

10707

Deep Learning: Spring 2021

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Lecture 8:

Intro to unsupervised
learning

Recap: unsupervised learning

Unsupervised learning

■ “Pure” Reinforcement Learning (cherry)

- ▶ The machine predicts a scalar reward given once in a while.
- ▶ **A few bits for some samples**

■ Supervised Learning (icing)

- ▶ The machine predicts a category or a few numbers for each input
- ▶ Predicting human-supplied data
- ▶ **10→10,000 bits per sample**

■ Unsupervised/Predictive Learning (cake)

- ▶ The machine predicts any part of its input for any observed part.
- ▶ Predicts future frames in videos
- ▶ **Millions of bits per sample**



■ (Yes, I know, this picture is slightly offensive to RL folks. But I'll make it up)

Slide by Yann LeCun

Unsupervised learning

Learning from data **without** labels.

What can we hope to do:

Task A: Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace, manifold) to data to reveal something meaningful about data. (**Structure learning**)

Task B: Learn a (parametrized) **distribution** *close* to data generating distribution. (**Distribution learning**)

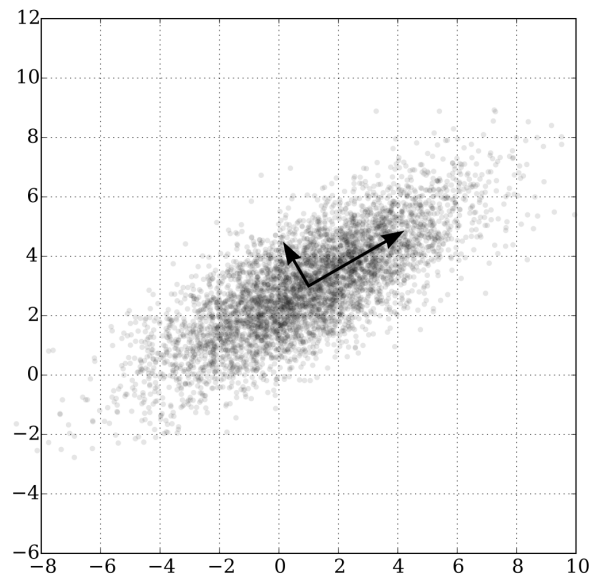
Task C: Learn a (parametrized) distribution that implicitly reveals an **“embedding”/“representation”** of data for downstream tasks. (**Representation/feature learning**)

Entangled! The “structure” and “distribution” often reveals an embedding.

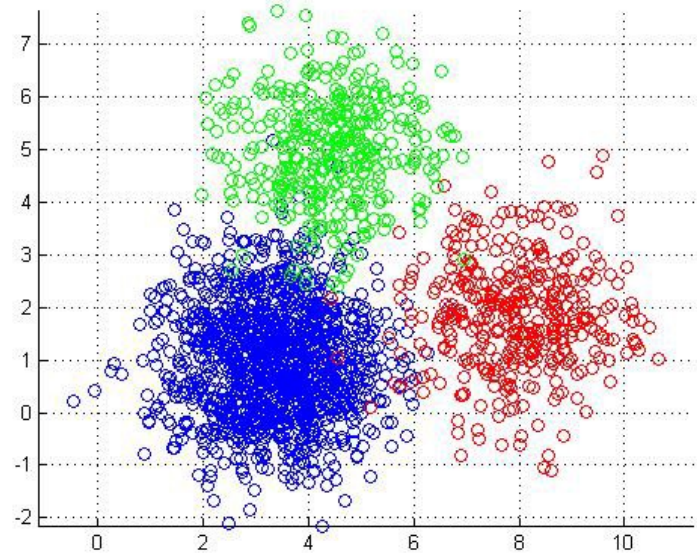
Structure learning

Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace) to data to reveal something meaningful about data.

PCA(principal component analysis),
direction of highest variance



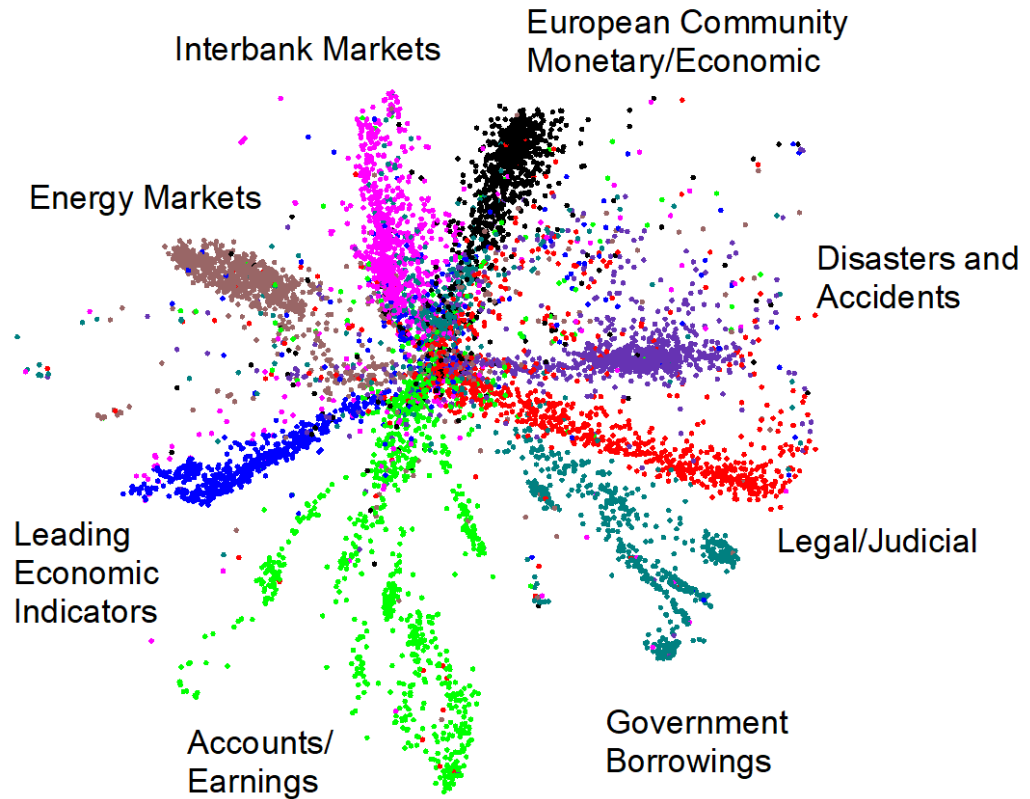
Clustering



Structure learning



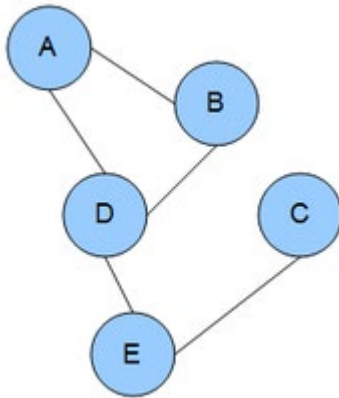
804,414 newswire stories



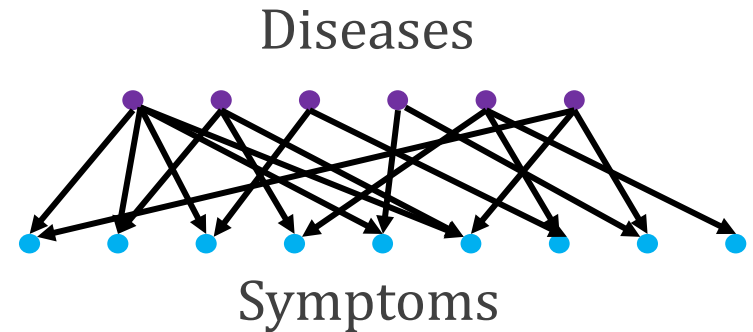
Distribution learning

Some typical choices of parametrized distributions:

Classical choices: **fully-observed** graphical models (undirected and directed), **latent-variable** graphical models (mixture models, sparse coding, topic models).



Markov Random Fields:
sparse independence
structure: “A is independent of
other vars, given B, D”

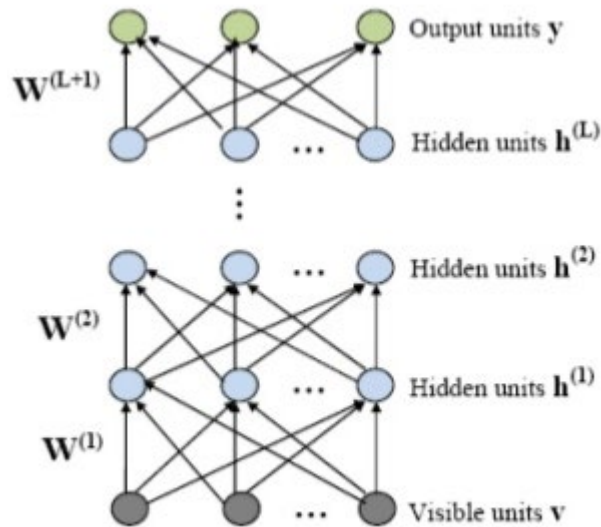


Latent variable models: data is
“simple” conditioned on some
unobserved (latent) variables

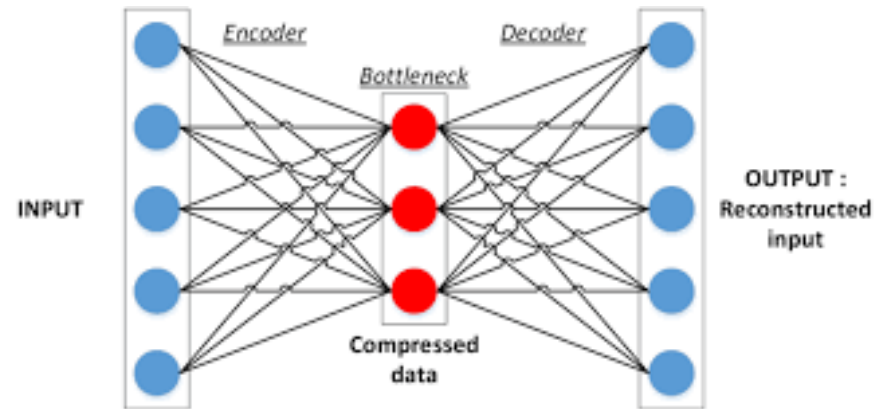
Distribution learning

Some typical choices of parametrized distributions:

Semi-modern choices: deep Boltzmann machines, deep belief networks, (variational) auto-encoders, energy models.



Deep Boltzmann machines, belief networks: graphical model analogues of deep neural networks.

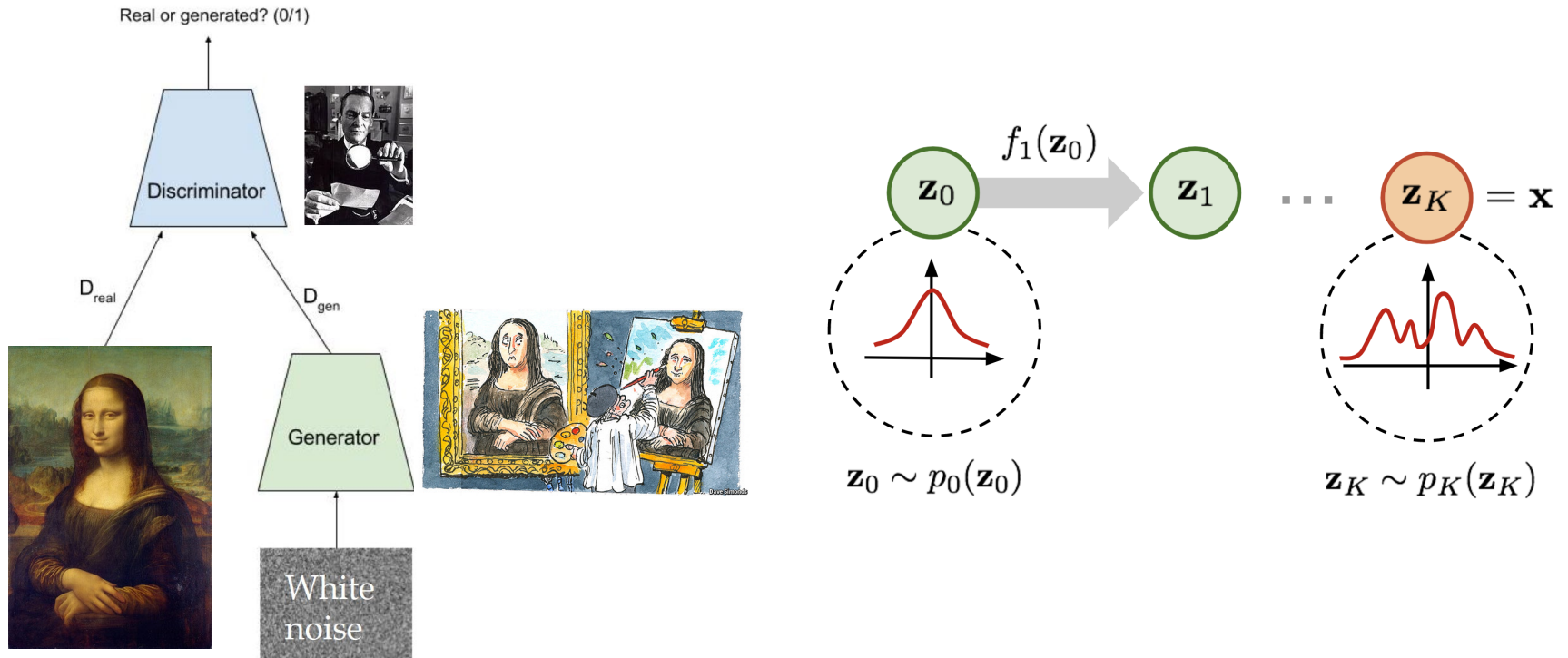


(Variational) autoencoders: model data by enforcing a latent space “bottleneck”:

Distribution learning

Some typical choices of parametrized distributions:

Modern choices: generative adversarial networks, autoregressive models (pixelRNN, pixelCNN), flow models, etc.



Distribution learning



Training
Data(CelebA)



Model Samples (Karras et.al.,
2018)

4 years of progression on Faces



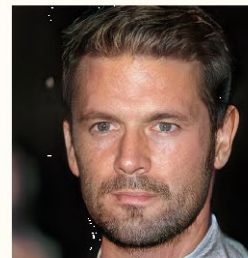
20 14



20 15



20 16



20 17

Brundage et al.,
2017

Distribution learning



Whichfaceisreal.com

Distribution learning



BigGAN, Brock et al '18

Distribution learning

Conditional generative model $P(\text{zebra images} | \text{horse images})$



Style Transfer



Input Image



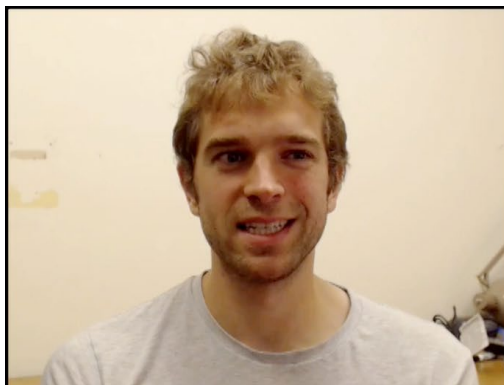
Monet



Van Gogh

Distribution learning

Source
actor



Target
actor



Real-time Reenactment



Real-time
reenactment

Reenactment Result

Representation learning and self-supervised learning

Given **unlabeled** data, **design supervised tasks** that induce a good representation for downstream tasks.

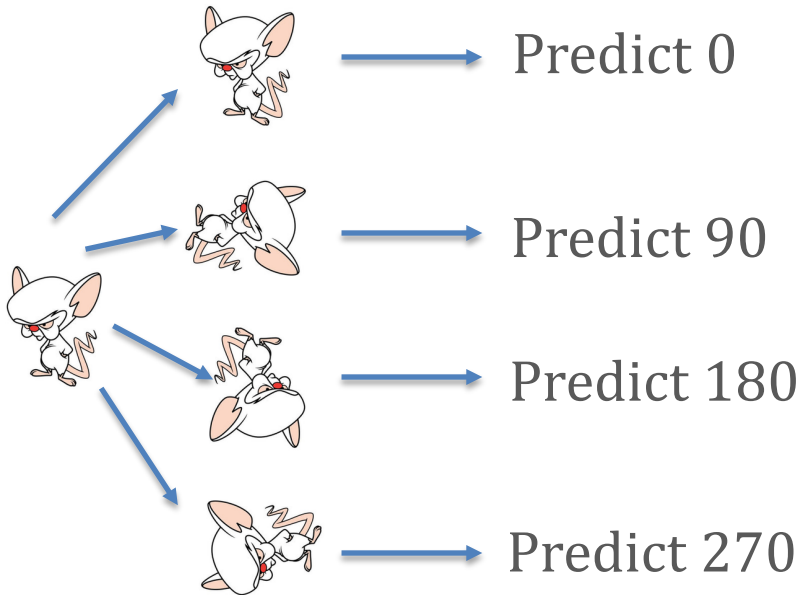
No good mathematical formalization, but the intuition is to “force” the predictor used in the task to learn something “**semantically meaningful**” about the data.

Examples in NLP: predict next word, given previous 5 words; predict middle word, given surrounding 5 words; etc.

Representation learning and self-supervised learning

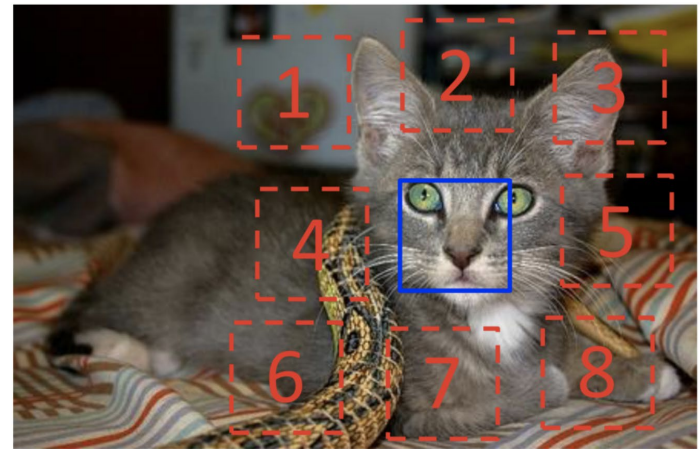
Examples in vision: a lot, and quite different in nature.

Rotation prediction



Predict one of four angles
an image is rotated by

Jigsaw puzzles



$$X = \left(\begin{array}{c} \text{cat face} \\ \text{cat ear} \end{array} \right); Y = 3$$

Predict position of second
piece wrt to first

Relationships between the tasks

Structure learning and feature learning often blend

E.g. low dimensional features in PCA or cluster a point belongs to in clustering can be viewed as features.

Structure learning/feature learning is in general weaker than distribution learning:

E.g. methods like PCA/clustering can't be used to generate new samples.

Feature, not a bug: it has been argued that self-supervised learning works because the task we are solving is **easier** (both computationally and statistically)

Relationships between the tasks

Distribution learning often implies representation learning:

Many distributions we fit are **latent-variable** models (i.e. model the joint distribution between some latent variables \mathbf{h} and the observed data \mathbf{x})

$$P_{\theta}(x, h) = P_{\theta}(h)P_{\theta}(x|h)$$


The latent variables are often viewed as a “**representation**”.

The **posterior** distribution $P_{\theta}(h|x)$ captures a distribution over representations, given some values of the observed data.

However, a-priori, distribution $P_{\theta}(h|x)$ is a-priori not an easy distribution to **approximate/sample** from!

$$P_{\theta}(h|x) = \frac{P_{\theta}(x|h)p(h)}{\int_{h'} p(h')p(x|h')}$$

*Hard high-dimensional
sum/integral*



Representation learning and distribution learning

Common ways to get a handle of $P_\theta(h|x)$: **variational methods** and **MCMC** methods.

Question: how accurately do we need to approximate $P_\theta(h|x)$ if we want a good representation?

(Arora-Risteski blogpost: <http://www.offconvex.org/2017/06/26/unsupervised1/>)

Answer: Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

$$KL(Q_\theta(h|x) || P_\theta(h|x)) \leq \epsilon$$

(KL is a natural metric, as a lot of the **variational methods** operate in this metric. Stay tuned!)

(Recall the definition of KL divergence: $KL(q || p) = \mathbb{E}_q \log \left(\frac{q}{p} \right)$)

Representation learning and distribution learning

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$$KL(Q_\theta(h|x) || P_\theta(h|x)) \leq \epsilon$$

Suppose the way we will use the representation h is to solve **classification tasks**. Namely, let's say the labels for task are:

$$(x_t, c(h_t)), \text{ where } (h_t, x_t) \sim P_\theta(h, x) \text{ and } c(h_t) \in \{\pm 1\}$$

*In other words, the labels are a function of the **latent** variables, and the observables are the data.*

Representation learning and distribution learning

Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

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$$(x_t, c(h_t)), \text{ where } (h_t, x_t) \sim P_\theta(h, x) \text{ and } c(h_t) = \{\pm 1\}$$

The natural way to measure the distance with an eye towards classification tasks is total variation distance:

$$TV(Q_\theta(\cdot | x) || P_\theta(\cdot | x)) = \sup_{\Omega} \left| \Pr_{h \sim Q_\theta(\cdot | x)}[\Omega] - \Pr_{h \sim P_\theta(\cdot | x)}[\Omega] \right|$$

Why is this useful? Take $\Omega = \{\text{"C(h) is the correct label"}\}$

$\Pr_{h \sim Q_\theta(\cdot | x)}[\Omega]$ is the probability of having the correct answer using $Q_\theta(\cdot | x)$

$\left| \Pr_{h \sim Q_\theta(\cdot | x)}[\Omega] - \Pr_{h \sim P_\theta(\cdot | x)}[\Omega] \right|$ is the *difference in probability* of having the correct answer between $Q_\theta(\cdot | x)$!

Representation learning and distribution learning

Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

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Why is this useful? Take $\Omega = \{\text{"C}(h) \text{ is the correct label"}\}$

Hence, $TV(Q_\theta(\cdot | x) || P_\theta(\cdot | x)) \leq \epsilon'$ implies that the difference in performance b/w using $P_\theta(\cdot | x)$ and $Q_\theta(\cdot | x)$ is at most ϵ' (on the input sample x)

Hence, $\mathbb{E}_x[TV(Q_\theta(\cdot | x) || P_\theta(\cdot | x))] \leq \epsilon'$ implies that the difference in performance on the classification task is at most ϵ' .

Representation learning and distribution learning

Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

$$KL(Q_\theta(h|x) || P_\theta(h|x)) \leq \epsilon$$

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To conclude, by Pinsker's inequality, we have

$$TV(Q_\theta(\cdot | x) || P_\theta(\cdot | x)) \leq \sqrt{\frac{1}{2} KL(Q_\theta(\cdot | x) || P_\theta(\cdot | x))} \leq \sqrt{\frac{1}{2} \epsilon}$$

So, if we want a good performance on classification task, we need an extremely close approximation to the posterior!

The classic unsupervised structure learning-methods

The classics: PCA

Figure 1: Population structure within Europe.

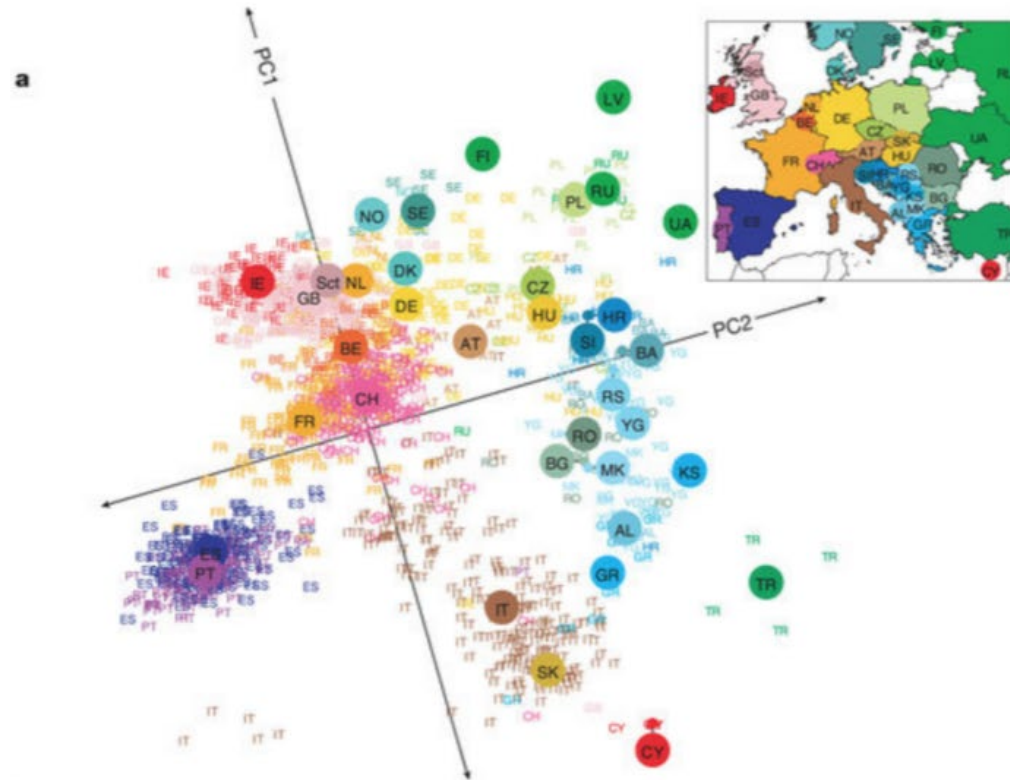


Figure 6: Plot from [1], depicting genomes for 1387 Europeans projected onto top 2 principal components. Colors/labels of datapoints correspond to geographic location of the individuals. Map of Europe (with same coloring) included in upper right for reference.

The classics: PCA

Goal: find a k -dimensional (linear) subspace explaining most of the variance in the data.

Assume the data is centered, that is $\mathbb{E}[x] = 0$

Warmup: let $k=1$.

$$\operatorname{argmax}_{\{v: \|v\|=1\}} \frac{1}{m} \sum_{\text{samples } x_i} \langle v, x_i \rangle^2$$

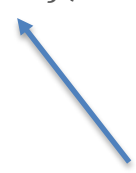


As $m \rightarrow \infty$, we get $\mathbb{E}[\langle v, x \rangle^2]$,
i.e. variance.

The classics: PCA

Goal: find a k-dimensional (linear) subspace explaining most of the variance in the data.

$$\operatorname{argmax}_{\{v_1, v_2, \dots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} (\text{length of } x_i \text{ on } \operatorname{span}(v_1, v_2, \dots, v_k))^2$$

$$= \operatorname{argmax}_{\text{orthonormal } \{v_1, v_2, \dots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^k \langle x_i, v_j \rangle^2$$


As $m \rightarrow \infty$, we get $\mathbb{E}[\sum_j \langle v_j, x \rangle^2]$

The classics: PCA

How to do this efficiently?

$$\operatorname{argmax}_{\text{orthonormal } \{v_1, v_2, \dots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^k \langle x_i, v_j \rangle^2$$

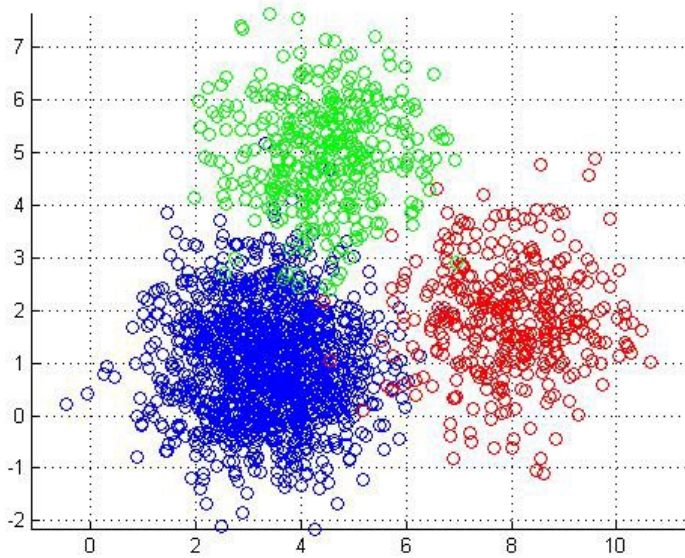
A convenient rewrite:

$$\operatorname{argmax}_{\text{orthonormal } \{v_1, v_2, \dots, v_k\}} \sum_{j=1}^k v_j^T \underbrace{\left(\frac{1}{m} \sum_{\text{samples } x_i} (x_i x_i^T) \right)}_{:= D, \text{ (covariance matrix)}} v_j$$

*How to do this efficiently? – **Singular Value Decomposition!!***

Argmax are the **top k eigenvectors** of D

The classics: clustering

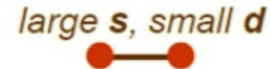
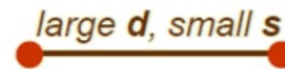


Goal: group the data into clusters of nearby points.

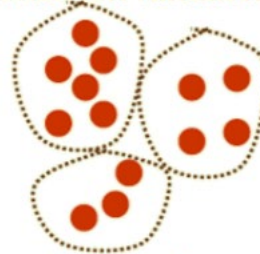
What's needed for clustering?

1. Proximity measure, *either*

- similarity measure $s(x_i, x_k)$: large if x_i, x_k are similar
- dissimilarity (or distance) measure $d(x_i, x_k)$: small if x_i, x_k are similar



2. Criterion function to evaluate a clustering



good clustering



bad clustering

3. Algorithm to compute clustering

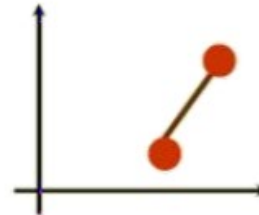
The classics: clustering

Popular distance metrics:

- Euclidean distance

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{k=1}^d (\mathbf{x}_i^{(k)} - \mathbf{x}_j^{(k)})^2}$$

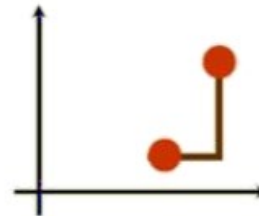
- translation invariant



- Manhattan (city block) distance

$$d(\mathbf{x}_i, \mathbf{x}_j) = \sum_{k=1}^d |\mathbf{x}_i^{(k)} - \mathbf{x}_j^{(k)}|$$

- approximation to Euclidean distance, cheaper to compute



- They are special cases of **Minkowski distance**:

$$d_p(\mathbf{x}_i, \mathbf{x}_j) = \left(\sum_{k=1}^m |\mathbf{x}_{ik} - \mathbf{x}_{jk}|^p \right)^{\frac{1}{p}}$$

(p is a positive integer)

The classics: clustering

Criterion functions:

Intra-cluster cohesion

- Cohesion measures how near the data points in a cluster are to the cluster “center”.

Inter-cluster separation

- Separation means that different cluster centroids should be far away from one another.

In most applications, expert judgments are still the key.

K-means clustering

If the distance metric is the **Euclidean distance**, and the measure of cohesion is the **average distance from the centroid**: we get the **k-means objective**.

$$\operatorname{argmin}_{\{r_{nk}, \mu_k\}} \sum_{n=1}^N \sum_{k=1}^K r_{nk} \|\mathbf{x}_n - \mu_k\|^2$$

Is point n in cluster k ?

Centroid of k -th cluster

K-means clustering

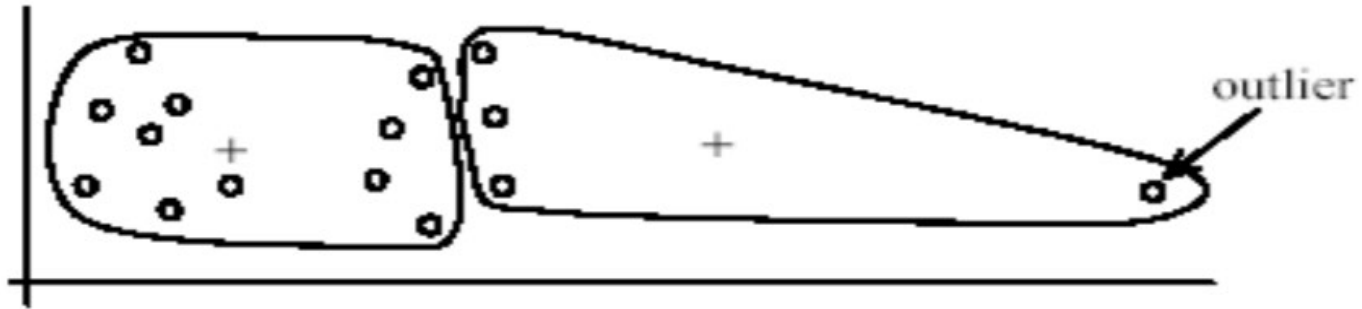
A natural iterative algorithm, which as we will see later is a variant of the **EM (expectation-maximization)** algorithm:

```
Input: Data set  $X = \{x^{(1)}, x^{(2)}, \dots, x^{(m)} | x^{(i)} \in \mathbb{R}^n\}$ 
Output: Cluster centroids  $\mu_{i=1, \dots, k} \in \mathbb{R}^n$ ; Cluster assignments  $c \in \mathbb{Z}$ 
1 Initialize  $k$  cluster centroids  $\mu_1, \dots, \mu_k \in \mathbb{R}^n$  randomly from  $X$ ;
2 repeat
3   for  $i = 1, \dots, m$  do // Update cluster assignments
4     | set  $c^{(i)} = \arg \min_j \|x^{(i)} - \mu_j\|^2$ ;
5   end
6   for  $j = 1, \dots, k$  do // Update cluster centroids
7     | set  $\mu_j = \frac{\sum_{i=1}^m 1_{\{c^{(i)}=j\}} x^{(i)}}{\sum_{i=1}^m 1_{\{c^{(i)}=j\}}}$ ;
8   end
9 until Convergence;
10 return  $\mu$  and  $c$ ;
```

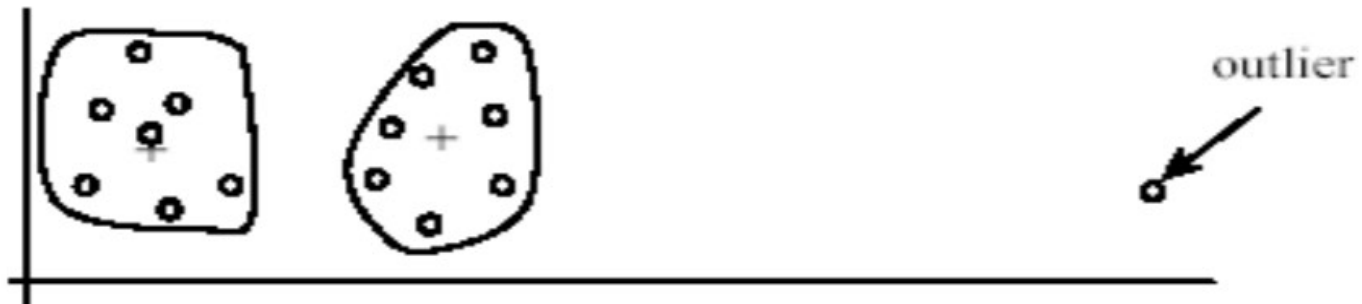
Algorithm 1: Algorithm of batch-version for K-means

Some weaknesses

Very sensitive to outliers:



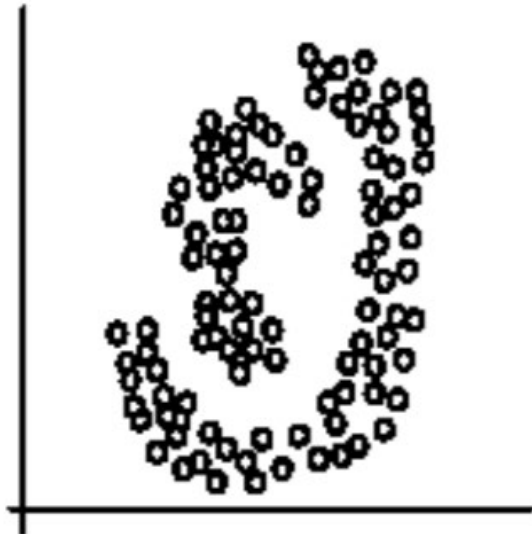
(A): Undesirable clusters



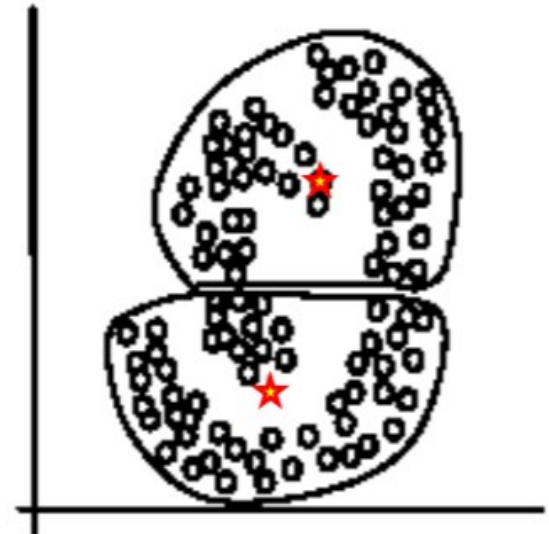
(B): Ideal clusters

Some weaknesses

Not suitable for non-spherical clusters:

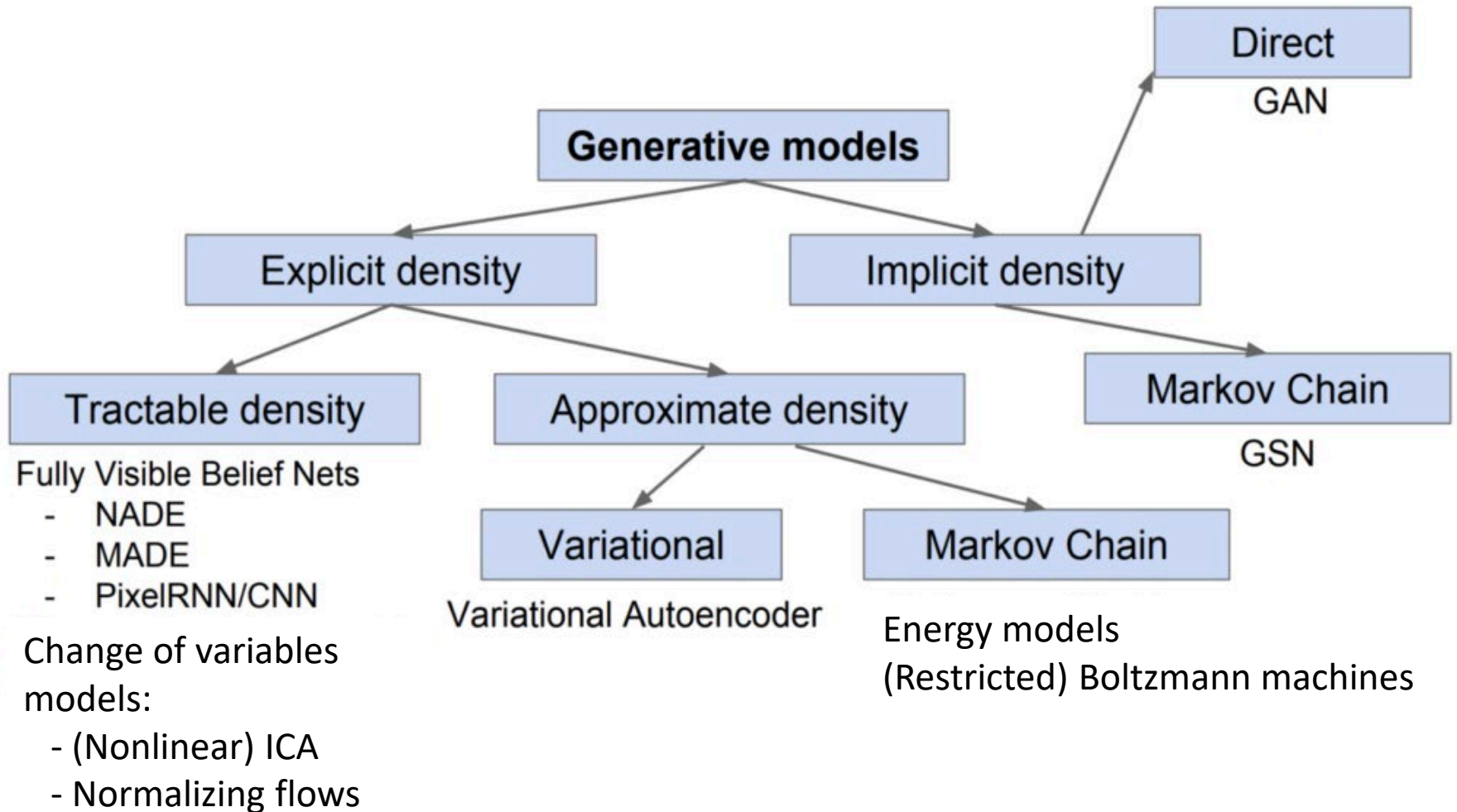


(A): Two natural clusters

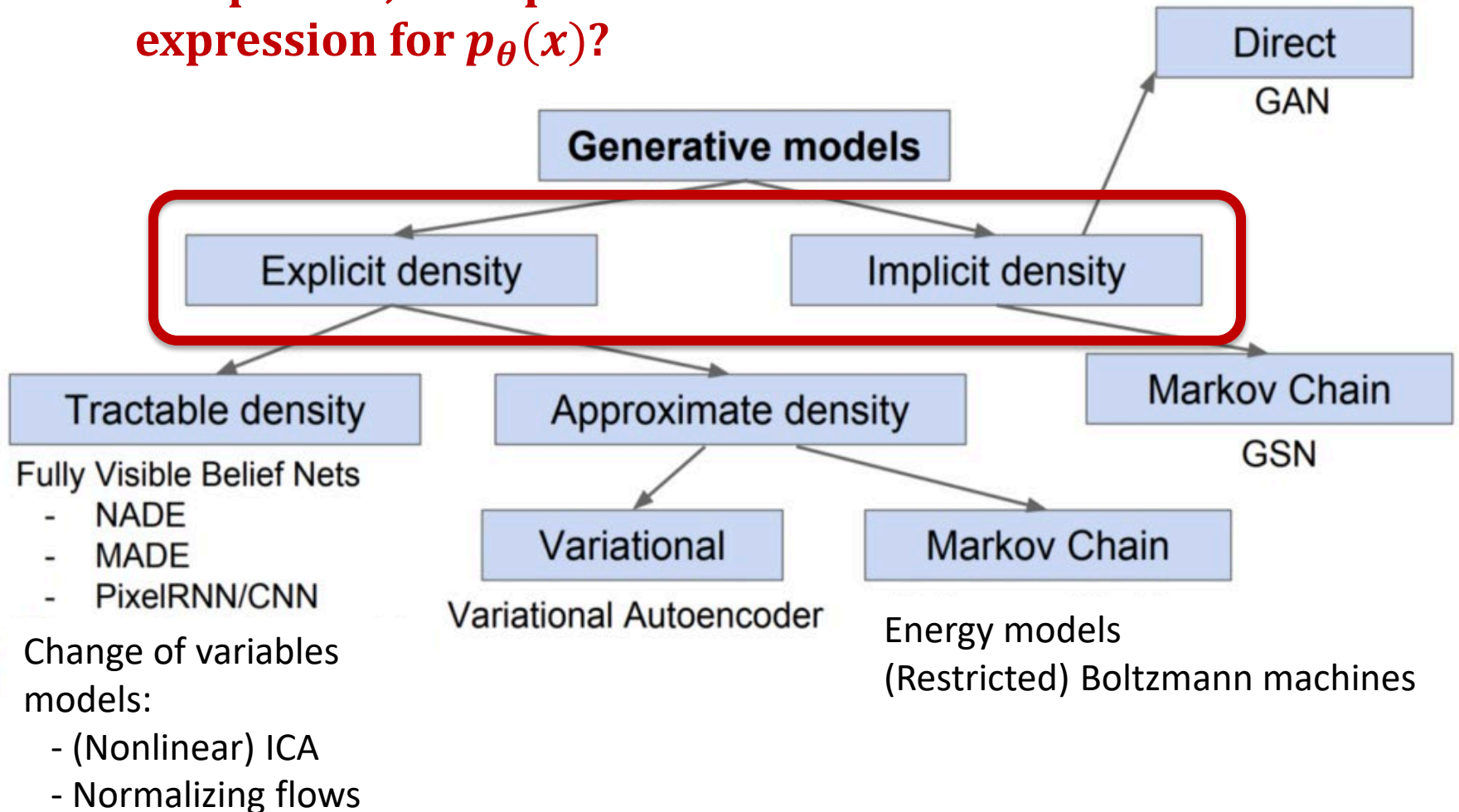


(B): k -means clusters

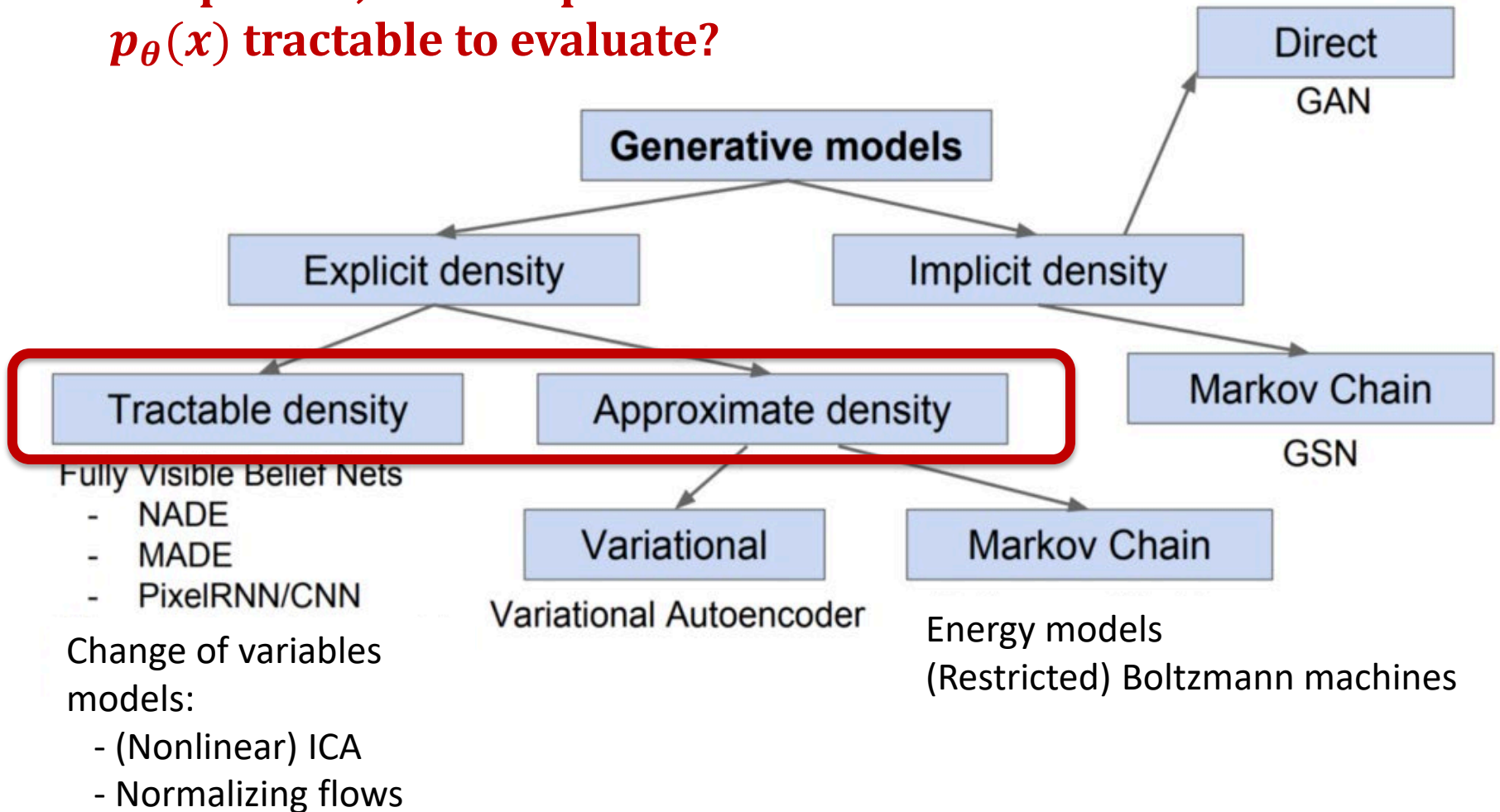
Taxonomy of generative models



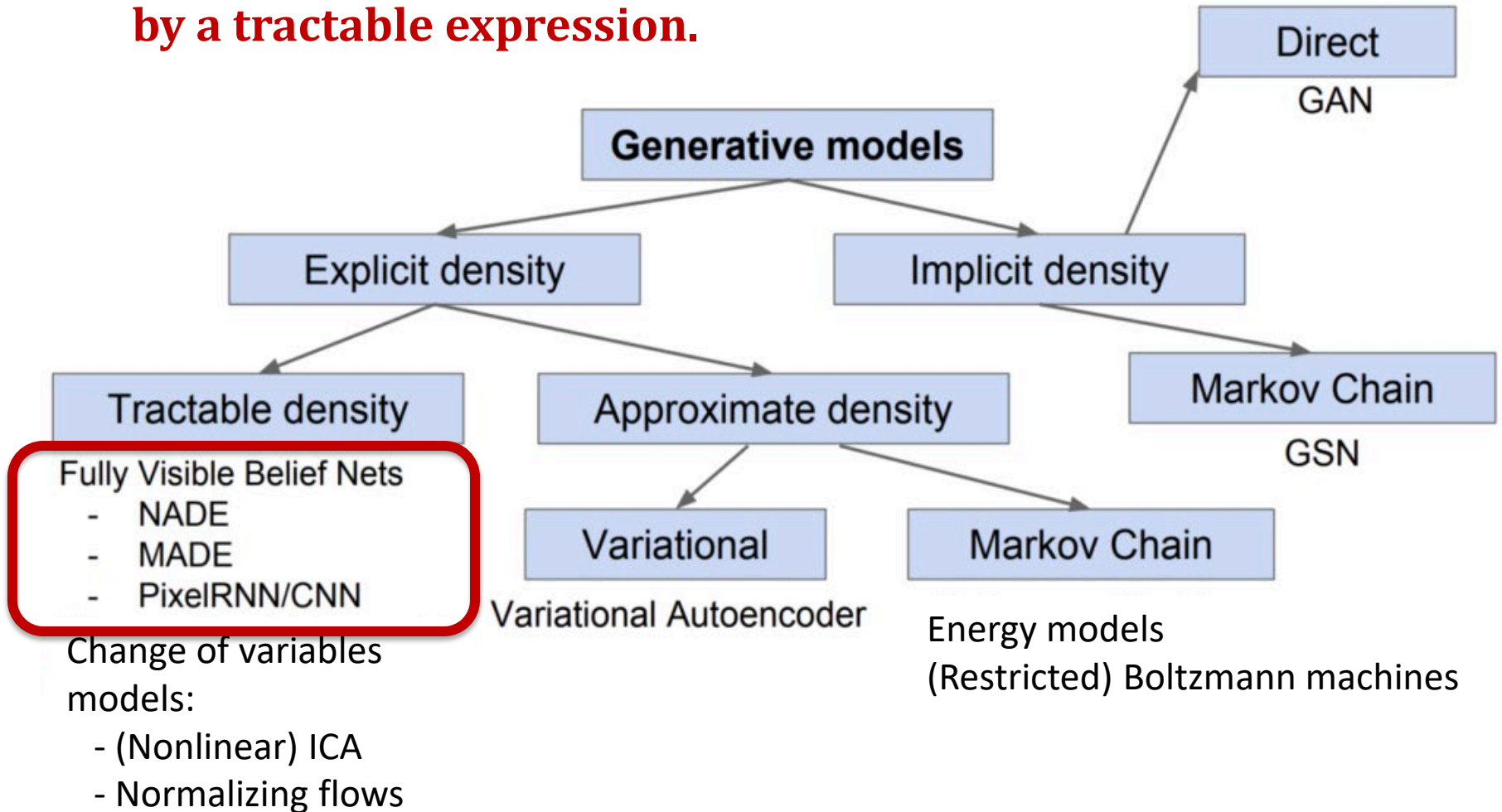
For a point x , an explicit expression for $p_{\theta}(x)$?



For a point x , is the expression $p_{\theta}(x)$ tractable to evaluate?

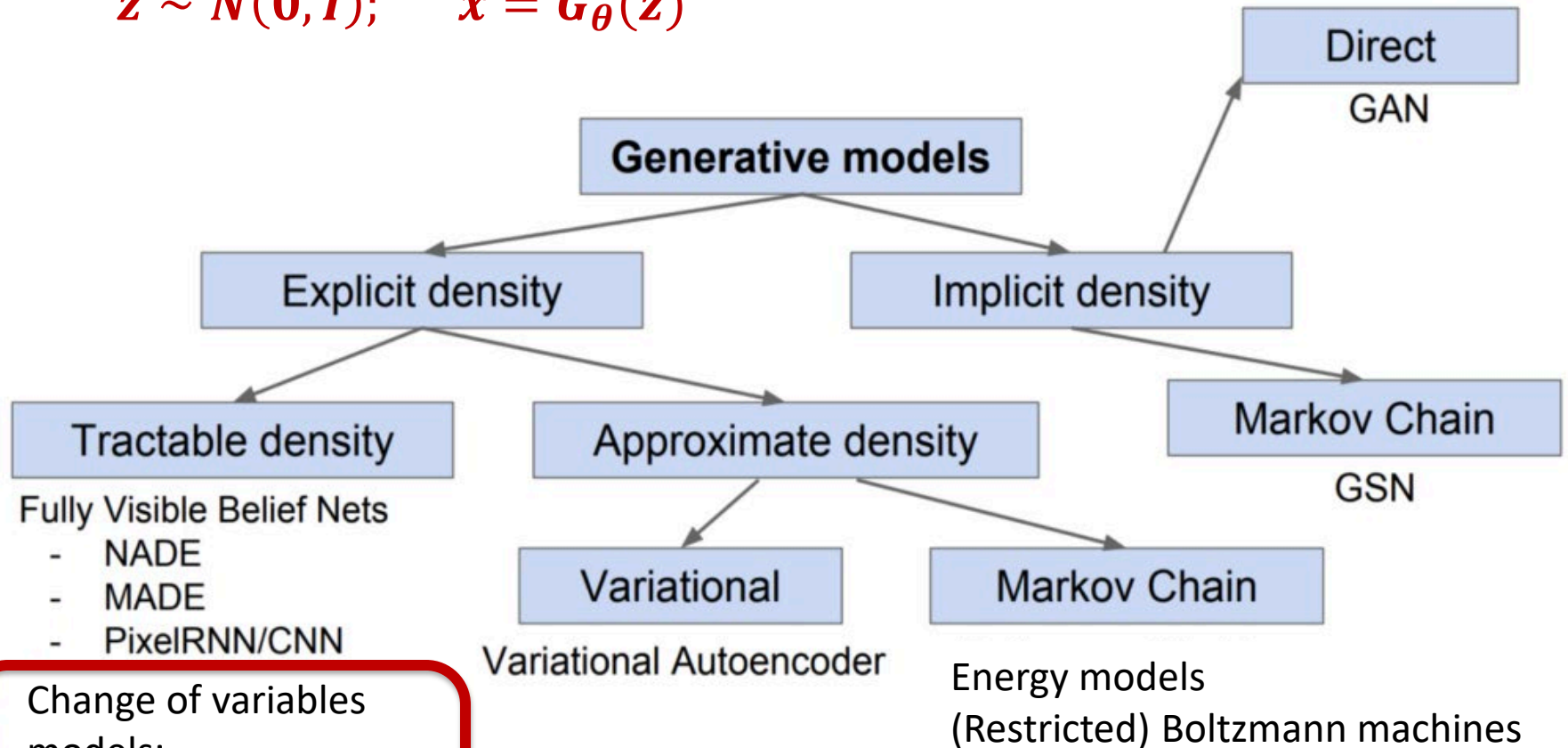


Autoregressive models, they model the distribution $p_{\theta}(x_t|x_{<t})$ by a tractable expression.



They model the distribution for x as an invertible transformation of an (easy) distribution over z :

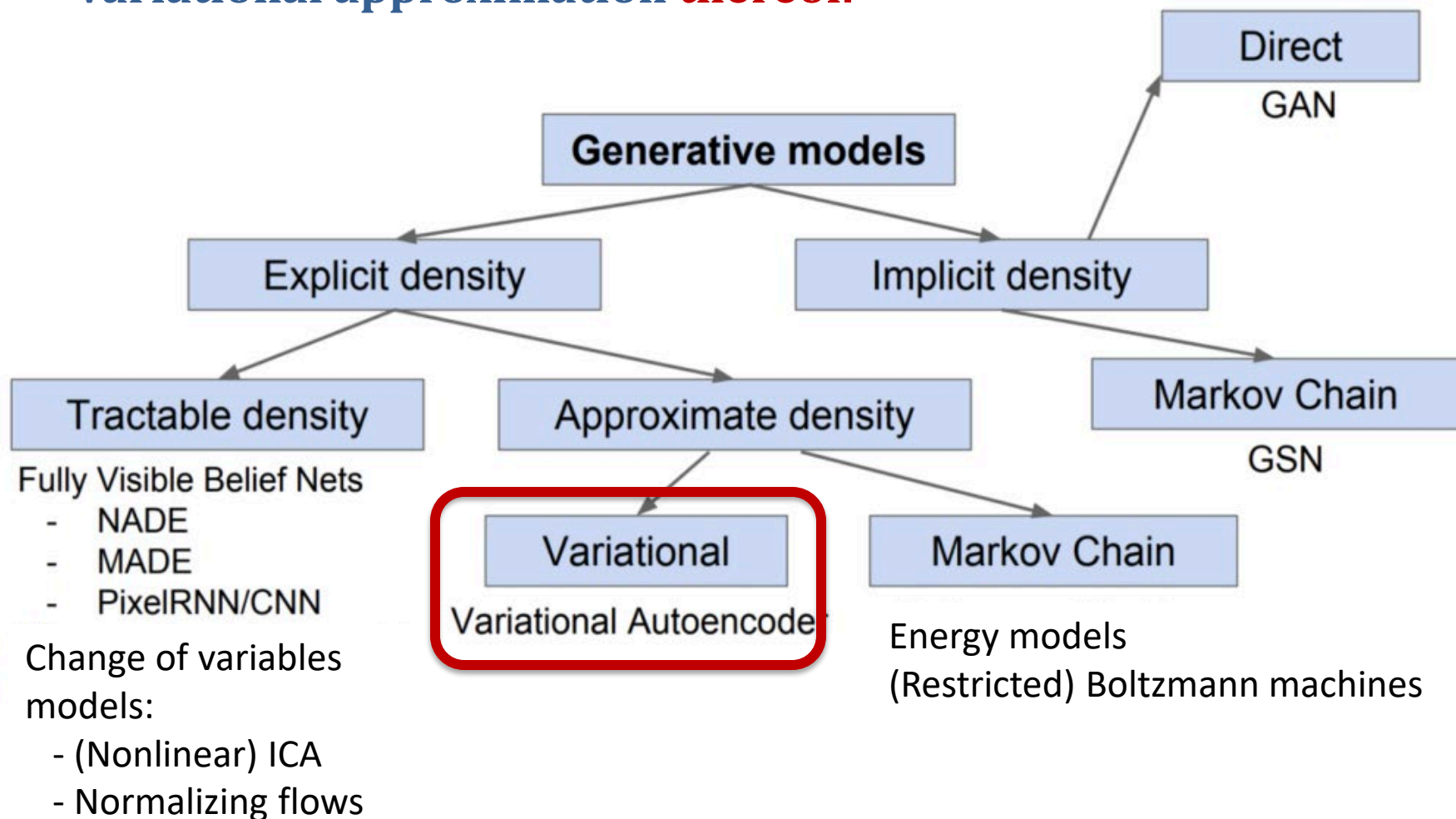
$$z \sim N(0, I); \quad x = G_{\theta}(z)$$



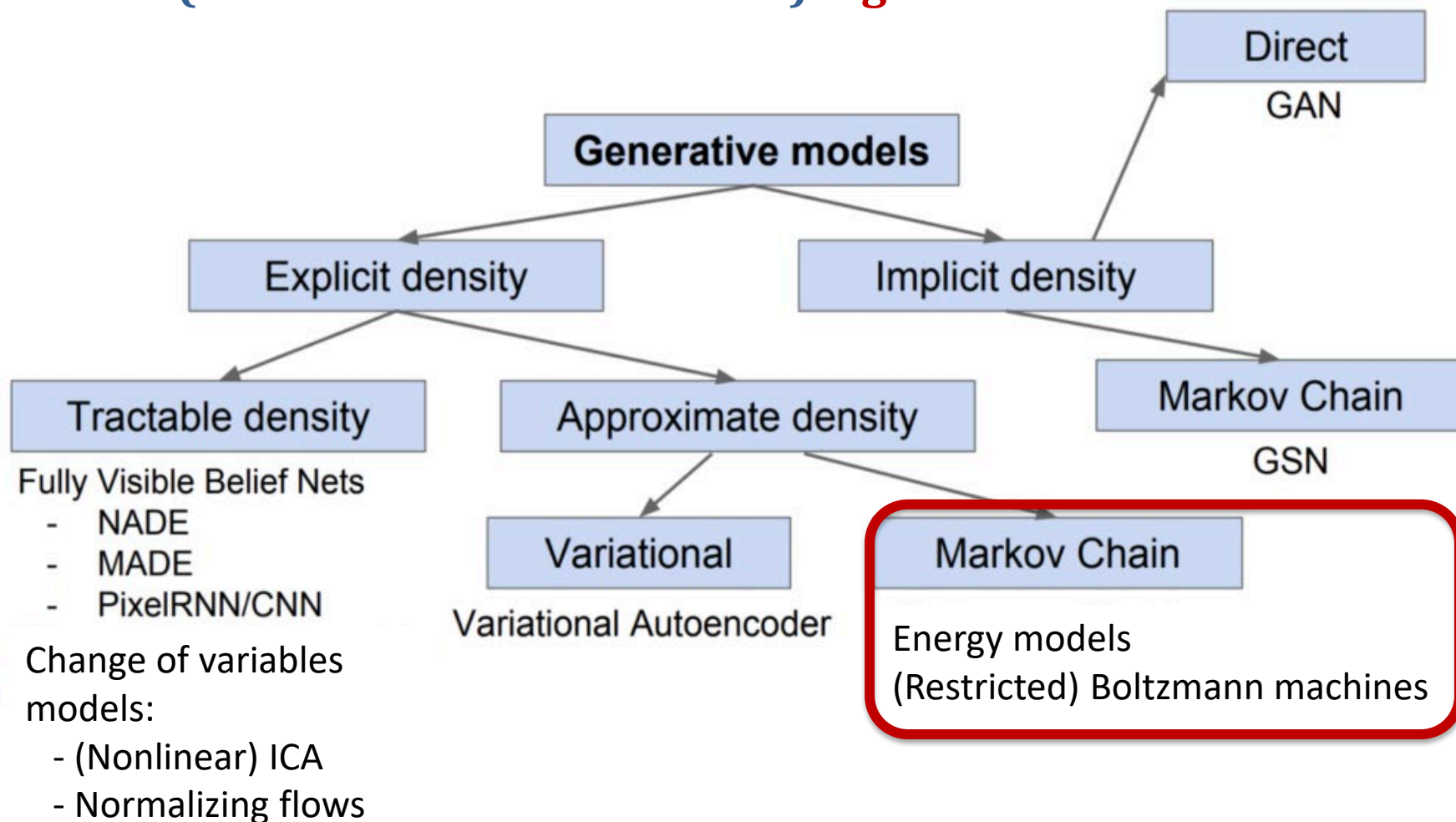
Change of variables models:

- (Nonlinear) ICA
- Normalizing flows

The distribution $p_{\theta}(x)$ does not have a tractable form, but we can write down a variational approximation thereof.

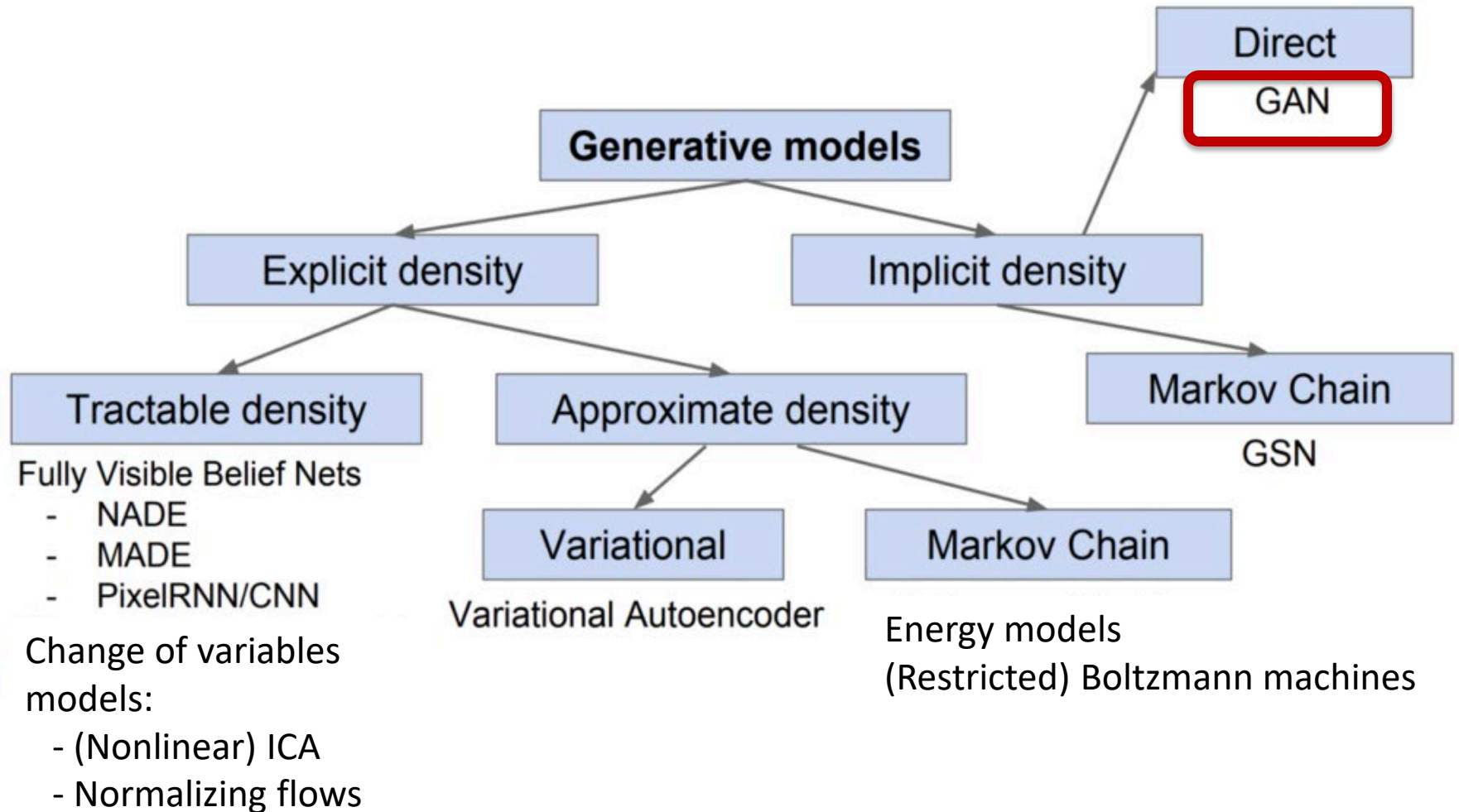


The distribution $p_{\theta}(x)$ does not have a tractable form, but we can approximate it by running a MCMC (Markov Chain Monte Carlo) algorithm.



The distribution $p_{\theta}(x)$ does not have an explicit form, but we can draw samples from it. e.g.

$$z \sim N(0, I); \quad x = G_{\theta}(z)$$



Training explicit density models

Likelihood-based: maximize the likelihood of the data under the model (possibly with variational or MCMC approximations)

$$\max_{\theta} \sum_{\text{samples } x_i} \log p_{\theta}(x_i)$$

In the limit of infinite number of samples:

$$\begin{aligned} \max_{\theta} \mathbb{E}_{x \sim p} \log p_{\theta}(x) &= -(\mathbb{E}_{x \sim p} \log \frac{1}{p_{\theta}(x)} + \mathbb{E}_{x \sim p} \log p(x) - \mathbb{E}_{x \sim p} \log p(x)) \\ &= -(\quad \quad \quad KL(p||p_{\theta}) \quad \quad \quad + \quad H(p)) \end{aligned}$$

Hence, we are minimizing KL divergence ($H(p)$ is a constant).

Training explicit density models

Likelihood-based: maximize the likelihood of the data under the model (possibly with variational or MCMC approximations)

Pros

Easy training: can just maximize via gradient descent.

Evaluation: evaluating the fit of the model can be done by evaluating the likelihood (on test data)

Cons

Larger models needed: likelihood objective is hard, to fit well need very big model

Likelihood encourages averaging: produced samples tend to be blurrier, as likelihood encourages “coverage” of training data.

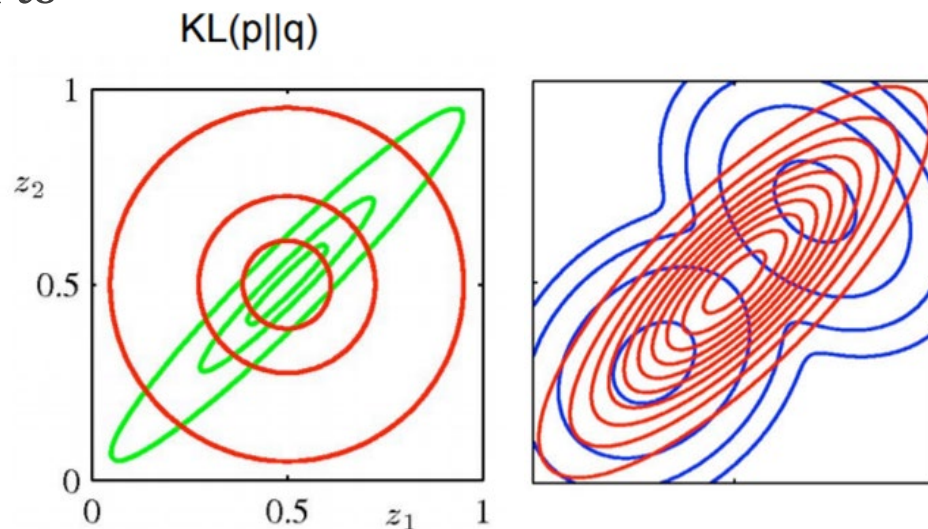
Training explicit density models

$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} d\mathbf{Z}.$$

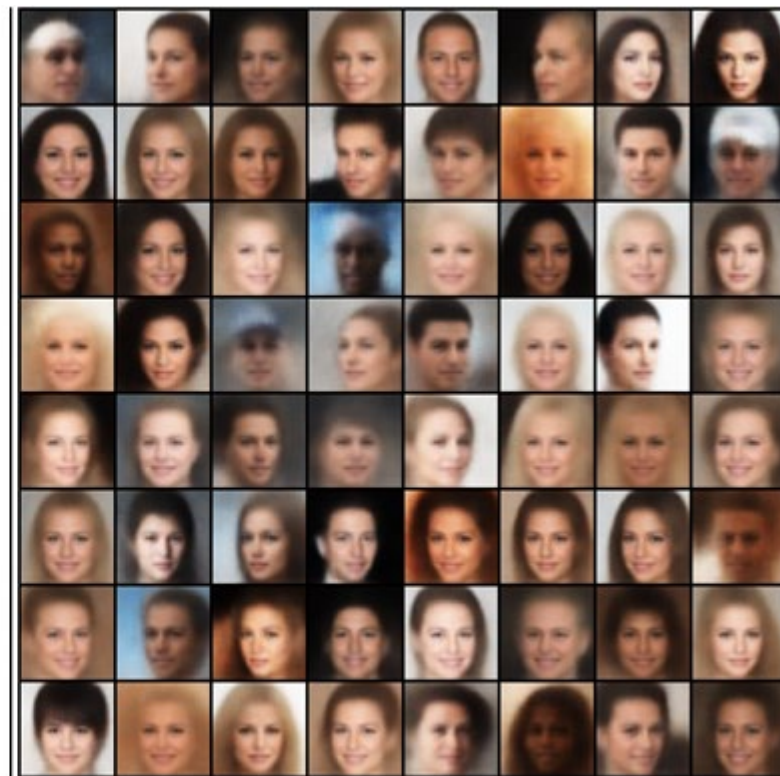
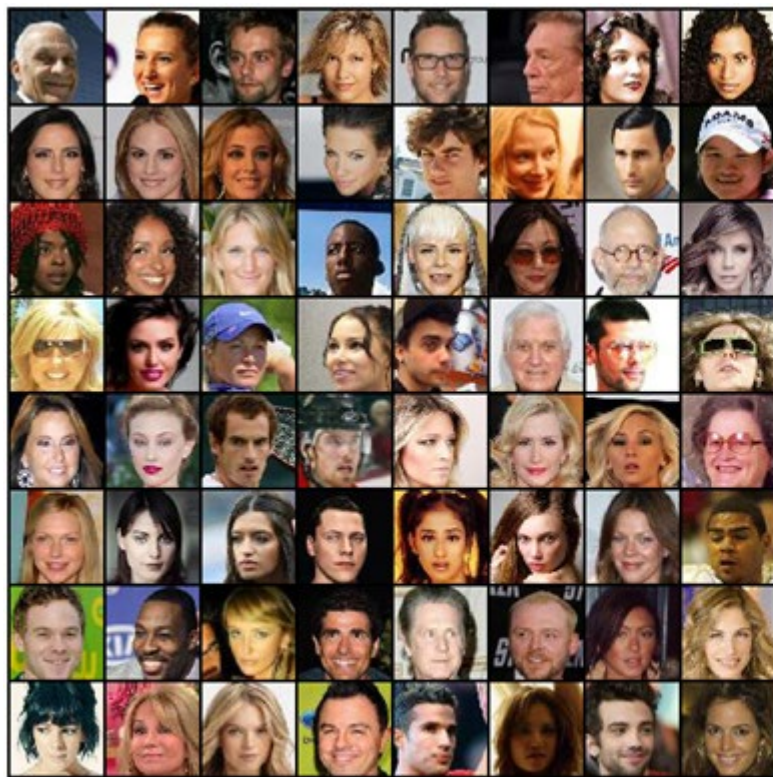
There is a large positive contribution to the KL divergence from regions of \mathbf{Z} space in which:

- $q(\mathbf{Z})$ is near zero,
- unless $p(\mathbf{Z})$ is also close to zero.

Minimizing $\text{KL}(p||q)$ leads to distributions $q(\mathbf{Z})$ that **are nonzero in regions where $p(\mathbf{Z})$ is nonzero.**



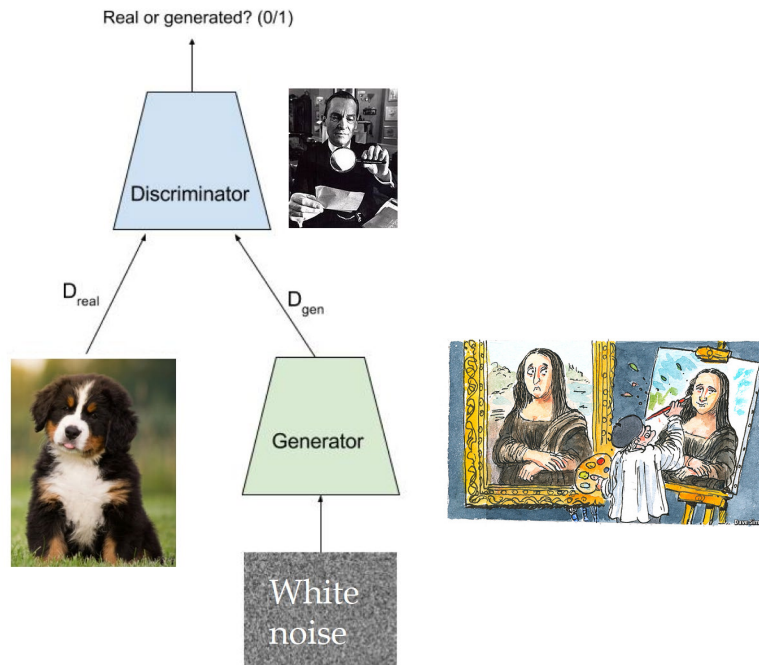
Training explicit density models



Faces generated using a trained VAE

Training implicit density models

Likelihood-free: use a **surrogate loss** – e.g. in GANs, train a discriminator to tell real and generated samples apart;



Training implicit density models

Likelihood-free: use a **surrogate loss** – e.g. in GANs, train a discriminator to tell real and generated samples apart;

Pros

Better objective, smaller models needed: objective itself (i.e. discriminator) is “learned” – can result in visually better images w/ smaller models.

Cons

Unstable training: typically min-max (saddle point) problems.

Evaluation: no way to evaluate likelihood, so no way to evaluate quality of fit.