenezhad, Madani, and Beigy 2021).
2. In structured distributions, the graph structure of the variables declares their conditional dependencies.
3. Therefore, having a graph structure, each of the chain rule conditional terms might be presentable by a conditional probability on a smaller set of variables.
4. In other words, for each i, we can assume that there is a subset $B_i \subseteq \{1, \dots, i-1\}$ such that $p(x_i|x_{<i}) = p(x_i|x_{B_i})$.
5. We call B_i as Looking-back Markov blanket of the i-th dimension. Then

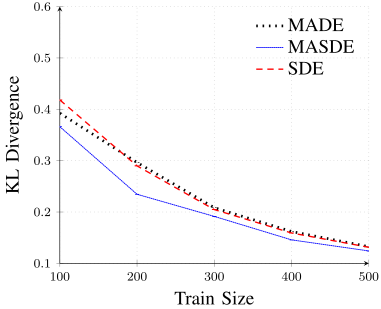
$$p(x_1, \dots, x_d) = P(x_1)p(x_2|x_{B_2}) \dots P(x_d|x_{B_d})$$

6. Use an auoencoder that has the above autoregressive property.
7. Mask matrix is constructed by a labeling process.

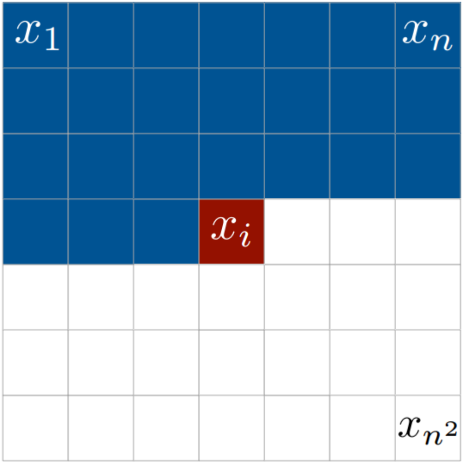
1. MASDE needs a smaller training set in comparison with its counterparts.

Size of the Hidden Layers = 100

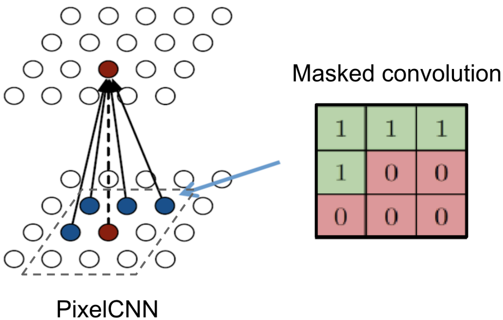




1. PixelRNN is a deep generative model for images (Oord, Kalchbrenner, and Kavukcuoglu 2016).
2. Dependency on previous pixels modeled using an RNN (LSTM).

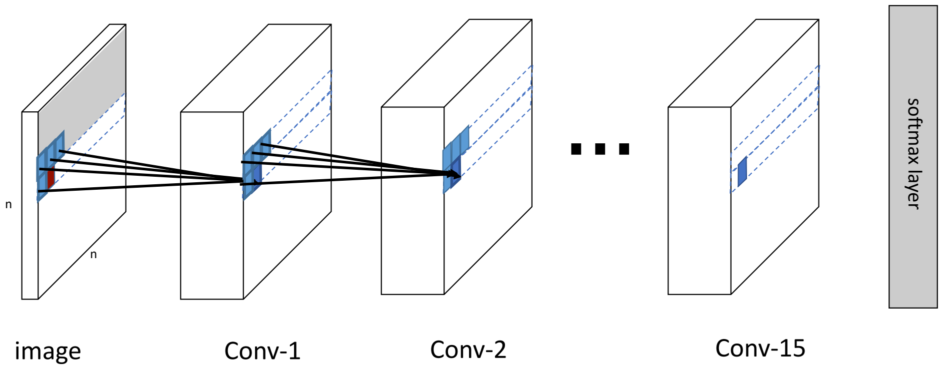


1. The main drawback of PixelRNN is that training is very slow.
2. PixelCNN uses standard convolutional layers to capture a bounded receptive field and compute features for all pixel positions at once (Oord, Kalchbrenner, Espeholt, et al. 2016).
3. In PixelCNN, pooling layers are not used.
4. Masks are adopted in the convolutions to restrict the model from violating the conditional dependence.



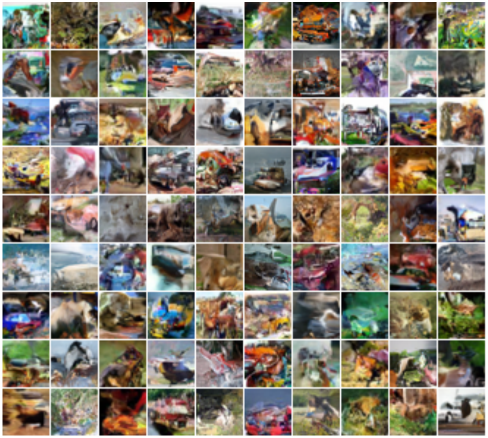
5. Please also PixelCNN++ (Salimans, Karpathy, et al. 2017).

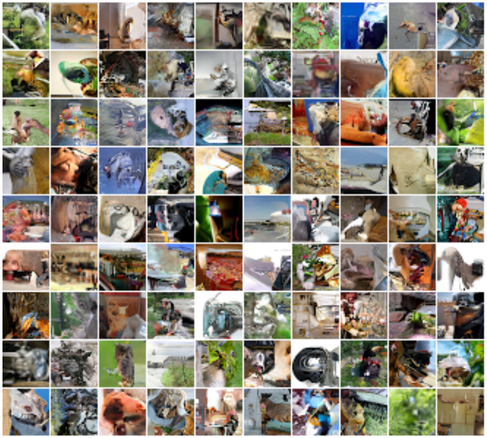
PixelCNN



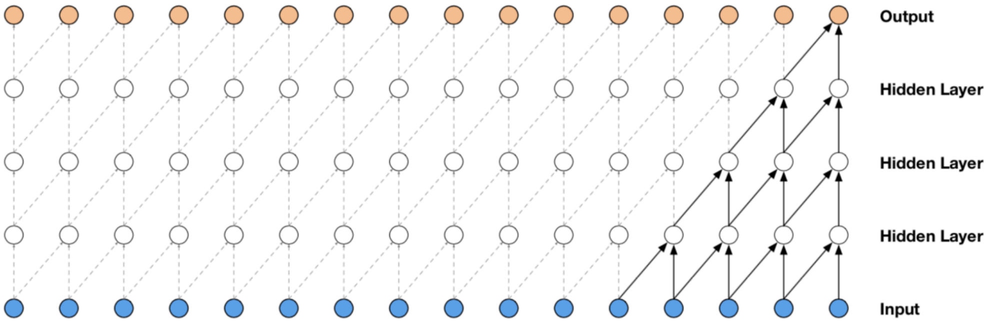
PixelCNN

1. The training set (CIFAR-10 (left)) and the samples generated by the PixelCNN (right).



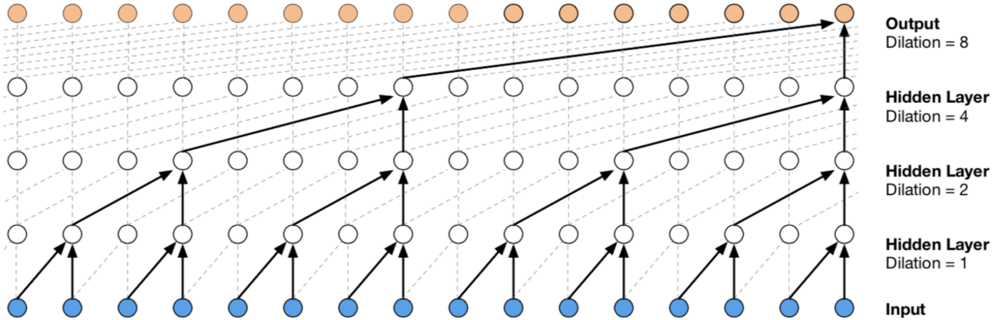


1. WaveNet is very similar to PixelCNN but applied to 1-D audio signals (Oord, Dieleman, et al. 2016).
2. WaveNet consists of a stack of causal convolution which is a convolution operation designed to respect the ordering.
3. Causal convolutions are a type of convolution used for temporal data which ensures the model cannot violate the ordering in which we model the data: the prediction $p(x_{t+1}|x_1, \ldots, x_t)$.
4. The causal convolution in WaveNet is simply to shift the output by a number of timestamps to the future so that the output is aligned with the last input element.


Output
Hidden Layer
Hidden Layer
Hidden Layer
Input

WaveNet

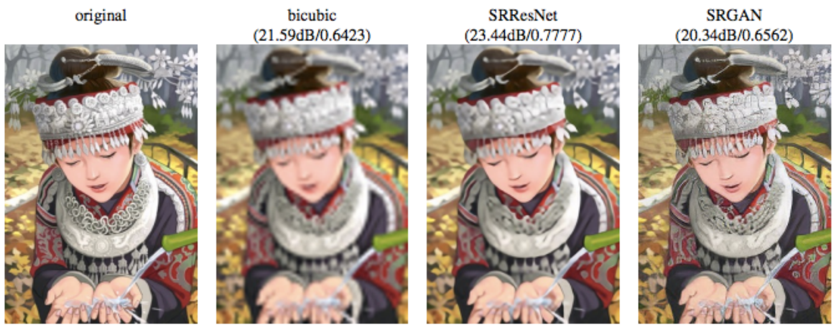
1. One big drawback of convolution layer is a very limited size of receptive field.
2. WaveNet therefore adopts dilated convolution, where the kernel is applied to an evenly-distributed subset of samples in a much larger receptive field of the input.



Generative Adversarial Networks

Generative Adversarial Networks

1. Generative adversarial networks (GANs) are a new way to implicitly build generative models $P(x)$ (I. J. Goodfellow et al. 2014).
2. Generative adversarial networks
   - Generative: Learns a generative model.
   - Adversarial: Trained in an adversarial setting
   - Networks: Use Deep Neural Networks
3. Which one is Computer generated?



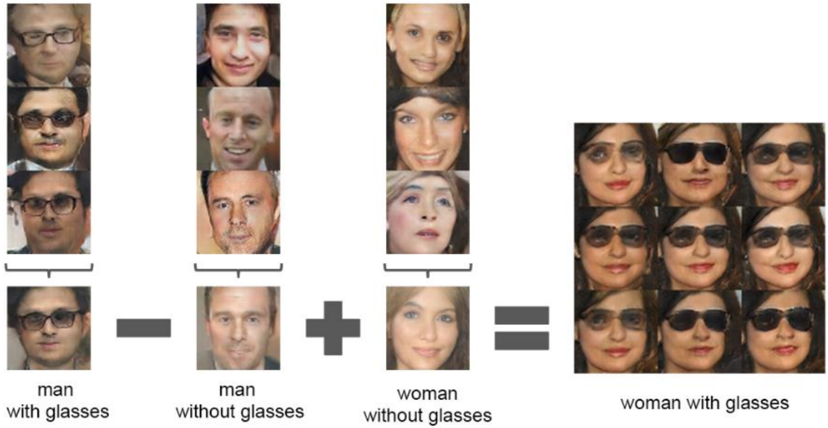
4. How do we generate a fake image?
5. Can we generate a fake image from a random number?

GAN results

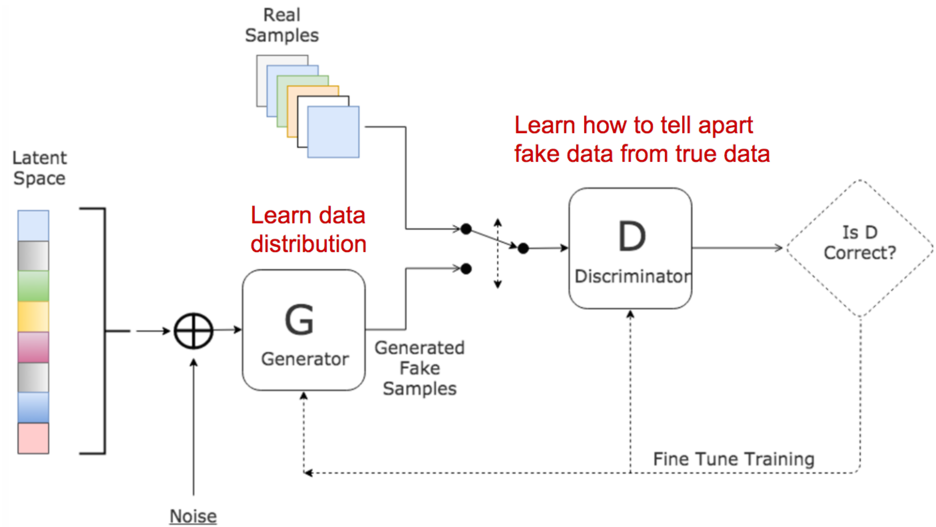
1. Results obtained from GAN (Radford, Metz, and Chintala 2016).

GAN results

1. Results obtained from GAN (Radford, Metz, and Chintala 2016).

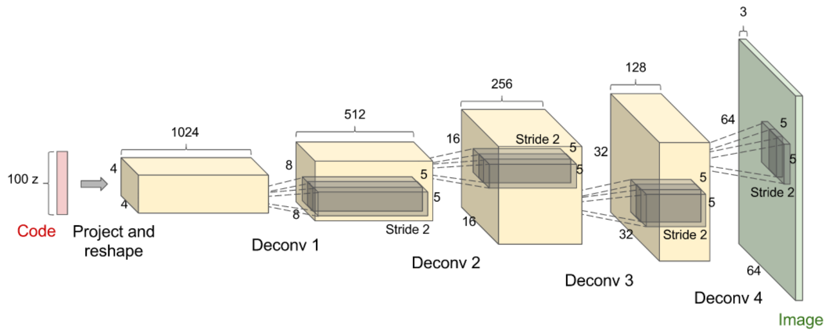


1. GAN has the following architecture

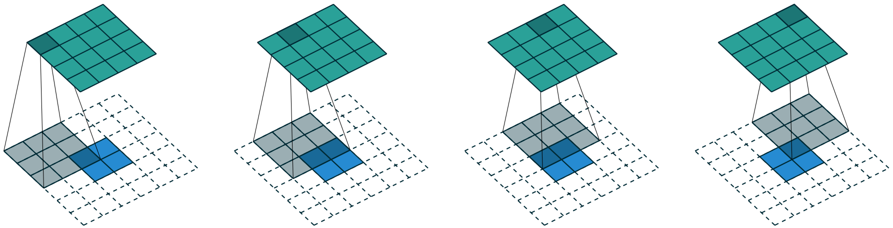


2. Z (input to generator) is some random noise (Gaussian/Uniform).
3. Z can be thought as the latent representation of the image.

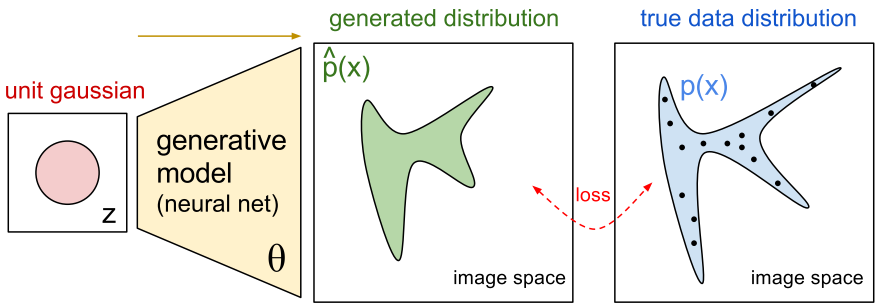
1. Opposite of convolutional neural nets.



2. Deconvolution layer or transposed convolutional layer is pad the original input (blue entries) with zeroes (white entries) (Dumoulin and Visin 2016).

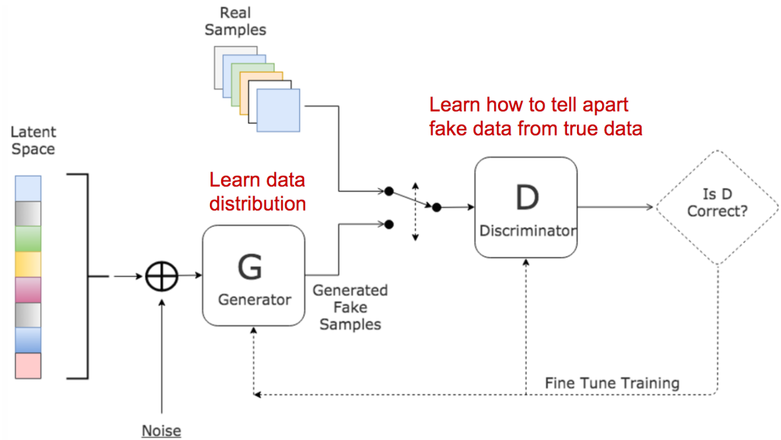


1. The generator tries to learn $P(x|z)$.
2. Inputs are directly sampled from $Q(z)$.
3. Problem: No true data x is provided when training the generator
4. Instead of a traditional loss function, gradient is provided by a discriminator (another network)



Discriminator

1. The discriminator attempts to tell the difference between real and fake images.
2. It tries to learn $P(y|x)$: y is label: real / generated and x is real/generated data.
3. Trained using standard cross entropy loss to assign the correct label.
4. Generator weights are frozen while training discriminator.
5. From generator's point-of-view, discriminator is a black-box loss function.



1. Let p_g / p_r be probability of generating a fake / real sample.
2. Let output of discriminator, $D(x)$, be the probability that x is real sample.
3. For a fake sample $G(z)$, the discriminator is expected to output a probability, $D(G(z))$, close to zero by **maximizing** $\mathbb{E}_{z\sim p_z(z)}[\log(1-D(G(z)))]$.
4. For a real data, the sample is expected to output a probability $D(x)$, close to one by **maximizing** $\mathbb{E}_{x\sim p_r(x)}[\log D(x)]$.
5. The generator is trained to increase the chances of D producing a high probability for a fake example, thus to **minimize** $\mathbb{E}_{z\sim p_z(z)}[\log(1-D(G(z)))]$.
6. When combining both aspects together, D and G are playing a minimax game in which we should optimize the following loss function:

$$\begin{aligned}\min_G \max_D V(D,G) &= \min_G \max_D \mathbb{E}_{x\sim p_r(x)}[\log D(x)] + \mathbb{E}_{z\sim p_z(z)}[\log(1-D(G(z)))] \\ &= \min_G \max_D \mathbb{E}_{x\sim p_r(x)}[\log D(x)] + \mathbb{E}_{x\sim p_g(x)}[\log(1-D(x)]\end{aligned}$$

7. Thus, $\mathbb{E}_{x\sim p_r(x)}[\log D(x)]$ has no impact on G during gradient descent updates.

1. Loss function is

$$
\begin{aligned}
V(G, D) &= \int_x p_r(x) \log(D(x))dx + \int_z p_z(z) \log(1 - D(G(z)))dz \\
&= \int_x \Big(p_r(x) \log(D(x)) + p_g(x) \log(1 - D(x)) \Big) dx
\end{aligned}
$$

2. The full two-player game can be summarily described by the below.

$$
\min_G \max_D V(D, G)
$$

Training GAN

1. It is important to understand that both the generator and discriminator are trying to learn moving targets. Both networks are trained simultaneously.
2. The discriminator needs to update based on how well the generator is doing.
3. The generator is constantly updating to improve performance on the discriminator.
4. These two need to be balanced correctly to achieve stable learning instead of chaos.

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

Discriminator updates

- **for** k steps **do**
  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

- **end for**

Generator updates

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by descending its stochastic gradient:

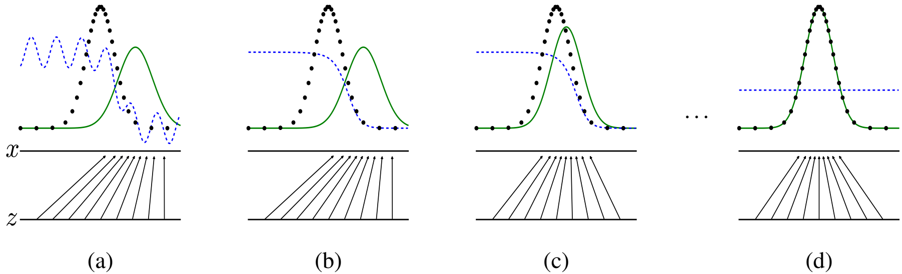
$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for

The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

Training GAN (An example)

1. How GAN is trained?



2. discriminative distribution $D(x)$, real data p_r, generative distribution p_g.

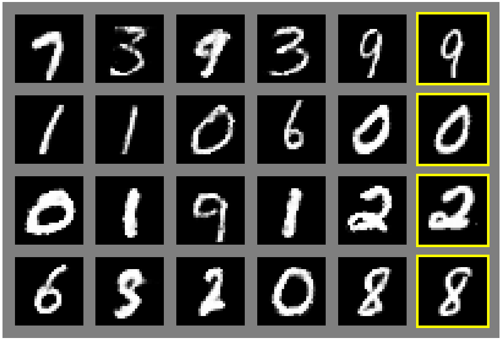
   (a) An adversarial pair near convergence: p_g is similar to p_r and D is a partially accurate classifier.

   (b) In inner loop of algorithm, D is trained to discriminate samples from data, converging to $D^*(x)$.

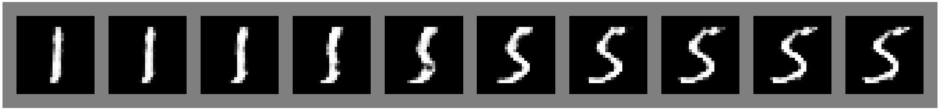
   (c) After an update to G, gradient of D has guided $G(z)$ to flow to regions that are more likely to be classified as data.

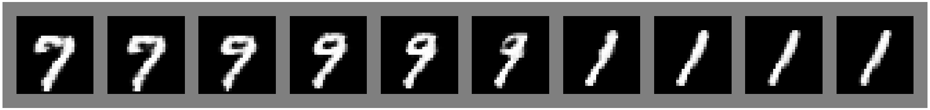
   (d) After several steps of training, if G and D have enough capacity, they will reach a point at which both cannot improve because $p_g = p_r$.

1. Rightmost column shows the nearest training example of the neighboring sample.



2. Digits obtained by linearly interpolating between coordinates in z space of the full model.





Theorem (Optimality of GAN)

For G fixed, the optimal discriminator D is

$$D^*(x) = \frac{p_r(x)}{p_r(x) + p_g(x)}$$

Theorem (Convergence of training algorithm of GAN)

If G and D have enough capacity, and at each step of training Algorithm, the discriminator is allowed to reach its optimum given G, and p_g is updated so as to improve the criterion $V(D, G)$, then, p_g converges to p_r

What is the global optimal?

When both G and D are at their optimal values, we have $p_g = p_r$ and $D^*(x) = \frac{1}{2}$, and the loss function becomes:

$$\begin{aligned} V(G, D^*) &= \int_x \Big(p_r(x) \log(D^*(x)) + p_g(x) \log(1 - D^*(x)) \Big) dx \\ &= \log \frac{1}{2} \int_x p_r(x) dx + \log \frac{1}{2} \int_x p_g(x) dx \\ &= -2 \log 2 \end{aligned}$$

What does the loss function represent?

1. KL divergence measures how one probability distribution p diverges from a second distribution q.

$$D_{KL}(p\|q) = \int_x p(x) \log \frac{p(x)}{q(x)} dx$$

2. KL divergence is asymmetric.
3. In cases where $p(x)$ is close to zero, but $q(x)$ is significantly non-zero, the q's effect is disregarded.
4. Jensen–Shannon Divergence is a measure of similarity between two probability distributions, bounded by $[0, 1]$.

$$D_{JS}(p\|q) = \frac{1}{2} D_{KL}\left(p\|\frac{p+q}{2}\right) + \frac{1}{2} D_{KL}\left(q\|\frac{p+q}{2}\right)$$

5. JS divergence is symmetric and more smooth.

What does the loss function represent?

1. JS divergence between p_r and p_g can be computed as:

$$
\begin{aligned}
D_{JS}(p_r \| p_g) =& \frac{1}{2} D_{KL}\left(p_r || \frac{p_r + p_g}{2}\right) + \frac{1}{2} D_{KL}\left(p_g || \frac{p_r + p_g}{2}\right) \\
=& \frac{1}{2}\left(\log 2 + \int_x p_r(x) \log \frac{p_r(x)}{p_r + p_g(x)} dx\right) \\
+& \frac{1}{2}\left(\log 2 + \int_x p_g(x) \log \frac{p_g(x)}{p_r + p_g(x)} dx\right) \\
=& \frac{1}{2}\left(\log 4 + V(G, D^*)\right)
\end{aligned}
$$

2. Thus

$$V(G, D^*) = 2D_{JS}(p_r | p_g) - 2 \log 2$$

3. The best G^* that replicates the real data distribution leads to the minimum $V(G^*, D^*) = -2 \log 2$, which is aligned to the optimal solution.

1. Hard to achieve Nash equilibrium (Salimans, I. J. Goodfellow, et al. 2016).
2. Low dimensional supports: When the intrinsic dimension is low, then training GAN will be instable (Arjovsky and Bottou 2017).
3. Vanishing gradient: When the discriminator is perfect, loss function is zero and there is not any training.
4. Mode collapse: During the training, the generator may collapse to a setting where it always produces same outputs.
5. Lack of a proper evaluation metric

Generative Adversarial Networks

Wasserstein GAN

1. Wasserstein Distance is a measure of the distance between two probability distributions.
2. When dealing with the continuous probability domain, the distance becomes

$$W(p_r, p_g) = \inf_{\gamma \sim \Pi(p_r, p_g)} \mathbb{E}_{(x,y)\sim\gamma}[\|x - y\|]$$

where $\Pi(p_r, p_g)$ is the set of all possible joint probability distributions between p_r and p_g.
3. It is intractable to exhaust all the possible joint distributions in $\Pi(p_r, p_g)$ to compute $\inf_{\gamma \sim \Pi(p_r, p_g)}$, the following metric is used.

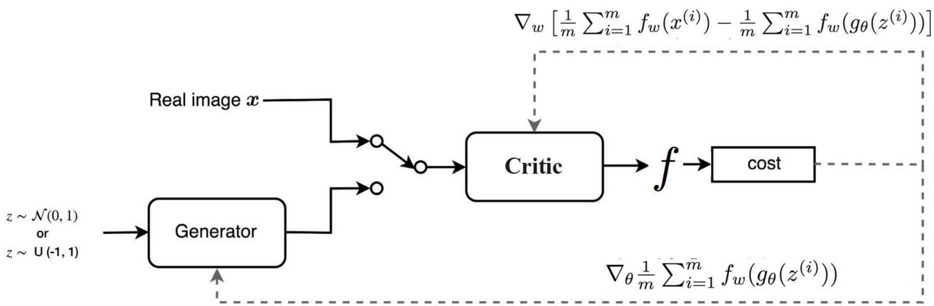
$$W(p_r, p_g) = \frac{1}{K} \sup_{\|f\|_L \leq K} \mathbb{E}_{x\sim p_r}[f(x)] - \mathbb{E}_{x\sim p_g}[f(x)]$$

where $\|f\|_L \leq K$ means that f is K-Lipschitz.

1. The discriminator network produces a scaler score (Arjovsky and Bottou 2017).
2. This score can be interpreted as how real the input images are.
3. In reinforcement learning, we call it the value function which measures how good a input is.
4. We rename the discriminator to critic to reflect its new role.
5. The loss function for WGAN is

$$V(p_r, p_g) = W(p_r, p_g) = \max_{w \in W} \mathbb{E}_{x \sim p_r}[f_w(x)] - \mathbb{E}_{z \sim p_z(z)}[f_w(g_\theta(z))]$$

   f comes from a family of K-Lipschitz continuous functions $\{f_w\}_{w \in W}$ parameterized by w.
6. The discriminator model is used for learning w to find a good f_w.



Generative Adversarial Networks

Conditional GAN

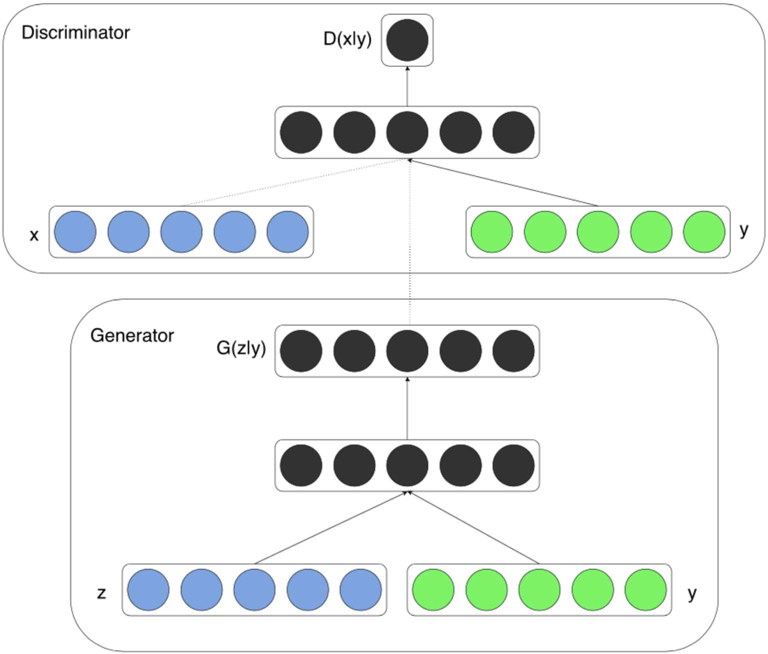
1. Now, as we want to condition those networks with some vector y.
2. The easiest way to do it is to feed y into both networks (Mirza and Osindero 2014).
3. Hence, generator and discriminator are now $G(z, y)$ and $D(x, y)$, respectively.
4. $G(z, y)$ models distribution of data, given z and y, that is $x_G \sim G(x|z, y)$.
5. Discriminator tries to find labels for x and x_G, that are modeled with $d \sim D(d|x, y)$.
6. Hence, we see that both D and G is jointly conditioned to two variables z or x and y.
7. Now, the objective function is given by:

$$
\begin{aligned}
\min_G \max_D V(D, G) = & \mathop{\mathbb{E}}_{x \sim p_r(x)} [\log D(x, y)] \\
& + \mathop{\mathbb{E}}_{z \sim p_z(z)} [\log(1 - D(G(z, y), y))]
\end{aligned}
$$

8. If we compare the above loss to GAN loss, the difference only lies in the additional parameter y in both D and G.

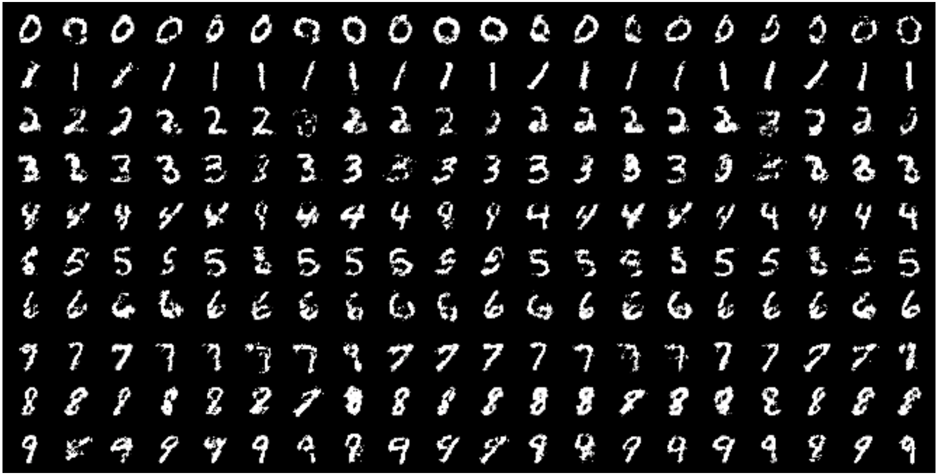
Conditional GAN architecture

1. The architecture of CGAN is



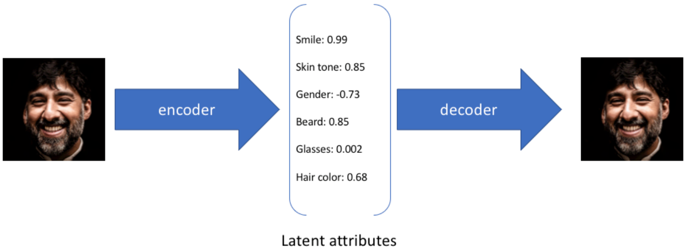
Conditional GAN results

1. The following figure shows some of the generated samples.
2. Each row is conditioned on one label and each column is a different generated sample.

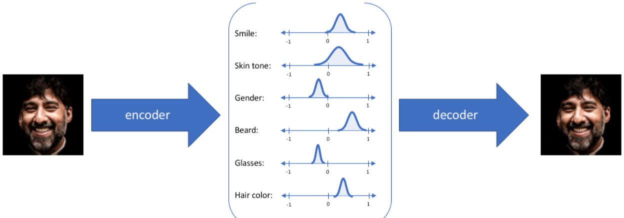


Variational Autoencoder models

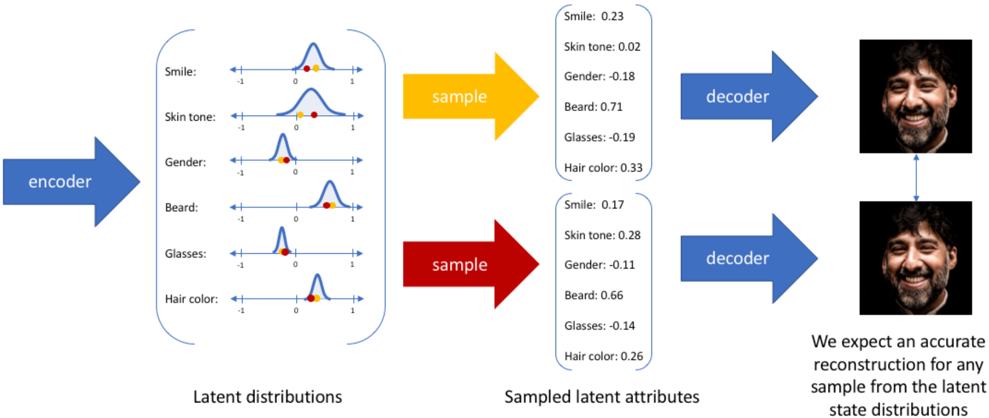
1. An ideal autoencoder learns attributes of input to describe an observation in some compressed representation.



2. However, we may prefer to represent each latent attribute as a range of possible values.



1. For any sampling of the latent distributions, we're expecting our decoder model to be able to accurately reconstruct the input.



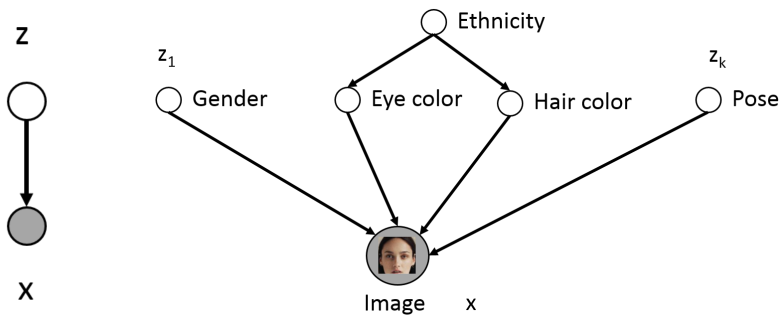
Latent Variable Models[6]

1. Lots of variability in images x due to gender, eye color, hair color, pose, etc.
2. However, unless images are annotated, these factors of variation are not explicitly available (latent).

3. **Idea:** explicitly model these factors using latent variables z.

[6] Some slides of this lecture are from S. Ermon and A. Grover slides.

1. Consider an image x, and some of its latent factors such as gender, eye color, hair color, pose, etc.



2. Only shaded variables x are observed in the data (pixel values).
3. Latent variables z correspond to high level features.
    - If z chosen properly, $p(x|z)$ could be much simpler than $p(x)$.
    - If we trained this model, then we could identify features via $p(z|x)$.
4. **Challenge:** Very difficult to specify these conditionals by hand.

1. Consider an observed variable x, and latent variable z.

2. Instead of modelling $p(x)$ directly, we use an unobserved latent variable z and define $p(x|z)$ for the data.
3. We can use prior distribution $p(z)$ over the z and

$$p(x, z) = p(x|\, z)p(z).$$

4. Generative process for the observed data x.

$$z \sim p(z)$$
$$x \sim p(x|\, z).$$

1. Given a set of observed random variables $x = \{x_1, x_2, \cdots, x_n\}$ and a set of latent random variables $z = \{z_1, z_2, \cdots, z_m\}$, we need to compute the posterior $p(z|x)$.
2. Using Bayes' theorem, we have

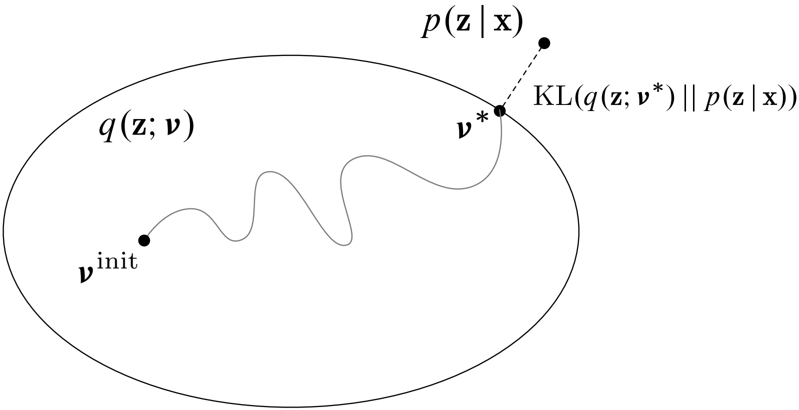
$$\begin{aligned} p(z|x) &= \frac{p(x,z)}{p(x)} \\ &= \frac{p(x|z)p(z)}{p(x)} \end{aligned}$$

3. $p(x)$ is the marginal density which is also called evidence.

$$p(x) = \int_z p(x,z)dz$$

4. For most of the models, computing $p(x)$ is **intractable**. Hence computing $p(z|x)$ is also **intractable**.

1. Since directly computing $p(z|x)$ is intractable, we have to do some approximate inference.
2. Variational inference considers a family of parametric distributions that approximates $p(z|x)$.



$v = \theta$ is parameter of q.

Variational Inference: Optimization Goal

1. Variational inference leverages optimization to find the best distribution $q(z;\theta)$.
2. In variational inference, we specify a family of distributions $\mathcal{Q}$ over the latent random variables.
3. Each $q(z) \in \mathcal{Q}$ is a candidate approximation to the posterior.
4. Our goal is to find the best candidate that has the smallest KL divergence to the posterior we want to compute.
5. Mathematically, the optimization goal is

$$q^*(z) = argmin_{q(z)\in\mathcal{Q}} KL\big(q(z)||p(z|x)\big)$$

where $q^*(\cdot)$ is the best approximation to the posterior in distribution family $\mathcal{Q}$.

1. To measure the difference between two probability distributions over the same variable x, Kullback-Leibler divergence is used.
2. The KL divergence between two distributions p and q with discrete support is defined as

$$KL(p\|q) = \sum_x p(x) \log \frac{p(x)}{q(x)}.$$

3. The KL divergence has the following properties
   - $KL(p\|q) \geq 0$ for all p, q.
   - $KL(p\|q) = 0$ if and only if $q = p$
4. KL divergence is not symmetric, i.e.

$$KL(q\|p) \neq KL(p\|q)$$

1. The KL divergence between two distributions p and q with discrete support is defined as

$$KL(p\|q) = \sum_x p(x) \log \frac{p(x)}{q(x)} = \mathbb{E}_p \log \frac{p(x)}{q(x)}.$$

2. It is hard to compute $KL(p\|q)$, because taking expectation wrt p is assumed to be intractable.
3. An alternative is the reverse KL divergence, which is

$$KL(q\|p) = \sum_x q(x) \log \frac{q(x)}{p(x)} = \mathbb{E}_q \log \frac{q(x)}{p(x)}.$$

4. The main advantage is that computing expectation wrt q is tractable, by choosing a suitable form of q.
5. The above equation is still not tractable because $p(x) = p(x|S)$ is intractable, where S is the given dataset.

1. We'll assume that p is a general undirected model of the following form

$$p(x_1, \dots, x_n; \theta) = \frac{\bar{p}(x_1, \dots, x_n; \theta)}{Z(\theta)} = \frac{1}{Z(\theta)} \prod_k \phi_k(x_k; \theta),$$

   where the ϕ_k are the factors and $Z(\theta)$ is the normalization constant.

2. Given this formulation, optimizing $KL(q \| p)$ directly is not possible because of the potentially intractable normalization constant $Z(\theta)$.

3. Evaluating $KL(q \| p)$ is not possible, because we need to evaluate p.

4. Instead, we work with the following objective (the same form as the KL divergence), but only involves the unnormalized probability $\bar{p}(x) = \prod_k \phi_k(x_k; \theta)$.

$$J(q) = \sum_x q(x) \log \frac{q(x)}{\bar{p}(x)}.$$

1. We use the following objective function

$$J(q) = \sum_x q(x) \log \frac{q(x)}{\bar{p}(x)}.$$

2. This function is not only tractable, it also has the following important property

$$\begin{aligned} J(q) &= \sum_x q(x) \log \frac{q(x)}{\bar{p}(x)} \\ &= \sum_x q(x) \log \frac{q(x)}{p(x)} - \log Z(\theta) \\ &= KL(q \| p) - \log Z(\theta) \end{aligned}$$

3. Since $KL(q \| p) \geq 0$, we get by rearranging terms that

$$\log Z(\theta) = KL(q \| p) - J(q) \geq -J(q).$$

1. Thus, $-J(q)$ is a lower bound on the $\log Z(\theta)$.
2. Because of this property, $-J(q)$ is called **variational lower bound** or **evidence lower bound (ELBO)**.
3. ELBO it often written in the form

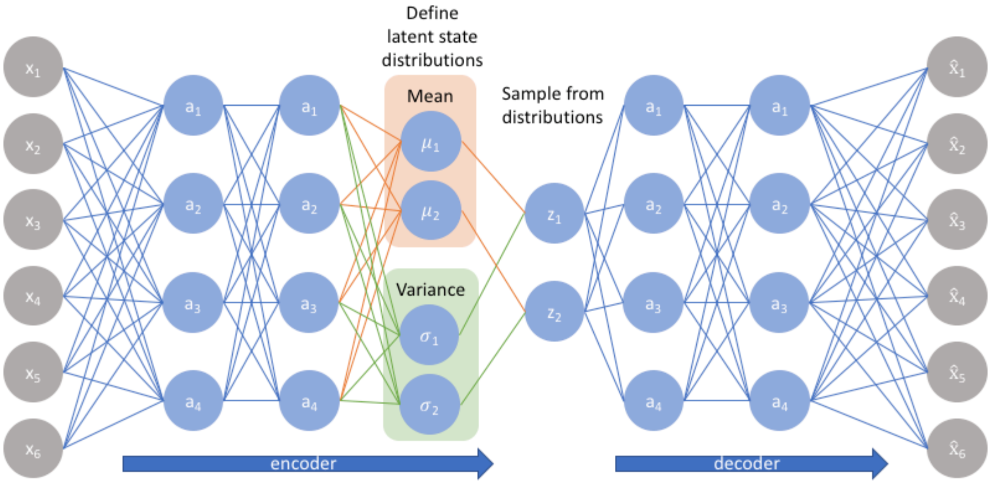
$$\log Z(\theta) \geq \mathbb{E}_{q(x)}[\log \bar{p}(x) - \log p(x)].$$

4. The difference between $\log Z(\theta)$ and $-J(q)$ is $KL(q\|p)$.
5. Thus, by maximizing ELBO, we are minimizing $KL(q\|p)$.

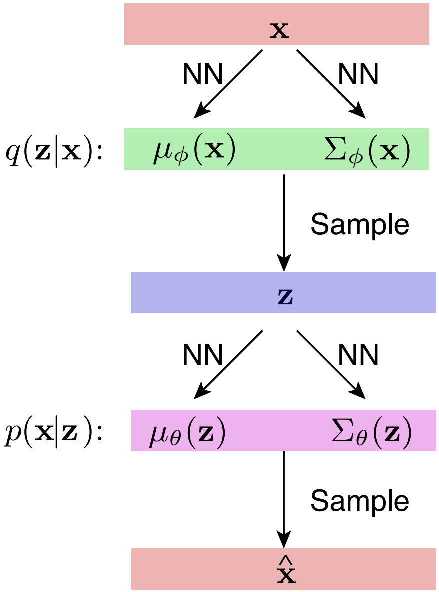
Variational Autoencoder models

1. The idea of VAE is actually less similar to all the autoencoder models, but deeply rooted in graphical models (Kingma and Welling 2014).
2. Instead of mapping the input into a fixed vector, we want to map it into a distribution (in practice, a Gaussian distribution) over encodings.
3. The decoder will then sample an encoding from that probability distribution, and try to reconstruct the original input.
4. This forces the decoder to produce reasonable outputs over a range of different encodings.
5. Since a Gaussian distribution can be parametrized by its mean vector and covariance matrix, we have the encoder output a mean vector μ and a covariance matrix Σ (restricted to a diagonal matrix for simplicity).

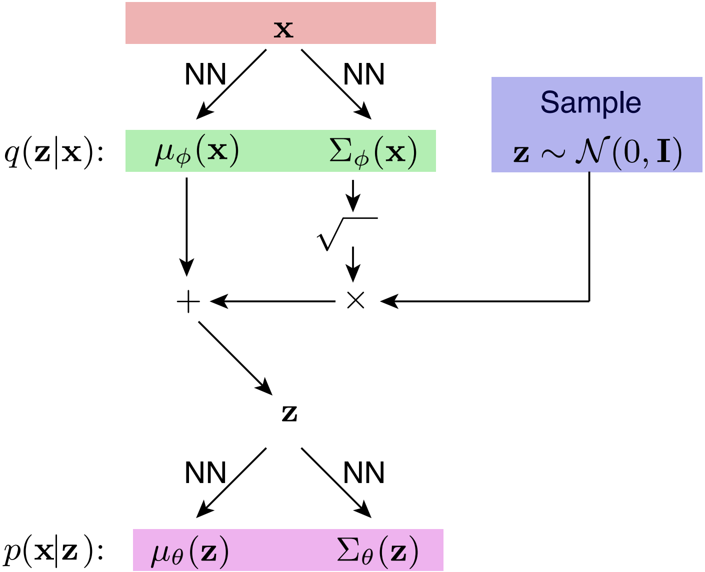
1. The VAE has the following architecture.



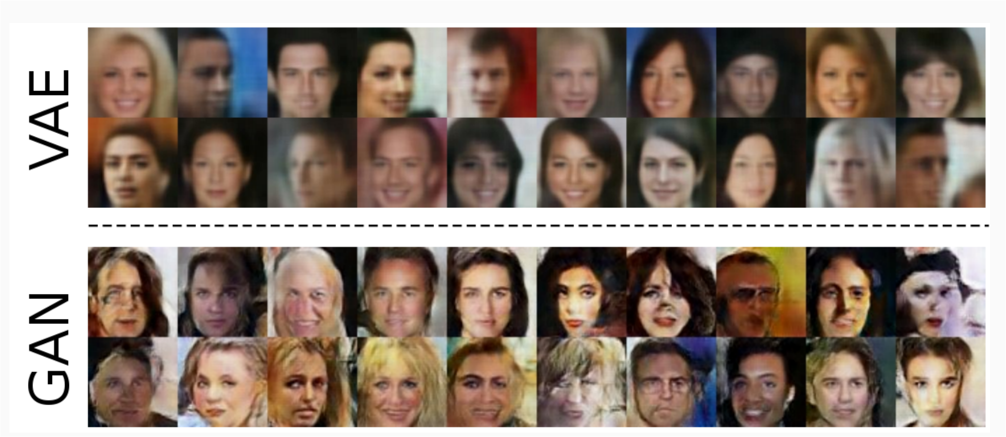
1. We can generate through VAE as



1. VAEs are not as simple to optimize though.
2. The key problem is that the sampling operation is not differentiable and we cannot propagate gradients to encoder.
3. We resolve this problem through reparameterization trick.



1. The comparison between VAE and GAN.



Normalizing Flow Models

1. Given a function of mapping a n-dimensional input vector $\mathbf{x}$ to a m-dimensional output vector, $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^m$, the Jacobian matrix, $\mathbf{J}$, is

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

2. The determinant of a $n \times n$ matrix M is

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

$\tau(.)$ indicates the signature of a permutation.[7]

[7] Most slides of this section are adopted from
https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html

1. Given a random variable z and its known probability density function $z \sim \pi(z)$, we would like to construct a new random variable using a one-one mapping function $x = f(z)$.
2. The function f is invertible, so $z = f^{-1}(x)$.
3. The question is how to infer the unknown probability density function of the new variable, $p(x)$?

$$\int_x p(x)dx = \int_z \pi(z)dz = 1$$

Definition of probability distribution.

$$p(x) = \pi(z)\left|\frac{dz}{dx}\right| = \pi(f^{-1}(x))\left|\frac{df^{-1}}{dx}\right| = \pi(f^{-1}(x))|(f^{-1})'(x)|$$

4. By definition, the integral $\int_z \pi(z)dz$ is the sum of an infinite number of rectangles of infinitesimal width Δz.
5. The height of such a rectangle at position z is the value of the density function $\pi(z)$.

1. When we substitute the variable, $z = f^{-1}(x)$ yields $\frac{\Delta z}{\Delta x} = (f^{-1}(x))'$ and $\Delta z = (f^{-1}(x))'\Delta x$.
2. Here $|(f^{-1}(x))'|$ indicates the ratio between the area of rectangles defined in two different coordinate of variables z and x, respectively.
3. The multivariable version has a similar format:

$$\mathbf{z} \sim \pi(\mathbf{z}), \mathbf{x} = f(\mathbf{z}), \mathbf{z} = f^{-1}(\mathbf{x})$$

$$\begin{aligned} p(\mathbf{x}) &= \pi(\mathbf{z}) \left| \det\left(\frac{d\mathbf{z}}{d\mathbf{x}}\right) \right| \\ &= \pi(f^{-1}(\mathbf{x})) \left| \det\left(\frac{df^{-1}}{d\mathbf{x}}\right) \right| \end{aligned}$$

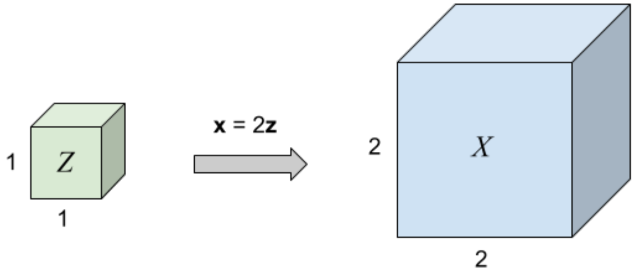
where $\det\left(\frac{\partial f}{\partial \mathbf{z}}\right)$ is the Jacobian determinant of the function f.

Change of Variable Theorem (example)

1. Consider a random variable Z that is uniformly distributed over the unit cube $\mathbf{z} \in [0, 1]^3$.
2. We can scale Z by a factor of 2 to get a new random variable X,

$$\mathbf{x} = f(\mathbf{z}) = \mathbf{A}\mathbf{z} = \begin{vmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{vmatrix} \mathbf{z}$$

   where X is uniform over a cube with side length 2.



Change of Variable Theorem (example)

1. How is the density $p(x)$ related to $\pi(z)$?
2. Since every distribution sums to 1 and the unit cube has volume $V_Z = 1$.

$$\pi(\mathbf{z})V_Z = 1$$

   and $\pi(z) = 1$ for all z in the unit cube.
3. The volume of the larger cube is easy to compute: $V_X = 2^3 = 8$.
4. The total probability mass must be conserved, so we can solve for the density of X.

$$p(\mathbf{x}) = \frac{\pi(\mathbf{z})V_Z}{V_X} = \frac{1}{8}.$$

5. The new density is equal to the original density multiplied by the ratio of the volumes.

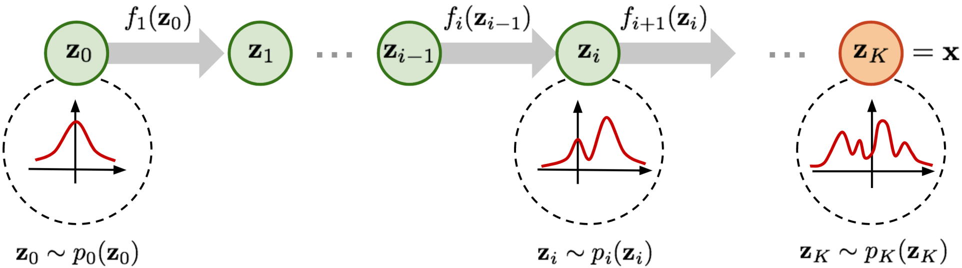
1. The change of variables formula allows us to tractably compute normalized probability densities when we apply an invertible transformation f.

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

2. The invertible function is just multiplication by a scaling matrix, so the determinant of the Jacobian matrix is easy to compute:

$$\det \left(\frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \right) = \det(\mathbf{A}) = 8.$$

1. Normalizing flow transforms a simple distribution into a complex one by applying a sequence of invertible transformation functions (Rezende and Mohamed 2015).



2. We need the embedded probability distribution is expected to be simple enough to calculate the derivative easily and efficiently.
3. This is why Gaussian distribution is often used in latent variable generative models.

1. From the previous slide, we have

$$\begin{aligned} \mathbf{z}_{i-1} &\sim p_{i-1}(\mathbf{z}_{i-1}) \\ \mathbf{z}_i &= f_i(\mathbf{z}_{i-1}), \text{ thus } \mathbf{z}_{i-1} = f_i^{-1}(\mathbf{z}_i) \\ p_i(\mathbf{z}_i) &= p_{i-1}(f_i^{-1}(\mathbf{z}_i)) \left| \det \left(\frac{df_i^{-1}}{d\mathbf{z}_i} \right) \right| \end{aligned}$$

2. Repeating above, we can do inference using base distribution.

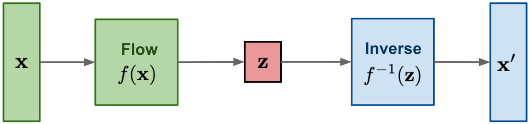
$$\begin{aligned} p_i(\mathbf{z}_i) &= p_{i-1}(\mathbf{z}_{i-1})(f_i^{-1}(\mathbf{z}_i)) \\ &= p_{i-1}(\mathbf{z}_{i-1}) \left| \det \left(\left(\frac{df_i}{d\mathbf{z}_{i-1}} \right)^{-1} \right) \right| \quad \text{According to the inverse func theorem.} \\ &= p_{i-1}(\mathbf{z}_{i-1}) \left| \det \left(\frac{df_i}{d\mathbf{z}_{i-1}} \right) \right|^{-1} \quad \text{Using property of Jacobians of invertible func.} \\ \log p_i(\mathbf{z}_i) &= \log p_{i-1}(\mathbf{z}_{i-1}) - \log \left| \det \left(\frac{df_i}{d\mathbf{z}_{i-1}} \right) \right| \end{aligned}$$

1. Given chain of pdfs, we can expand the equation of the output x step by step until tracing back to the initial distribution $\mathbf{z}_0$.

$$
\begin{aligned}
\mathbf{x} = \mathbf{z}_K &= f_K \circ f_{K-1} \circ \cdots \circ f_1(\mathbf{z}_0) \\
\log p(\mathbf{x}) = \log \pi_K(\mathbf{z}_K) &= \log \pi_{K-1}(\mathbf{z}_{K-1}) - \log \left| \det \left(\frac{df_K}{d\mathbf{z}_{K-1}} \right) \right| \\
&= \log \pi_{K-2}(\mathbf{z}_{K-2}) - \log \left| \det \left(\frac{df_{K-1}}{d\mathbf{z}_{K-2}} \right) \right| \\
&- \log \left| \det \left(\frac{df_K}{d\mathbf{z}_{K-1}} \right) \right| \\
&= \dots \\
&= \log \pi_0(\mathbf{z}_0) - \sum_{i=1}^{K} \log \left| \det \left(\frac{df_i}{d\mathbf{z}_{i-1}} \right) \right|
\end{aligned}
$$

Normalizing Flows

1. The path traversed by the random variables is the flow.



2. The full chain formed by the successive distributions π_i is called a normalizing flow.
3. A transformation function f_i should satisfy two properties:
   - It is easily invertible.
   - Its Jacobian determinant is easy to compute.
4. With normalizing flows, the exact log-likelihood of input data $\log p(\mathbf{x})$ becomes tractable.
5. The training criterion is simply the negative log-likelihood (NLL) over training dataset S.

$$\mathcal{L}(S) = -\frac{1}{|S|} \sum_{\mathbf{x} \in S} \log p(\mathbf{x})$$

Real-valued Non-Volume Preserving (RealNVP)

1. The RealNVP model implements a normalizing flow by stacking a sequence of invertible bijective transformation functions (Dinh, Sohl-Dickstein, and S. Bengio 2017).
2. In each bijection $f : \mathbf{x} \mapsto \mathbf{y}$, the input dimensions are split into two parts:
   - The first d dimensions stay same (x_1);
   - The second part, $d+1$ to D dimensions (x_2) transformed using

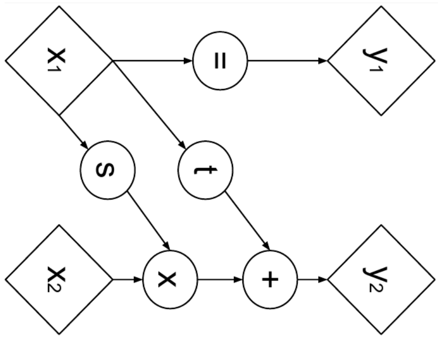
$$
\begin{aligned}
\mathbf{y}_{1:d} &= \mathbf{x}_{1:d} \\
\mathbf{y}_{d+1:D} &= \mathbf{x}_{d+1:D} \odot \exp(s(\mathbf{x}_{1:d})) + t(\mathbf{x}_{1:d})
\end{aligned}
$$

   where

   $s(.)$ and $t(.)$ are scale and translation functions and both map $\mathbb{R}^d \mapsto \mathbb{R}^{D-d}$.

   The $\odot$ operation is the element-wise product.

1. This network has
   - Stack many invertible coupling layers.
   - Each has simple inverse and determinant



Real-valued Non-Volume Preserving (RealNVP)

1. This transformation satisfy two properties of flow transformations.

   - It is easily invertible.

$$\begin{cases} \mathbf{y}_{1:d} &= \mathbf{x}_{1:d} \\ \mathbf{y}_{d+1:D} &= \mathbf{x}_{d+1:D} \odot \exp(s(\mathbf{x}_{1:d})) + t(\mathbf{x}_{1:d}) \end{cases}$$

$$\Leftrightarrow \begin{cases} \mathbf{x}_{1:d} &= \mathbf{y}_{1:d} \\ \mathbf{x}_{d+1:D} &= (\mathbf{y}_{d+1:D} - t(\mathbf{y}_{1:d})) \odot \exp(-s(\mathbf{y}_{1:d})) \end{cases}$$

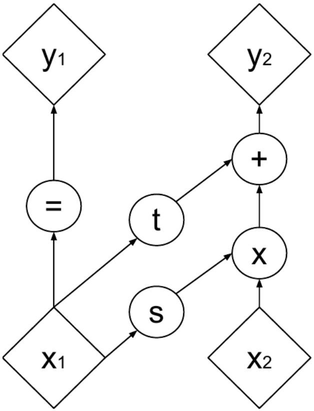
   - Its Jacobian determinant is easy to compute. The Jacobian is a lower triangular matrix.

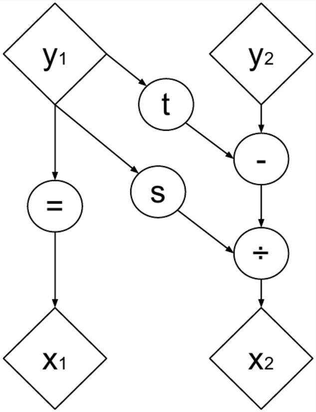
$$\mathbf{J} = \begin{bmatrix} \mathbb{I}_d & \mathbf{0}_{d\times(D-d)} \\ \frac{\partial \mathbf{y}_{d+1:D}}{\partial \mathbf{x}_{1:d}} & \operatorname{diag}(\exp(s(\mathbf{x}_{1:d}))) \end{bmatrix}$$

   Hence, the determinant is simply the product of terms on the diagonal.

$$\det(\mathbf{J}) = \prod_{j=1}^{D-d} \exp(s(\mathbf{x}_{1:d}))_j = \exp(\sum_{j=1}^{D-d} s(\mathbf{x}_{1:d})_j)$$

1. The inverse transformation





Real-valued Non-Volume Preserving (RealNVP)

Data space $\mathcal{X}$ Latent space $\mathcal{Z}$

Inference

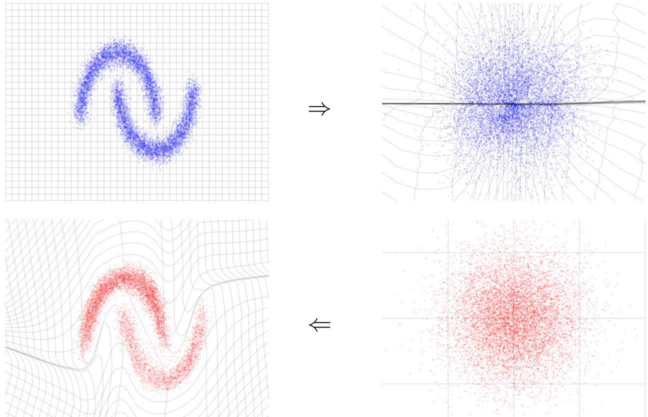
$x \sim \hat{p}_X$

$z = f(x)$

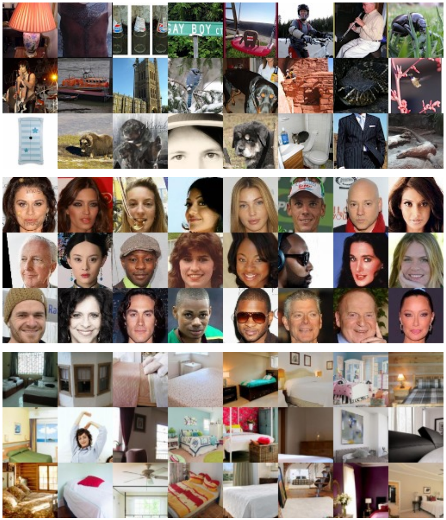
Generation

$z \sim p_Z$

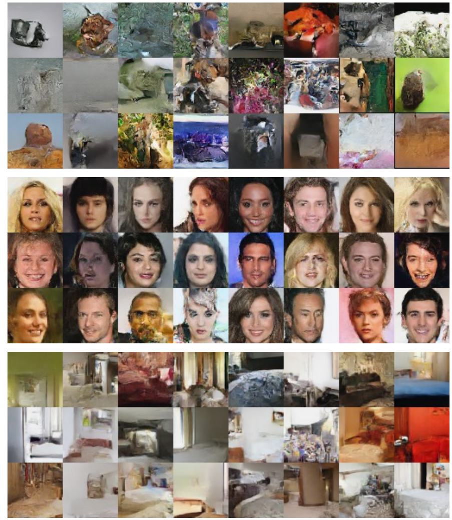
$x = f^{-1}(z)$



Real-valued Non-Volume Preserving (RealNVP)

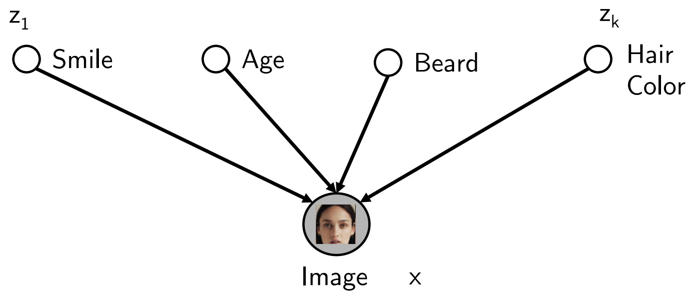


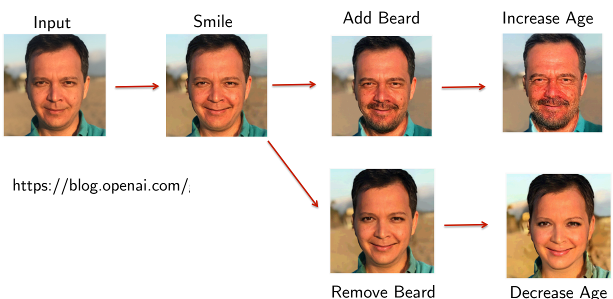
Dataset



samples from model

1. The Glow model extends RealNVP, and simplifies the architecture by replacing the reverse permutation operation on the channel ordering with invertible 1×1 convolutions (Kingma and Dhariwal 2018).
2. Latent factors

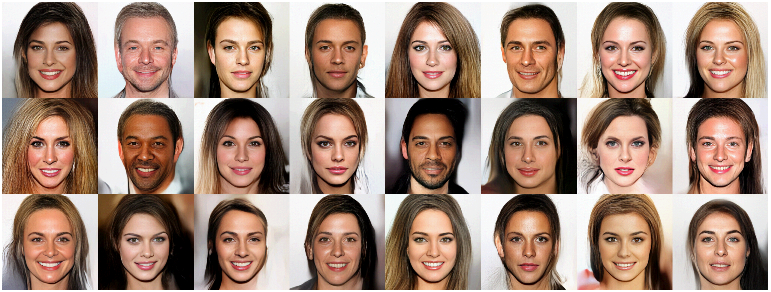




https://blog.openai.com/;

Glow Results

Synthetic celebrities sampled from Glow model



Random samples from the Glow model

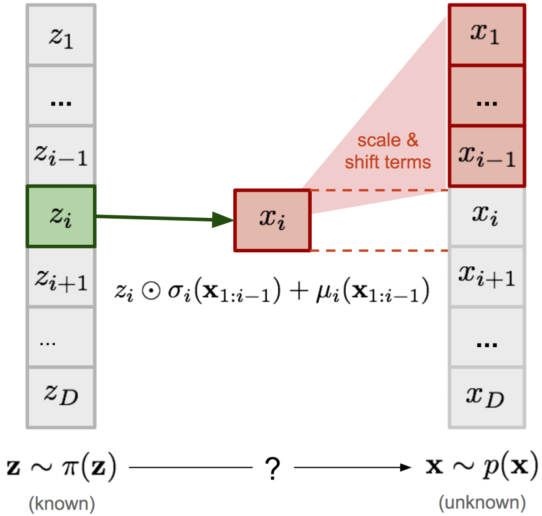
See also `https://openai.com/blog/glow/`.

1. In autoregressive models, the probability of observing x_i is conditioned on $x_1, \ldots, x_{i-1}$ and the product of these conditional probabilities gives us the probability of observing the full sequence:

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

2. If a flow transformation in a normalizing flow is framed as an autoregressive model, the model is an autoregressive flow.

1. MAF is a type of normalizing flows, where the transformation layer is built as an autoregressive neural network (Papamakarios, Murray, and Pavlakou 2017).



1. Given two random variables $\mathbf{z} \sim \pi(\mathbf{z})$ and $\mathbf{x} \sim p(\mathbf{x})$, and the probability density function $\pi(z)$ is known, MAF aims to learn $p(x)$.
2. MAF generates each x_i, conditioned on the past dimensions $\mathbf{x}_{1:i-1}$.
   - Data generation, producing a new $\mathbf{x}$.

$$x_i = z_i \exp \alpha_i + \mu_i$$

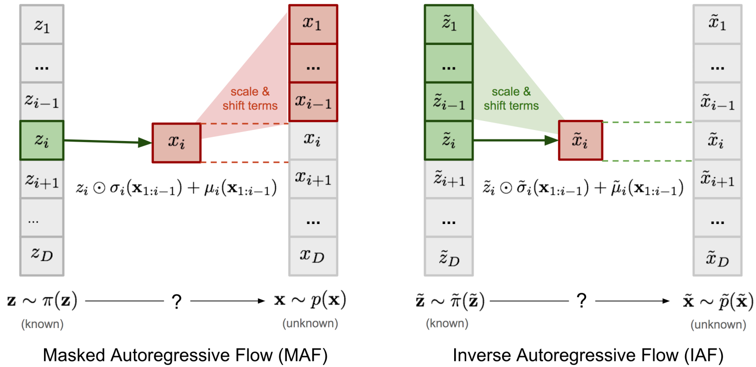
where

$$p(x_i|\mathbf{x}_{1:i-1}) = \mathcal{N}\left(x_i|\mu_i, (\exp \alpha_i)^2\right)$$
$$\mu_i = f_{\mu_i}(\mathbf{x}_{1:i-1})$$
$$\alpha_i = f_{\alpha_i}(\mathbf{x}_{1:i-1})$$

   - Density estimation, given a known $\mathbf{x}$.

$$p(\mathbf{x}) = \prod_{i=1}^{D} p(x_i|\mathbf{x}_{1:i-1})$$

1. IAF models the conditional probability of the target variable as an autoregressive model too, but with a reversed flow (for efficient sampling process) (Kingma, Salimans, and Welling 2016).



2. In IAF, the nonlinear shift/scale statistics are computed using the previous noise variates $\mathbf{z}_{1:i-1}$, instead of the data samples:

$$x_i = z_i \exp \alpha_i + \mu_i$$

$$\mu_i = f_{\mu_i}(\mathbf{z}_{1:i-1})$$

$$\alpha_i = f_{\alpha_i}(\mathbf{z}_{1:i-1})$$

1. The reverse transformation in MAF is

$$z_i = \frac{x_i - \mu_i(\mathbf{x}_{1:i-1})}{\sigma_i(\mathbf{x}_{1:i-1})} = -\frac{\mu_i(\mathbf{x}_{1:i-1})}{\sigma_i(\mathbf{x}_{1:i-1})} + x_i \odot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}$$

2. If we consider

$$\tilde{\mathbf{x}} = \mathbf{z},\ \tilde{p}(.) = \pi(.),\ \tilde{\mathbf{x}} \sim \tilde{p}(\tilde{\mathbf{x}})$$
$$\tilde{\mathbf{z}} = \mathbf{x},\ \tilde{\pi}(.) = p(.),\ \tilde{\mathbf{z}} \sim \tilde{\pi}(\tilde{\mathbf{z}})$$
$$\tilde{\mu}_i(\tilde{\mathbf{z}}_{1:i-1}) = \tilde{\mu}_i(\mathbf{x}_{1:i-1}) = -\frac{\mu_i(\mathbf{x}_{1:i-1})}{\sigma_i(\mathbf{x}_{1:i-1})}$$
$$\tilde{\sigma}(\tilde{\mathbf{z}}_{1:i-1}) = \tilde{\sigma}(\mathbf{x}_{1:i-1}) = \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}$$

3. Then, $\tilde{x}_i \sim p(\tilde{x}_i|\tilde{\mathbf{z}}_{1:i}) = \tilde{z}_i \odot \tilde{\sigma}_i(\tilde{\mathbf{z}}_{1:i-1}) + \tilde{\mu}_i(\tilde{\mathbf{z}}_{1:i-1})$, where $\tilde{\mathbf{z}} \sim \tilde{\pi}(\tilde{\mathbf{z}})$
4. IAF intends to estimate the probability density function of $\tilde{\mathbf{x}}$ given that $\tilde{\pi}(\tilde{\mathbf{z}})$ is already known.

Evaluating deep generative models

1. Evaluation of generative models is tricky
2. The key questions is about underlying task of the generative model.
   - Density estimation
   - Sampling / generation
   - Latent representation learning
   - More than one task.
3. How do we evaluate generative models?

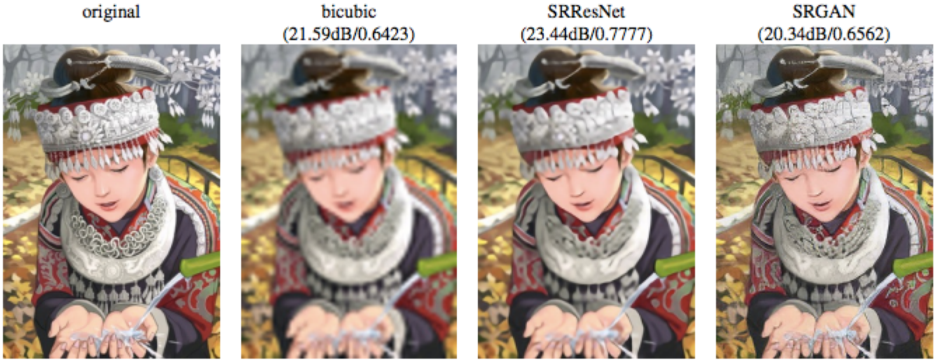
Example (Evaluating density estimation)

When the given model has tractable likelihood, the evaluation is straightforward.

- Split dataset into train, validation, and test sets.
- Evaluate gradients based on the train set.
- Tune hyper-parameters based on the validation set.
- Evaluate generalization by measuring likelihoods on the test set.

1. We have a dataset that sampled from p_{data} and generated samples from p_g.
2. Evaluating deep generative models (DGM) is hard because
   - the distributions of interest are often high dimensional,
   - the likelihood functions are not always available or easily computable.
3. A common way to evaluate a DGM is to measure how close p_{data} is to p_g.
4. Since sample complexity of traditional measure such as KL divergence or Wasserstein distance is exponential in the dimensionality of the distribution, they cannot be used for real world distributions.
5. The reduced sample complexity comes at the cost of reduced discriminative power.
6. These metrics cannot tell the difference between a model that memorizes the training data and a model that generalizes.

1. Some generative models, such as VAE, have intractable likelihoods.
2. For example, in VAE we can compare the evidence lower bounds (ELBO) to log-likelihoods.
3. For general case, kernel density estimates only via samples can be used.
4. Consider the following generated images, which of them is better?

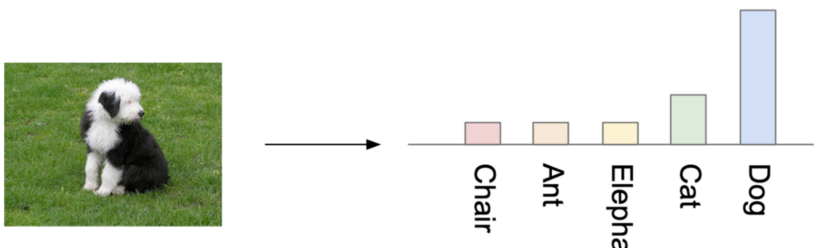


Human evaluations

1. One intuitive metric of performance can be obtained by having human annotators judge the visual quality of samples.
2. This process can be automated using Amazon Mechanical Turk (Salimans, I. J. Goodfellow, et al. 2016).
3. The task is to ask annotators to distinguish between **generated data** and **real data**.
4. For **MNIST** dataset and GAN model, annotators were able to distinguish samples in **52.4%** of cases (2000 votes total), where **50%** would be obtained by random guessing.
5. For **CIFAR-10** dataset and GAN model, annotators were able to distinguish samples in **78.7%** of cases.
6. A downside of using human annotators is that the metric varies depending on the setup of the task and the motivation of the annotators.
7. Also, results change drastically when we give annotators feedback about their mistakes.
8. By learning from such feedback, annotators are better able to point out the flaws in generated images, giving a more pessimistic quality assessment.

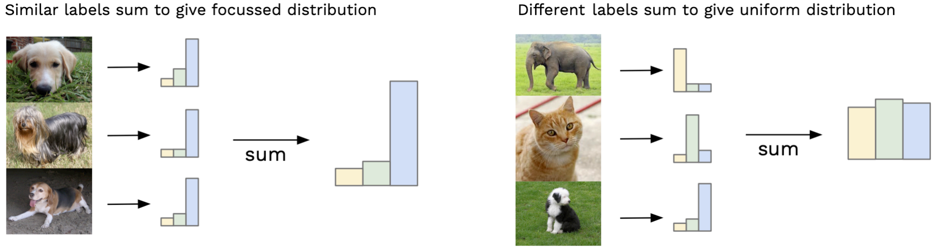
Inception score

1. The inception score takes a list of images and returns a single number, the score.
2. The score is a measure of how realistic the output of a generative model (GAN) is.
3. The score measures two things simultaneously:
   - The images have variety.
   - Each image distinctly looks like something.
4. If both things are true, the score will be high; otherwise, the score will be low.
5. The lower bound of this score is zero and the upper bound is ∞.
6. The inception score takes its name from the Inception classifier, an image classification network from Google.
7. Classifier takes an image, and returns probability distribution of labels for image.



Inception score

1. If image contains just one well-formed thing, then output of classifier is a narrow distribution.
2. If image is a jumble, or contains multiple things, it's closer to the uniform distribution of many similar height bars.
3. The next step is combine the label probability distributions for many of generated images (50,000 images).
4. By summing the label distributions of our images, a new label distribution (marginal distribution) will be obtained.
5. The marginal distribution tells the variety in the generator's output:



6. The final step is to combine these two different things into one single score.

1. The final step is to combine these two different things into one single score.
2. By comparing label distribution with marginal label distribution for images, a score will be obtained that shows how much those two distributions differ.
3. The more they differ, the higher a score we want to give, and this is the inception score.
4. To produce the inception score, the KL divergence between label distribution and marginal label distribution is used.
   - Construct an estimator of the Inception Score from samples $\mathbf{x}^{(i)}$ by constructing an empirical marginal class distribution,

$$\hat{p}(y) = \frac{1}{m}\sum_{i=1}^{m} p(y \mid \mathbf{x}^{(i)})$$

   - Then an approximation to the expected KLdivergence is computed by

$$IS(G) \approx \exp\left(\frac{1}{m}\sum_{i=1}^{m} D_{KL}(p(y \mid \mathbf{x}^{(i)}) \parallel \hat{p}(y))\right)$$

1. Several metrics have been proposed for evaluation of generative models (Thanh-Tung and Tran 2020).
2. Divergence based evaluation metrics
   - Inception score
   - Fréchet inception distance
   - Neural net divergence
3. Precision-Recall based evaluation metrics
   - k-means based Precision-Recall
   - k-NN based Precision-Recall
4. Other evaluation metrics
   - Metrics for class-conditional models
   - Topological/Geometrical approaches
   - Non-parametric approaches

Summary

1. Marginal distribution on x obtained by integrating out z

$$p(z) = \mathcal{N}(z; 0, I)$$
$$p_\theta(x) = \int_z p(z) p(x|f_\theta(z))$$

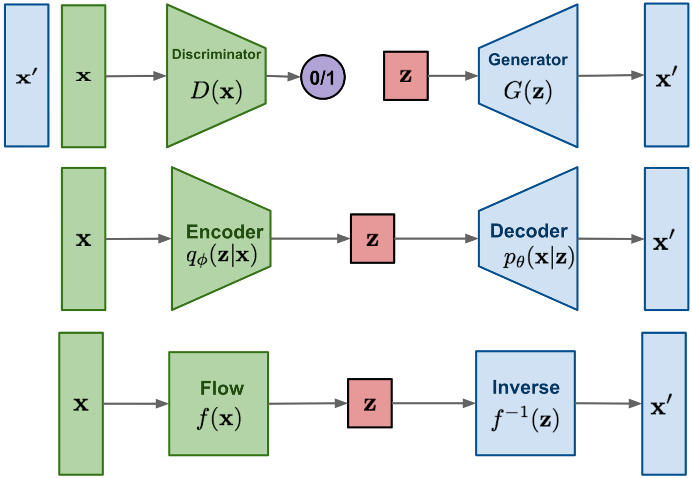
2. Problem: Evaluation of $p_\theta(x)$ intractable due to integral involving flexible non-linear deep net $f_\theta(z)$.
3. Solutions: by different unsupervised deep learning paradigms
   - Avoid integral: Generative adversarial networks (GAN)
   - Approximate integral: Variational autoencoders (VAE)
   - Tractable integral: constrain $f_\theta(z)$ to invertible flow. Please read (Kobyzev, Prince, and Brubaker 2020).
   - Avoid latent variables: autoregressive models

Different generative models using latent variables

GAN: minimax the classification error loss.

VAE: maximize ELBO.

Flow-based generative models: minimize the negative log-likelihood



Reading

1. Chapter 10 of Deep Learning Book[8]

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Questions?