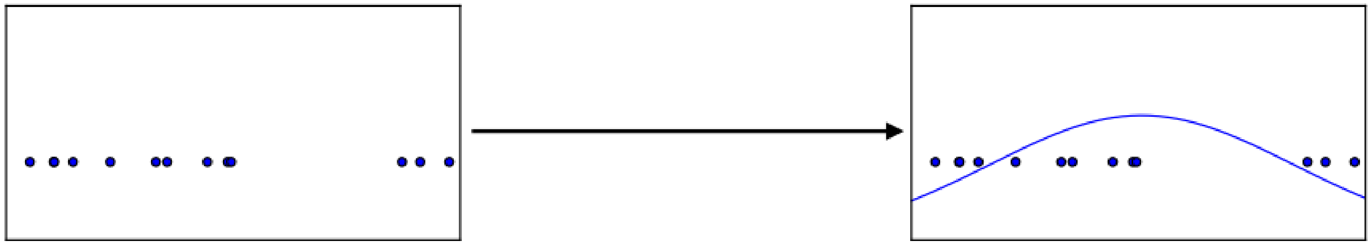
Chapter 20

Deep Generative Models

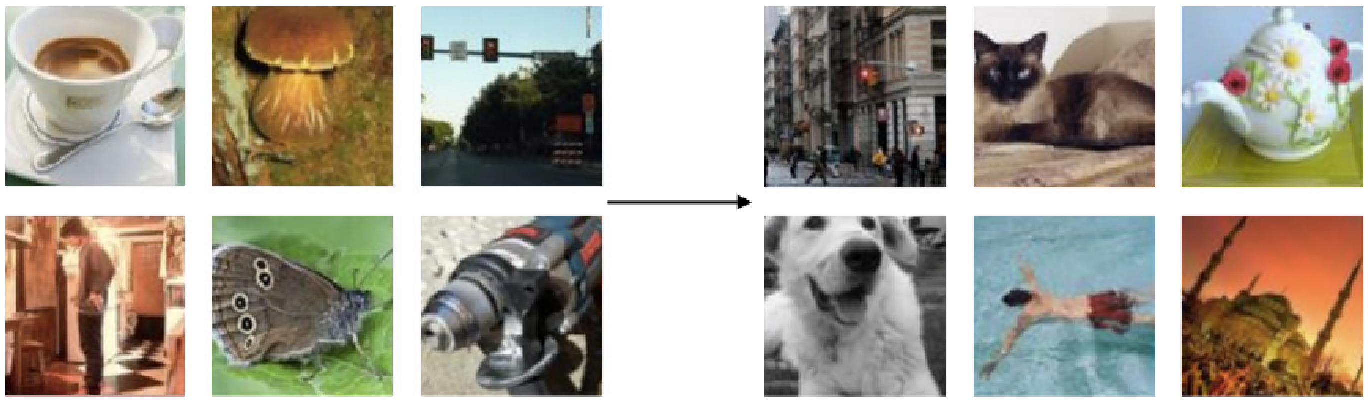
Generative Models

Models that are able to

- Provide an estimate of the probability distribution function, p_{data}, or



- Generate samples from a (likely implicit) distribution

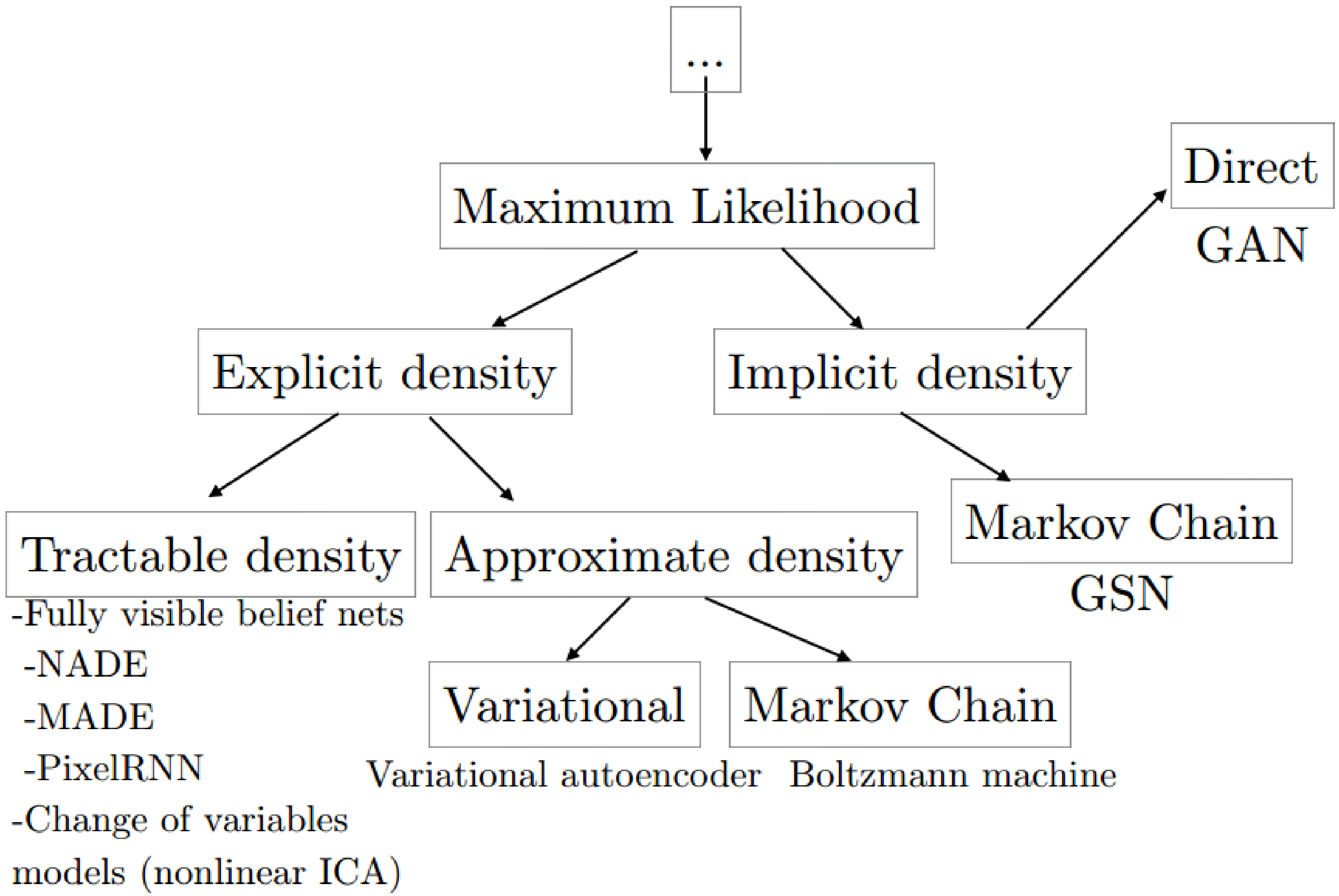


Training examples Model samples

Why Study Generative Models?

- Manipulation of high-dimensional, multi-modal distributions
- Potential uses in reinforcement learning, such as future state prediction
- Training with missing data (e.g. missing labels) and prediction on them
- Generation of realistic samples
- etc.

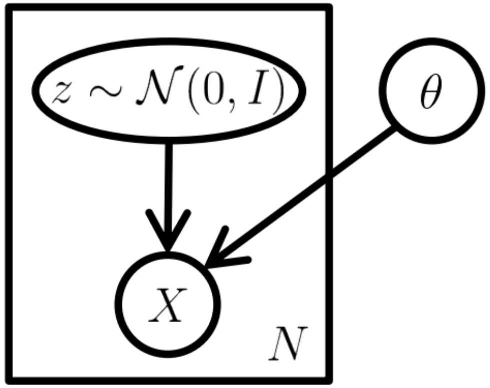
Taxonomy of Generative Models



- Explicit density, $p_{\mathsf{model}}(\boldsymbol{x}; \boldsymbol{\theta})$
  - Tractable (trained with the ordinary ML)
  - Intractable/approximate (trained with approximate inference and/or MCMC approximations)
- Implicit density
  - Single-step sample generation via a network
  - Multi-step sample generation via Markov chains

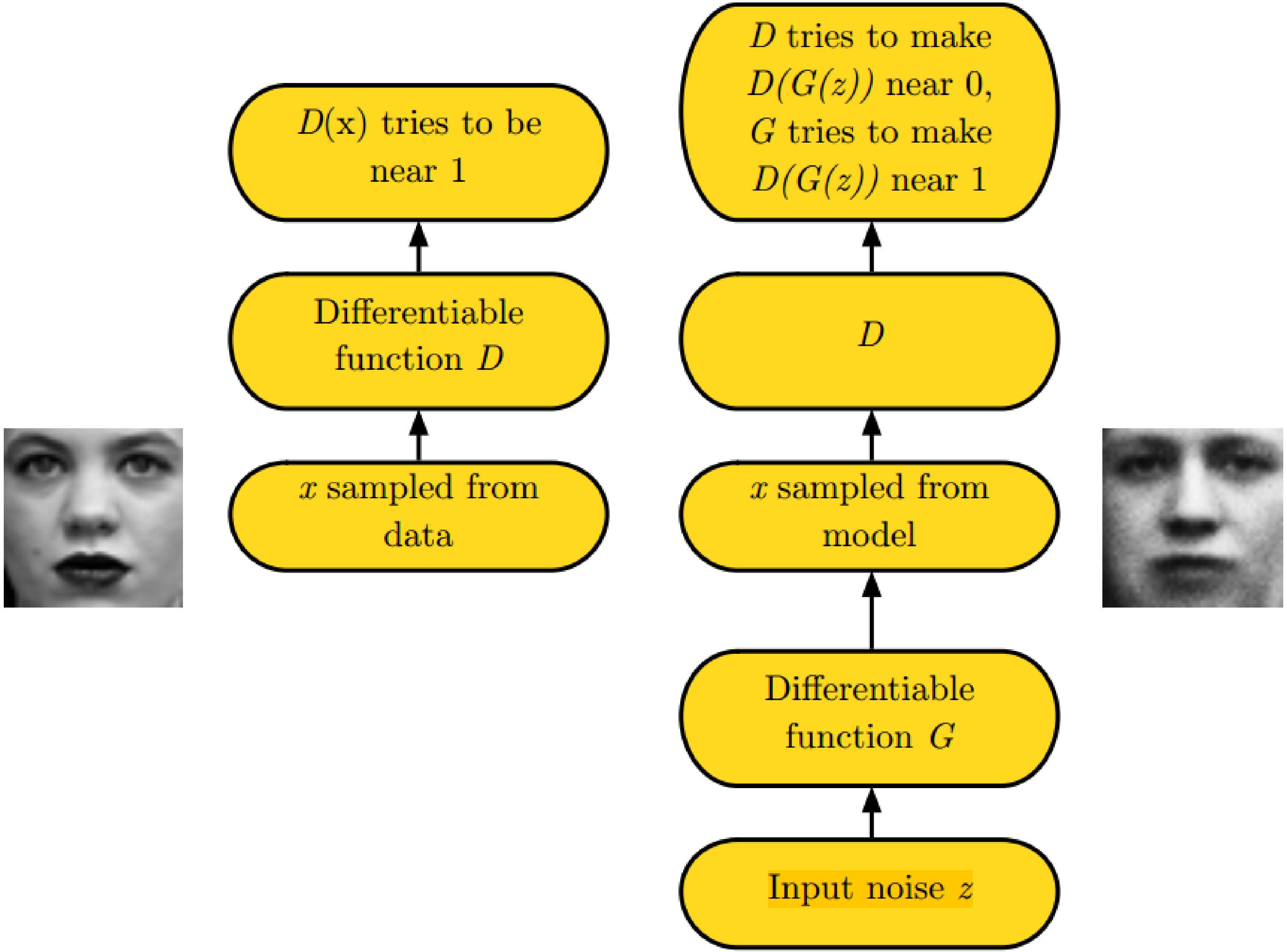
Generative Adversarial Networks (GAN)

- A differentiable generation network G, paired with a discriminator D for training
- Generator G maps latent noises $\boldsymbol{z} \sim p(\boldsymbol{z})$ to visible variables $\boldsymbol{x}$
  - Conceptually, a graphical model with the same structure as VAE
  - $\boldsymbol{x} = G(\boldsymbol{z})$ can be regarded as a sample drawn from some $p_{\mathrm{g}}(\boldsymbol{x})$



- Generator is what we are concerned with

- Discriminator D divides inputs into real and fake classes
  - An ordinary binary classifier trained supervisedly
  - Inputs are training examples (real) and generated samples (fake)


D(x) tries to be near 1
Differentiable function D
x sampled from data
D tries to make $D(G(z))$ near 0, G tries to make $D(G(z))$ near 1
D
x sampled from model
Differentiable function G
Input noise z

Training GANs: Two-Player Minimax Game

- $D(\boldsymbol{x}; \boldsymbol{\theta}^{(D)}), G(\boldsymbol{z}; \boldsymbol{\theta}^{(G)})$ can be implemented with neural networks, and each has their own cost to minimize

  – **Discriminator cost** (cross-entropy cost)

  $$J^{(D)}(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}) = -E_{\boldsymbol{x} \sim p_{\text{data}}} \log D(\boldsymbol{x}) - E_{\boldsymbol{z} \sim p_{\boldsymbol{z}}} \log(1 - D(G(\boldsymbol{z})))$$

  where $D(\boldsymbol{x})$ denotes the probability of $\boldsymbol{x}$ being real

  – **Generator cost**

  $$J^{(G)}(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}) = -J^{(D)}(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)})$$

- Note that the sum of all players' costs is zero (zero-sum game)

- The entire game can be summarized with a value function

$$V(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}) \equiv -J^{(D)}(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)})$$

and the objective is to find a generator

$$\boldsymbol{\theta}^{(G)*} = \arg\min_{\boldsymbol{\theta}^{(G)}} \max_{\boldsymbol{\theta}^{(D)}} V(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)})$$

Optimization vs. Game

- The solution to an optimization problem is generally a local minimum of an objective function in parameter space, e.g.

$$\arg \min_{\boldsymbol{\theta}^{(G)}, \boldsymbol{\theta}^{(D)}} V(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)})$$

where both $\boldsymbol{\theta}^{(G)}, \boldsymbol{\theta}^{(D)}$ are optimized simultaneously

- The solution to a game problem is generally a saddle point of an objective function in parameter space, e.g.

$$\arg \min_{\boldsymbol{\theta}^{(G)}} \max_{\boldsymbol{\theta}^{(D)}} V(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)})$$

where $\boldsymbol{\theta}^{(G)}, \boldsymbol{\theta}^{(D)}$ are optimized in turn by controlling one of them at a time with the other fixed

The Optimal Discriminator

- For a given generator G, the optimal discriminator is seen to be

$$D^*_G(\boldsymbol{x}) = \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_{\text{g}}(\boldsymbol{x})}$$

which can be obtained by having

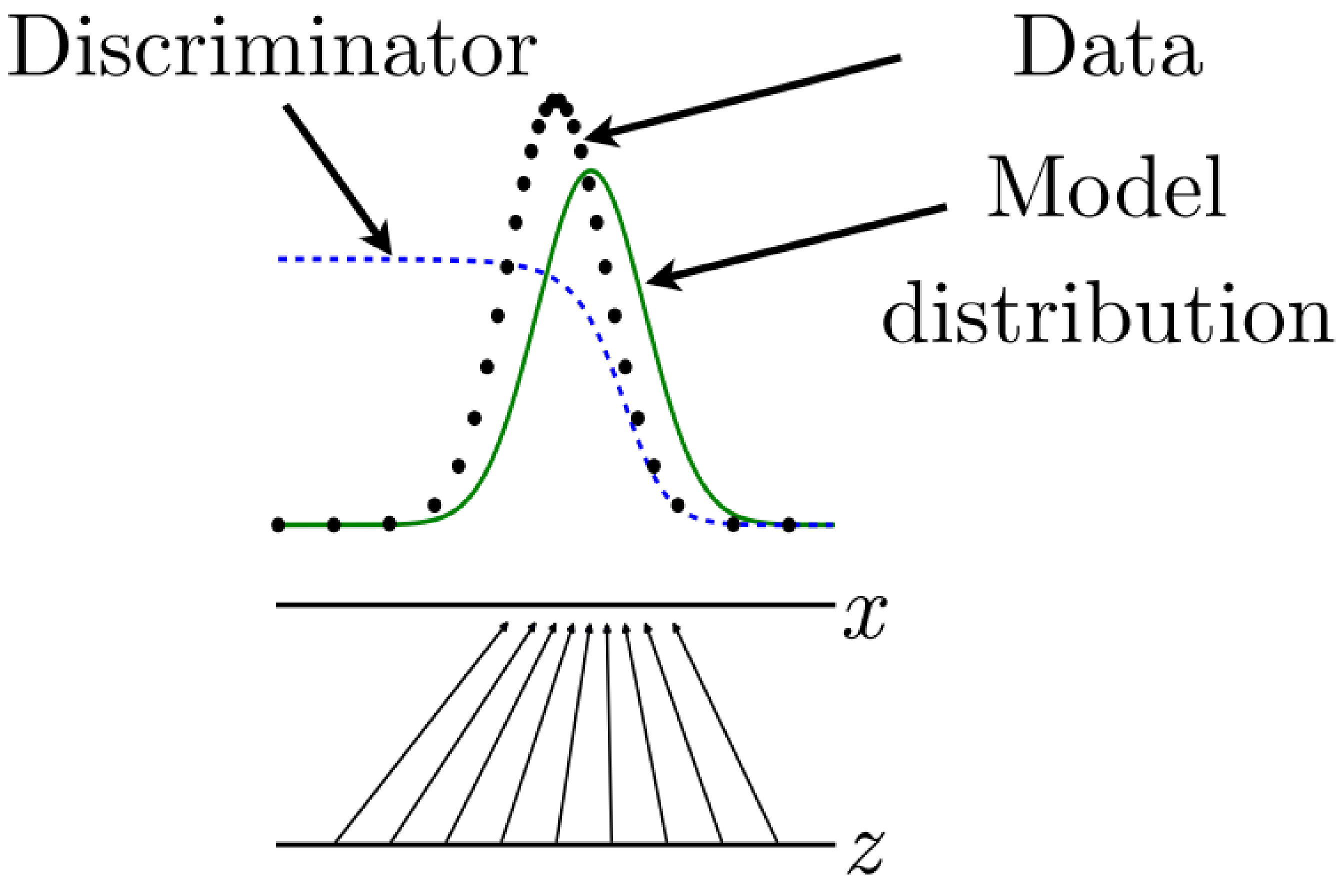
$$\frac{\delta}{\delta D(\boldsymbol{x})} J^{(D)}(\boldsymbol{x}) = 0$$

- When given enough capacity, the discriminator obtains an estimate

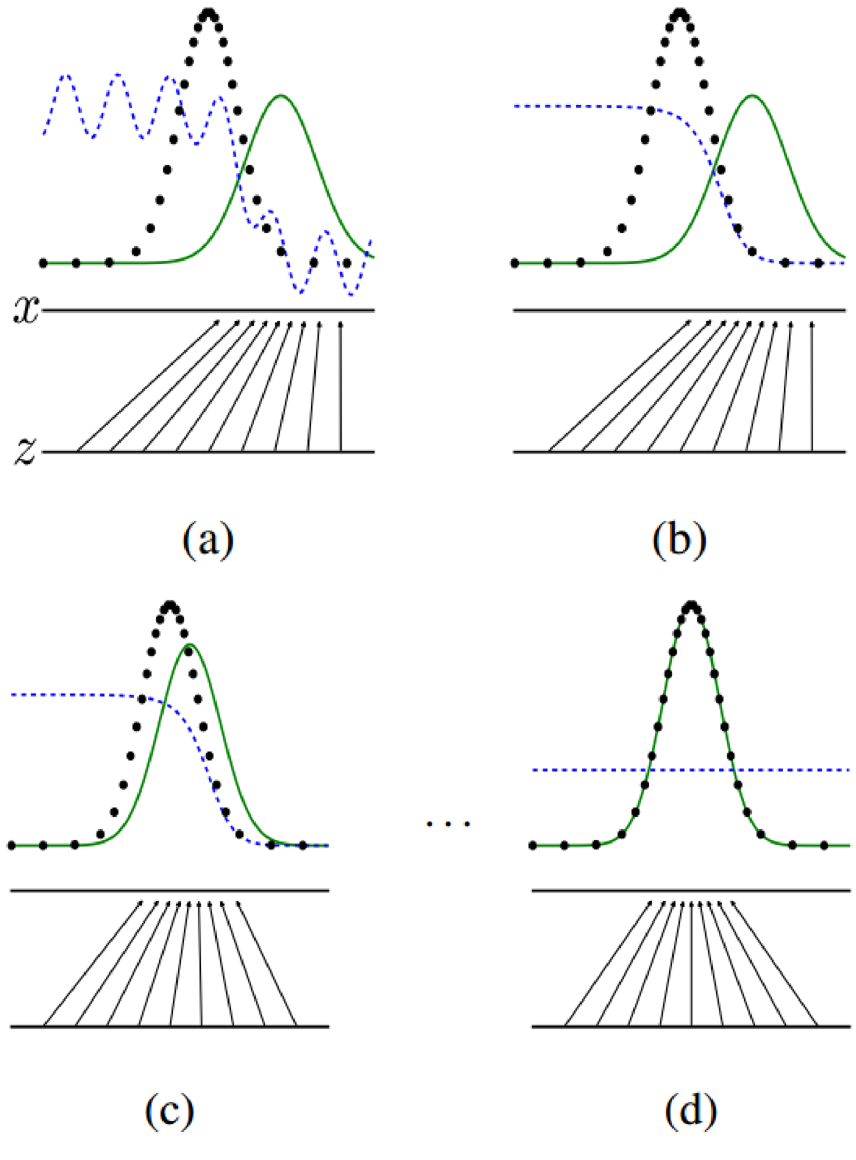
$$\frac{p_{\text{data}(\boldsymbol{x})}}{p_{\text{g}(\boldsymbol{x})}}$$

at every $\boldsymbol{x}$

- This is the key that sets GANs apart from other generative models


Discriminator
Data
Model
distribution
x
z

- The generator is to learn a model by following a discriminator uphill



The Optimal Generator

- Given $D^*_G(\boldsymbol{x})$ and enough capacity, the optimal generator is to minimize the Jensen-Shannon divergence between p_{data} and p_{g}

$$
\begin{aligned}
&\arg\min_{p_{\text{g}}} E_{\boldsymbol{x}\sim p_{\text{data}}} \log D^*_G(\boldsymbol{x}) + E_{\boldsymbol{x}\sim p_{\text{g}}} \log(1 - D^*_G(\boldsymbol{x})) \\
&= \arg\min_{p_{\text{g}}} E_{\boldsymbol{x}\sim p_{\text{data}}} \log \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_{\text{g}}(\boldsymbol{x})} + E_{\boldsymbol{x}\sim p_{\text{g}}} \log \frac{p_{\text{g}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_{\text{g}}(\boldsymbol{x})} \\
&= \arg\min_{p_{\text{g}}} -\log(4) + \text{KL}\left(p_{\text{data}} \parallel \frac{p_{\text{data}} + p_{\text{g}}}{2}\right) + \text{KL}\left(p_{\text{g}} \parallel \frac{p_{\text{data}} + p_{\text{g}}}{2}\right) \\
&= \arg\min_{p_{\text{g}}} -\log(4) + 2 \times \text{JSD}(p_{\text{data}} \parallel p_{\text{g}})
\end{aligned}
$$

- The minimum is achieved when $p_{\text{g}} = p_{\text{data}}$, i.e. $\text{JSD}(p_{\text{data}} \parallel p_{\text{g}}) = 0$

- Remarks
  - The optimization is done w.r.t. p_{g} directly
  - The analysis for the discriminator is done w.r.t. $D(\boldsymbol{x})$
  - Enough capacity in both contexts means that $D_G^*(\boldsymbol{x})$ and $p_{\mathrm{g}}^*(\boldsymbol{x})$ can be implemented by $D(\boldsymbol{x};\boldsymbol{\theta}^{(D)*})$ and $G(\boldsymbol{z};\boldsymbol{\theta}^{(G)*})$, respectively

Implementation

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**
  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
  • 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.

- (Convergence) If G and D have enough capacity, and at each step of Algorithm I, the discriminator is allowed to reach its optimum $D_G^*(\boldsymbol{x})$ given G, and p_{g} is updated to improve the criterion (reduce the cost)

$$E_{\boldsymbol{x}\sim p_{\mathsf{data}}} \log D_G^*(\boldsymbol{x}) + E_{\boldsymbol{x}\sim p_{\mathsf{g}}} \log(1 - D_G^*(\boldsymbol{x}))$$

  then p_{g} converges to p_{data}

- Nothing is said about the convergence when optimization is done based on simultaneous stochastic gradient descent in parameter space

Non-Convergence of Gradient Descent

- Toy problem

$$\min_x \max_y V(x,y) = xy$$

- x, y are optimized based on gradient descent with a tiny learning rate

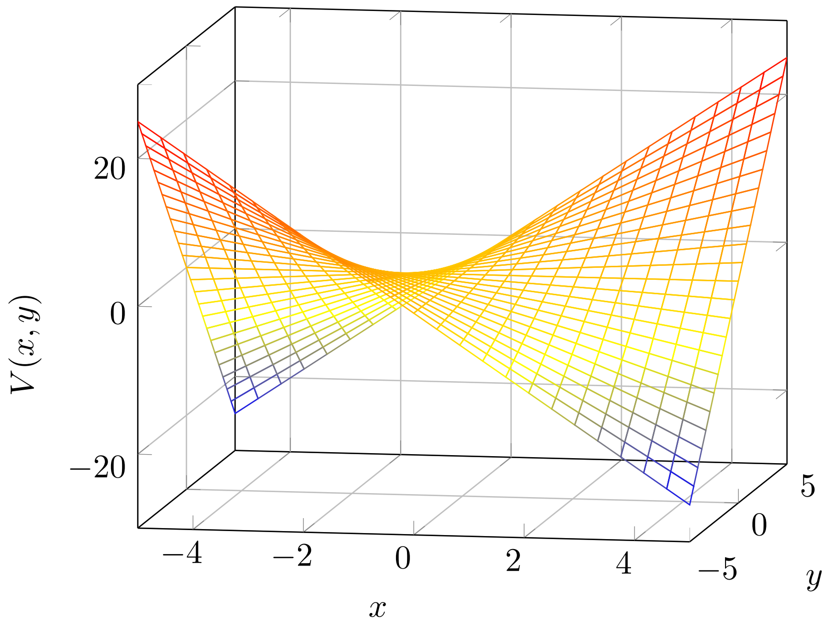
$$x(t+\Delta t) = x(t) - \Delta t \frac{\partial}{\partial x(t)} V(x(t), y(t))$$
$$y(t+\Delta t) = y(t) + \Delta t \frac{\partial}{\partial y(t)} V(x(t), y(t))$$

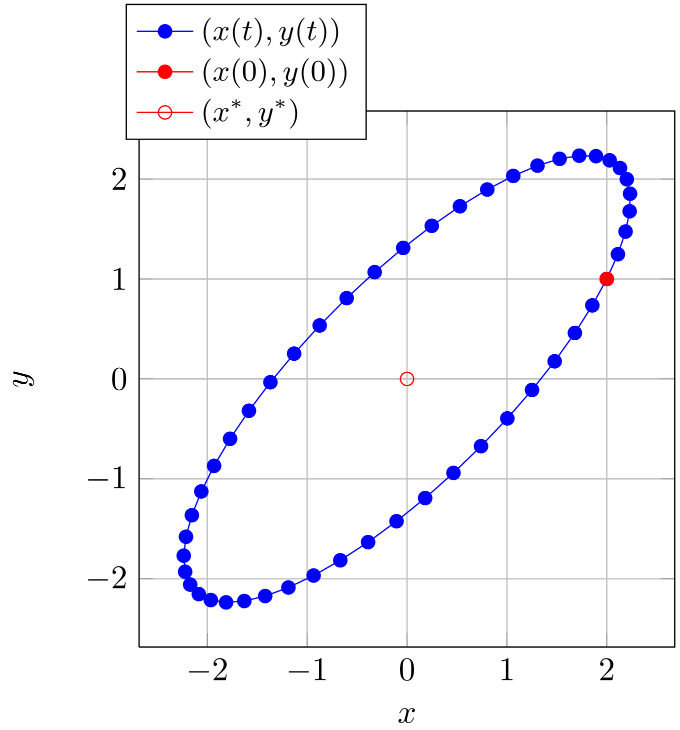
- This amounts to solving

$$\begin{cases} x'(t) = -y(t) \\ y'(t) = x(t) \end{cases} \rightarrow x''(t) = -x(t)$$

which has a solution of the form

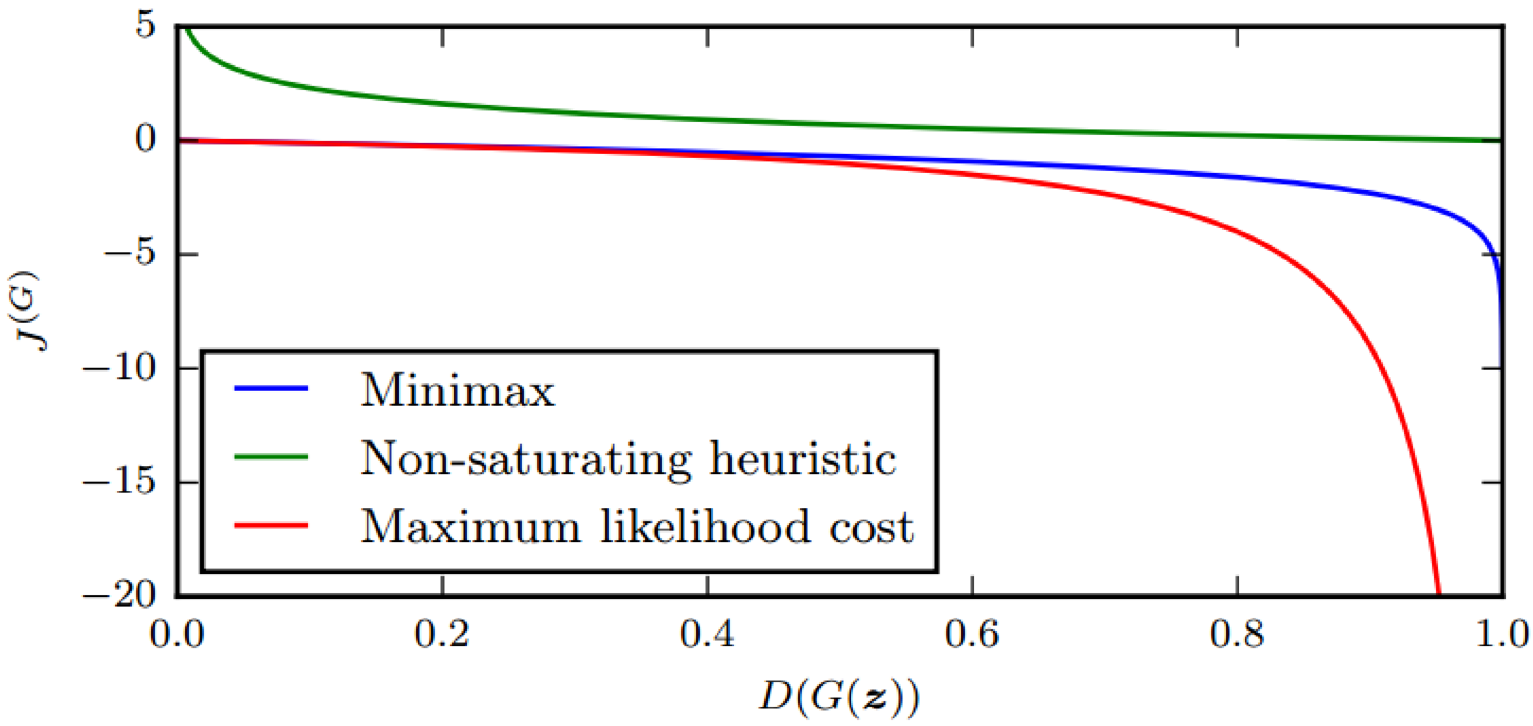
$$x(t) = x(0)\cos(t) + y(0)\sin(t)$$
$$y(t) = x(0)\sin(t) + y(0)\cos(t)$$





Other Games

- Zero-sum game does not perform well in learning generator: gradients of $J^{(G)}$ w.r.t $D(G(\boldsymbol{z}))$ vanish when the discriminator performs well



- Heuristic, non-saturating game (to ensure non-zero gradients)

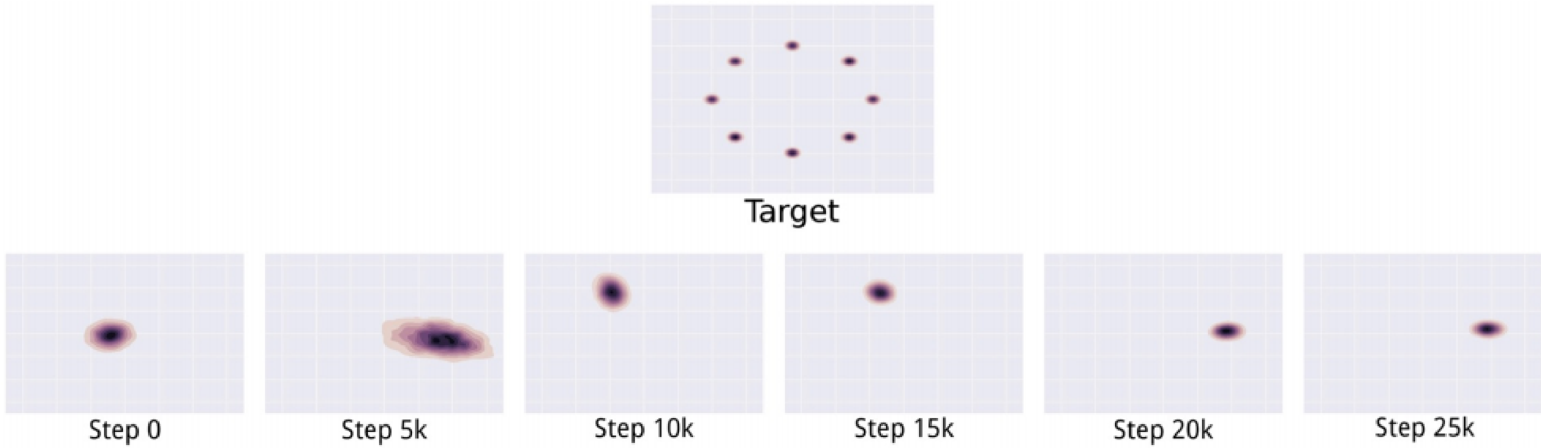
$$J^{(G)} = -E_z \log D(G(z))$$

- Maximum likelihood game (to minimize KL divergence)

$$J^{(G)} = -E_z \exp(\sigma^{-1}(D(G(z)))$$

Mode Collapse Problem

- The generator learns to map different $\boldsymbol{z}$ to the same $\boldsymbol{x}$



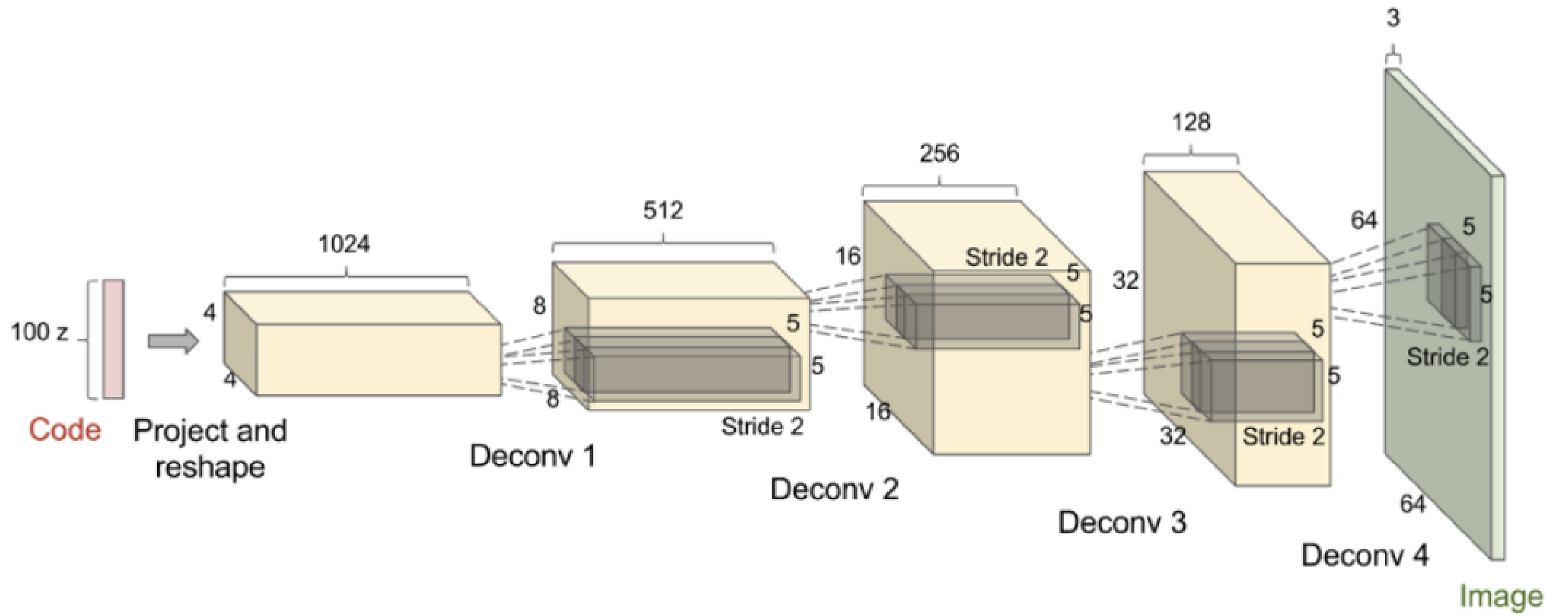
Top: Data distribution (Mixture Gaussian)

Bottom: Learned generator distribution over time

- The generator distribution produces only a single mode at a time and does not converge in this example
- This is acceptable in some applications but not all

DCGAN

- There are many different implementations for generators, such as DCGAN, LPGAN, and more (study by yourself)



Wasserstein GAN (WGAN)

- **Idea:** To adopt the Earth Mover distance (Wassertein distance) as the convergence criterion
- We have seen previously that training GAN is to learn a model distribution P_θ that should ideally converge to the data distribution P_r
- The convergence calls for a distance measure $\rho(P_r, P_\theta)$ to indicate how close these two distributions are
- To optimize the parameter θ, it is desirable that $\rho(P_r, P_\theta)$ is a continuous function in θ, or equivalently, the mapping $\theta \mapsto P_\theta$ is continuous (i.e., when $\theta_t \rightarrow \theta$, $P_{\theta_t} \rightarrow P_\theta$)
- The continuity depends on the distance measure

Elementary Distances

- The Kullback-Leibler (KL) divergence

$$KL(P_r||P_\theta) = \int P_r(x) \log \frac{P_r(x)}{P_\theta(x)} P_r(x) dx$$

(undefined when there are x's where $P_r(x) \neq 0$ and $P_\theta(x) = 0$)

- The Jensen-Shannon (JS) divergence

$$JS(P_r||P_\theta) = KL(P_r||P_m) + KL(P_\theta||P_m)$$

where

$$P_m = (P_r + P_\theta)/2$$

- The Earth Mover distance

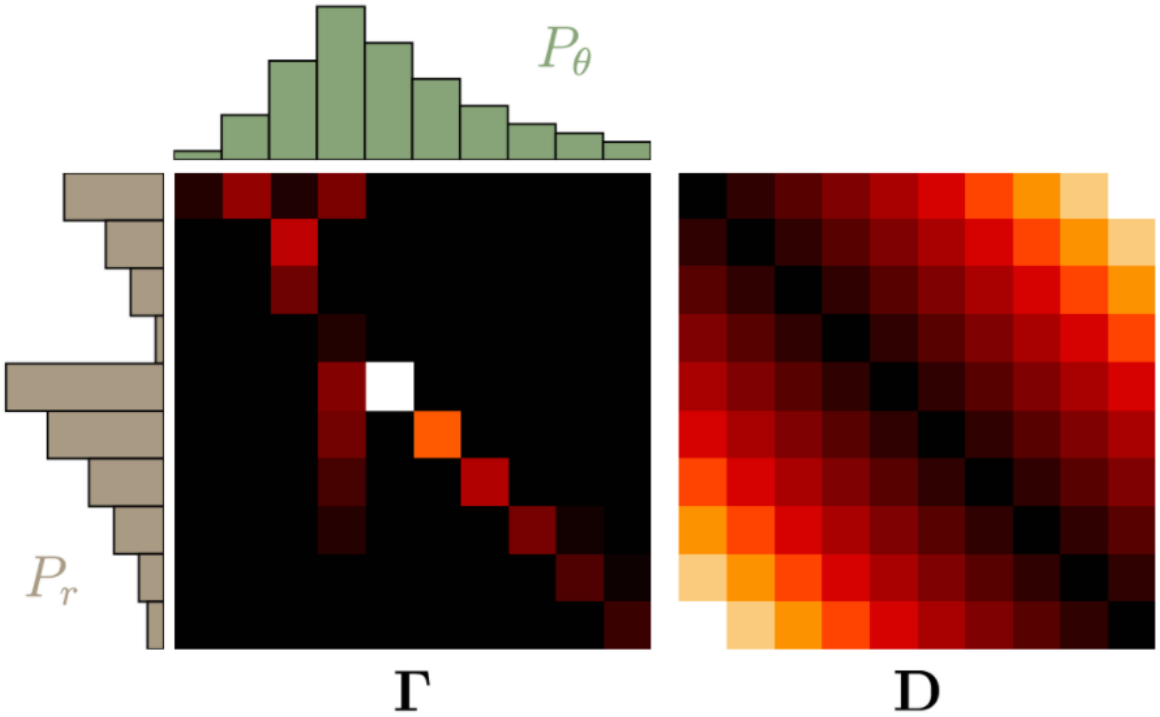
$$W(P_r, P_\theta) = \inf_{\gamma \in \Pi(P_r, P_\theta)} E_{(x,y)\sim\gamma}[\|x-y\|]$$
$$= \inf_{\gamma \in \Pi(P_r, P_\theta)} \sum_{x,y} \gamma(x,y)\|x-y\|$$

where $\Pi(P_r, P_\theta)$ is the set of all joint distributions $\gamma(x,y)$ whose marginals are P_r and P_θ, respectively; that is,

$$P_r(x) = \sum_y \gamma(x,y)$$
$$P_\theta(y) = \sum_x \gamma(x,y)$$

- Intuitively, $\gamma(x,y)$ indicates how much mass must be transported from y to x in order to transform the distribution P_θ into P_r
- The EM distance is the cost of the optimal transport plan

The Earth Mover (EM) Distance



$$\mathbf{\Gamma} = \gamma(\mathbf{x}, \mathbf{y}), \;\; \mathbf{D} = \|\mathbf{x} - \mathbf{y}\|$$

$$W(P_r, P_\theta) = \inf_{\gamma \in \Pi(P_r, P_\theta)} \langle \mathbf{\Gamma}, \mathbf{D} \rangle_F$$

Source: https://vincentherrmann.github.io/blog/wasserstein/

Comparison of Elementary Distances

- The EM distance is continuous and differentiable almost everywhere, whereas the JS divergence is not
- As such, the EM distance allows the model to learn a probability distribution over low dimensional manifolds by using gradient descent

Example 1 (Learning parallel lines)**.** Let $Z \sim U[0,1]$ the uniform distribution on the unit interval. Let $\mathbb{P}_0$ be the distribution of $(0, Z) \in \mathbb{R}^2$ (a 0 on the x-axis and the random variable Z on the y-axis), uniform on a straight vertical line passing through the origin. Now let $g_\theta(z) = (\theta, z)$ with θ a single real parameter. It is easy to see that in this case,

- $W(\mathbb{P}_0, \mathbb{P}_\theta) = |\theta|$,
- $JS(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} \log 2 & \text{if } \theta \neq 0 \ , \\ 0 & \text{if } \theta = 0 \ , \end{cases}$
- $KL(\mathbb{P}_\theta \| \mathbb{P}_0) = KL(\mathbb{P}_0 \| \mathbb{P}_\theta) = \begin{cases} +\infty & \text{if } \theta \neq 0 \ , \\ 0 & \text{if } \theta = 0 \ , \end{cases}$

Linear Programming

- The EM distance between two distributions can be solved by linear programming/optimization

$$\min_{\boldsymbol{x}} z = \boldsymbol{c}^T \boldsymbol{x} \ \ \text{s.t.} \ \begin{cases} \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \\ \boldsymbol{x} \geq \boldsymbol{0} \end{cases}$$

- The dual problem (https://vincentherrmann.github.io/blog/wasserstein/)

$$\max_{\boldsymbol{y}} \ \tilde{z} = \boldsymbol{b}^T \boldsymbol{y} \ \ \text{s.t.} \ \boldsymbol{A}^T \boldsymbol{y} \leq \boldsymbol{c}$$

- (Weak Duality Theorem) $\tilde{z}$ is a lower bound of z

$$z = \boldsymbol{c}^T \boldsymbol{x} \geq \boldsymbol{y}^T \boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}^T \boldsymbol{b} = \tilde{z}$$

- (Strong Duality Theorem) When we find an optimal solution to the dual problem, $\tilde{z} = \boldsymbol{z}$ (the EM distance)

- The term $\boldsymbol{Ax} = \boldsymbol{b}$

$$
\left[\begin{array}{cccc|cccc|c|cccc}
1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 1 \\
\hline
1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots & 1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c}
\gamma(x_1, y_1) \\
\gamma(x_1, y_2) \\
\vdots \\
\hline
\gamma(x_2, y_1) \\
\gamma(x_2, y_2) \\
\vdots \\
\hline
\vdots \\
\hline
\gamma(x_n, y_1) \\
\gamma(x_n, y_2) \\
\vdots
\end{array}\right]
=
\left[\begin{array}{c}
P_r(x_1) \\
P_r(x_2) \\
\vdots \\
P_r(x_n) \\
\hline
P_\theta(y_1) \\
P_\theta(y_2) \\
\vdots \\
P_\theta(y_n)
\end{array}\right]
$$

- The vector $\boldsymbol{c}$

$$\boldsymbol{c} = \begin{bmatrix} \|x_1 - y_1\| \\ \|x_1 - y_2\| \\ \vdots \\ \hdashline \|x_2 - y_1\| \\ \|x_2 - y_2\| \\ \vdots \\ \hdashline \vdots \\ \hdashline \|x_n - y_1\| \\ \|x_n - y_2\| \\ \vdots \end{bmatrix}$$

- Now we can compute the EM distance using the dual form

$$\max_{\boldsymbol{y}} \ \tilde{z} = \boldsymbol{b}^T \boldsymbol{y} \ \text{ s.t. } \boldsymbol{A}^T \boldsymbol{y} \leq \boldsymbol{c}$$

- The objective is to find $\boldsymbol{y}$ such that $\boldsymbol{b}^T \boldsymbol{y}$ is maximized

$$\boldsymbol{b}^T \boldsymbol{y} = \left[\begin{array}{ccc|ccc} p_r(x_1) & \cdots & p_r(x_n) & p_\theta(y_1) & \cdots & p_\theta(y_n) \end{array} \right] \left[\begin{array}{c} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \\ \hline g(x_1) \\ g(x_2) \\ \vdots \\ g(x_n) \end{array} \right]$$

where the components of $\boldsymbol{y}$ have been made functions of x_i

- The constraint $\boldsymbol{A}^T \boldsymbol{y} \le \boldsymbol{c}$ is given by

$$
\left[\begin{array}{cccc|cccc}
1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\
1 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
0 & 1 & \cdots & 0 & 1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\hline
0 & 0 & \cdots & 1 & 1 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 1 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c}
f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \\ \hline g(x_1) \\ g(x_2) \\ \vdots \\ g(x_n)
\end{array}\right]
\le
\left[\begin{array}{c}
\|x_1 - y_1\| \\ \|x_1 - y_2\| \\ \vdots \\ \hline \|x_2 - y_1\| \\ \|x_2 - y_2\| \\ \vdots \\ \hline \vdots \\ \hline \|x_n - y_1\| \\ \|x_n - y_2\| \\ \vdots
\end{array}\right]
$$

- It is seen that

$$f(x_i) + g(x_j) \le \|x_i - y_j\|, \ \forall i, j$$

- Because $x_i = y_i$, we further arrive at

$$f(x_i) + g(x_i) \le 0, \ \forall i = j$$
$$f(x_i) + g(x_j) \le \|x_i - x_j\|, \ \forall i \ne j$$

- For $\boldsymbol{b}^T \boldsymbol{y}$ to be maximized, both $f(x_i)$ and $g(x_i)$ need to be as large as possible since the components of $\boldsymbol{b}$ are all non-negative
- The optimal solution must thus have $f(x_i) + g(x_i) = 0$
- The constraint $\boldsymbol{A}^T \boldsymbol{y} \le \boldsymbol{c}$ then reduces to requiring

$$f(x_i) - f(x_j) \le \|x_i - x_j\|$$
$$f(x_j) - f(x_i) \le \|x_j - x_i\|$$

which suggests f is Lipschitz continuous (with Lipschitz constant 1)

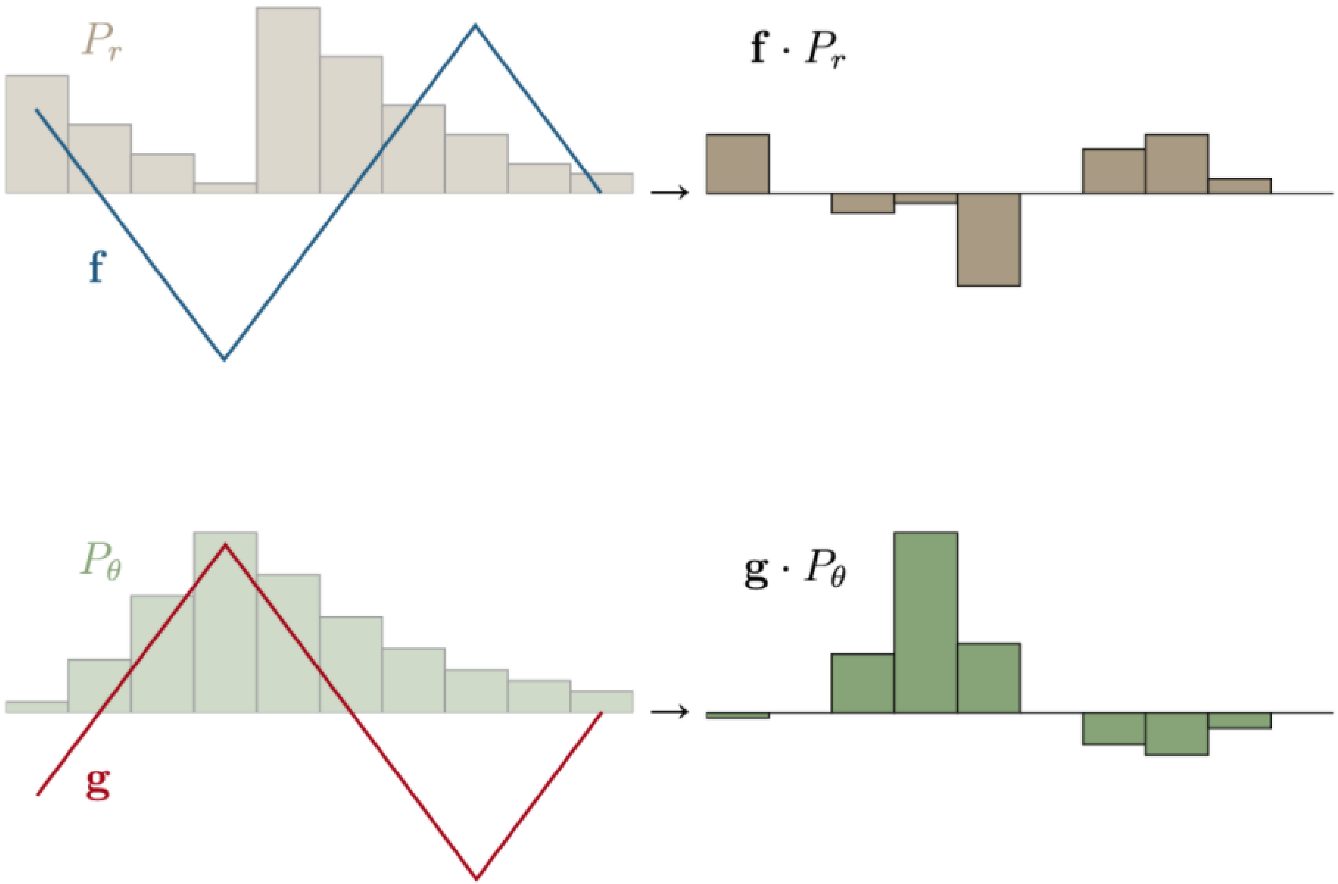
$$\|f(x_i) - f(x_j)\| \le \|x_i - x_j\|$$

- With this, searching for $\boldsymbol{y}$ to maximize $\boldsymbol{b}^T\boldsymbol{y}$

$$\boldsymbol{b}^T\boldsymbol{y} = \left[\begin{array}{ccc|ccc} p_r(x_1) & \cdots & p_r(x_n) & p_\theta(y_1) & \cdots & p_\theta(y_n) \end{array}\right] \left[\begin{array}{c} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \\ \hdashline -f(x_1) \\ -f(x_2) \\ \vdots \\ -f(x_n) \end{array}\right]$$

becomes to find a f among all the 1-Lipschitz functions such that

$$\max_{\|f\|_{L\leq 1}} E_{x\sim P_r} f(x) - E_{x\sim P_\theta} f(x)$$



Source: https://vincentherrmann.github.io/blog/wasserstein/

Training WGAN

- Training a generator $x = g_\theta(z), z \sim p(z)$ such that x has a distribution P_θ that converges to P_r in the EM distance

$$\theta^* = \arg\min_\theta W(P_r, P_\theta)$$

where the EM distance is evaluated by

$$W(P_r, P_\theta) = \max_{\|f\|_{L\leq 1}} E_{x\sim P_r} f(x) - E_{z\sim p(z)} f(g_\theta(z))$$

- Assuming $\{f_w\}_{w\in\mathcal{W}}$ is a family of 1-Lipschitz (or k-Lipschitz) functions

$$W(P_r, P_\theta) = \max_{\{f_w\}_{w\in\mathcal{W}}} E_{x\sim P_r} f_w(x) - E_{z\sim p(z)} f_w(g_\theta(z))$$

- The final objective becomes

$$\theta^* = \arg\min_\theta \max_{w\in\mathcal{W}} E_{x\sim P_r} f_w(x) - E_{z\sim p(z)} f_w(g_\theta(z))$$

where f_w (critic) and g_θ (generator) can be neural networks

- Under mild conditions, $W(P_r, P_\theta)$ is differentiable w.r.t. θ

$$\nabla_\theta W(P_r, P_\theta) = -E_{z \sim p(z)} \nabla_\theta f_w(g_\theta(z))$$

Algorithm 1 WGAN, our proposed algorithm. All experiments in the paper used the default values $\alpha = 0.00005$, $c = 0.01$, $m = 64$, $n_{\text{critic}} = 5$.

Require: : α, the learning rate. c, the clipping parameter. m, the batch size. n_{critic}, the number of iterations of the critic per generator iteration.
Require: : w_0, initial critic parameters. θ_0, initial generator's parameters.

while θ has not converged **do**
  for $t = 0, ..., n_{\text{critic}}$ **do**
    Sample $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$ a batch from the real data.
    Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.
    $g_w \leftarrow \nabla_w \left[\frac{1}{m}\sum_{i=1}^m f_w(x^{(i)}) - \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))\right]$
    $w \leftarrow w + \alpha \cdot \text{RMSProp}(w, g_w)$
    $w \leftarrow \text{clip}(w, -c, c)$
  end for
  Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.
  $g_\theta \leftarrow -\nabla_\theta \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))$
  $\theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, g_\theta)$
end while

GAN vs. WGAN

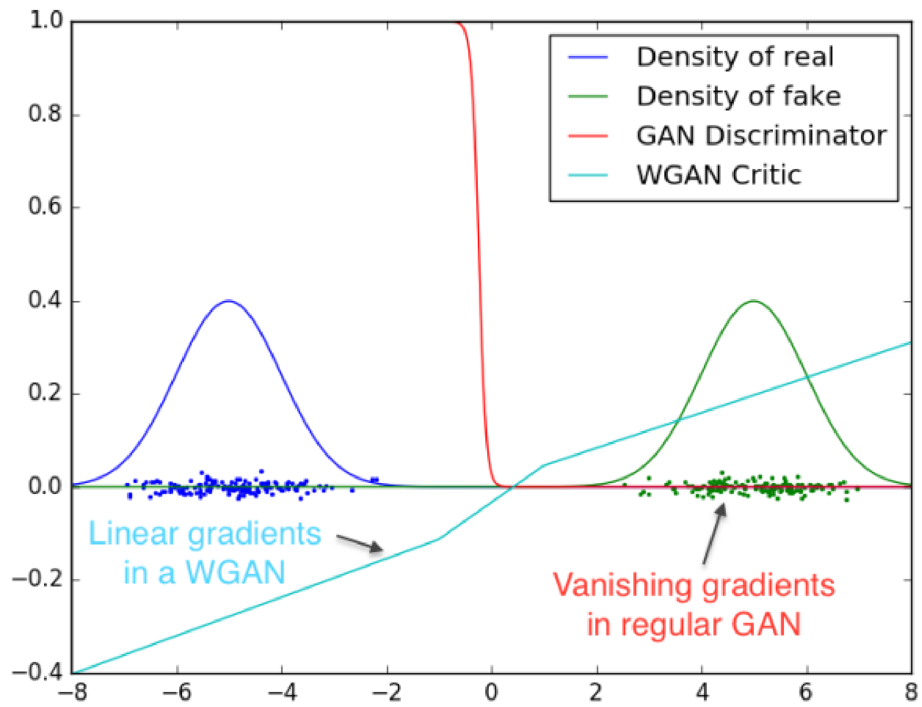


Figure 2: Optimal discriminator and critic when learning to differentiate two Gaussians. As we can see, the discriminator of a minimax GAN saturates and results in vanishing gradients. Our WGAN critic provides very clean gradients on all parts of the space.

InfoGAN

- **Idea:** To learn unsupervisedly disentangled representations for data through GAN
  1. Separate input noise into two parts z, c
  2. Learn a generator such that its output $x = G(z, c)$ correlates highly with c, by maximizing the mutual information $I(c; G(z, c))$
- Objective function

$$\arg\min_{\boldsymbol{\theta}^{(G)}} \max_{\boldsymbol{\theta}^{(D)}} V(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}) - \underbrace{\lambda I(c; G(z, c; \boldsymbol{\theta}^{(G)}))}$$

where $\lambda > 0$

Mutual Information

- (Definition) The mutual information between two random variables $\boldsymbol{x}, \boldsymbol{y}$ is given by

$$
\begin{aligned}
I(\boldsymbol{x};\boldsymbol{y}) &= \mathsf{KL}(p(\boldsymbol{x},\boldsymbol{y})||p(\boldsymbol{x})p(\boldsymbol{y})) \\
&= E[\log \frac{p(\boldsymbol{x},\boldsymbol{y})}{p(\boldsymbol{x})p(\boldsymbol{y})}] \\
&= H(\boldsymbol{x}) - H(\boldsymbol{x}|\boldsymbol{y}) \\
&= H(\boldsymbol{y}) - H(\boldsymbol{y}|\boldsymbol{x})
\end{aligned}
$$

  where $I(\boldsymbol{x};\boldsymbol{y}) = 0$ if and only if $\boldsymbol{x}, \boldsymbol{y}$ are independent

- $I(\boldsymbol{x};\boldsymbol{y})$ indicates the reduction of uncertainty about $\boldsymbol{x}$ (respectively, $\boldsymbol{y}$) after observing $\boldsymbol{y}$ (respectively, $\boldsymbol{x}$)

Variational Mutual Information Maximization

- Evaluating $I(c;x)$ with $x = G(z,c)$ needs to know the posterior $p(c|x)$, which is intractable

$$\begin{aligned} I(c;x) &= H(c) - H(c|x) \\ &= H(c) + E_{x\sim G(z,c)} E_{c'\sim p(c|x)}[\log p(c'|x)] \end{aligned}$$

- One way out of this difficulty is to introduce a variational function $q(c|x)$ for approximating $p(c|x)$

$$\begin{aligned} I(c;x) = H(c) &+ E_{x\sim G(z,c)} E_{c'\sim p(c|x)}[\log p(c'|x) - \log q(c'|x)] \\ &+ E_{x\sim G(z,c)} E_{c'\sim p(c|x)}[\log q(c'|x)] \end{aligned}$$

- It is readily seen that

$$\begin{aligned} I(c;x) = H(c) &+ E_{x\sim G(z,c)}[\mathsf{KL}(p(c'|x)||q(c'|x))] \\ &+ E_{x\sim G(z,c)} E_{c'\sim p(c|x)}[\log q(c'|x)] \end{aligned}$$

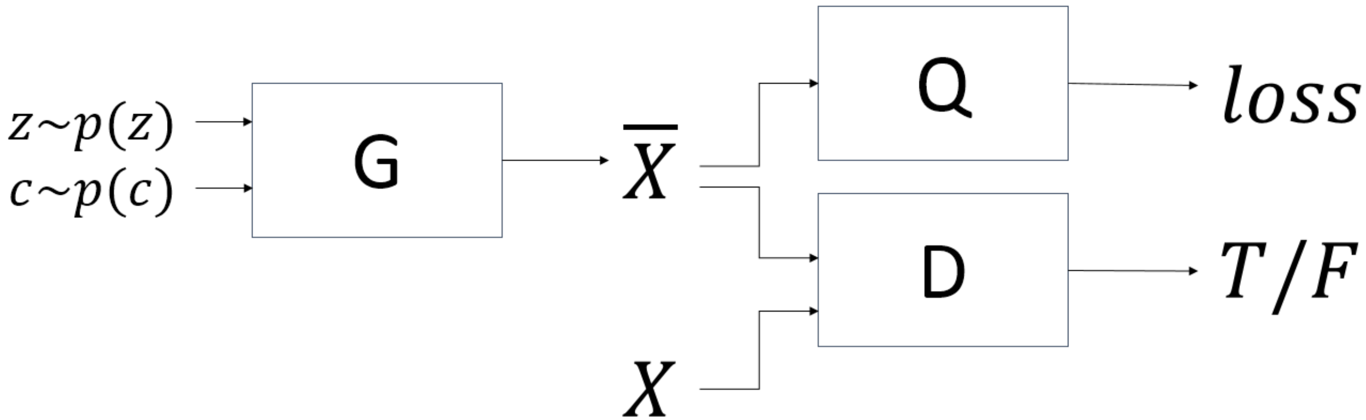
$$\geq H(c) + \underbrace{E_{x\sim G(z,c)}E_{c'\sim p(c|x)}[\log q(c'|x)]}$$

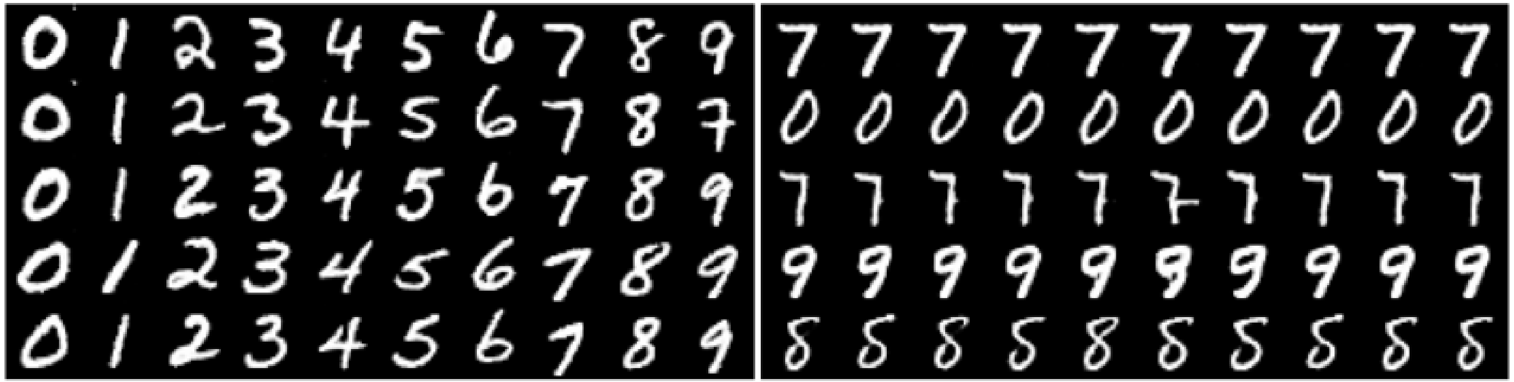
$$= H(c) + \underbrace{E_{c\sim p(c),x\sim G(z,c)}[\log q(c|x)]}$$

- The objective function of InfoGAN then becomes

$$\arg \min_{\boldsymbol{\theta}^{(G)},\boldsymbol{\theta}^{(Q)}} \max_{\boldsymbol{\theta}^{(D)}} V(\boldsymbol{\theta}^{(D)},\boldsymbol{\theta}^{(G)}) - \underbrace{\lambda(E_{c\sim p(c),x\sim G(z,c)}[\log q(c|x;\boldsymbol{\theta}^{(Q)})])}$$

- The term $E_{c\sim p(c),x\sim G(z,c)}[\log q(c|x;\boldsymbol{\theta}^{(Q)})]$ can be evaluated by using the reparameterization trick (i.e., by inputting different z samples while fixing c and requiring that the output of Q be c again)





(a) Varying c_1 on InfoGAN (Digit type) (b) Varying c_1 on regular GAN (No clear meaning)

Deep Boltzmann Machines (DBM)

- An energy-based generative model with an explicit density over binary visible $\boldsymbol{v}$ and hidden $\boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}$ variables

$$p(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}; \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp(-E(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}; \boldsymbol{\theta}))$$

where

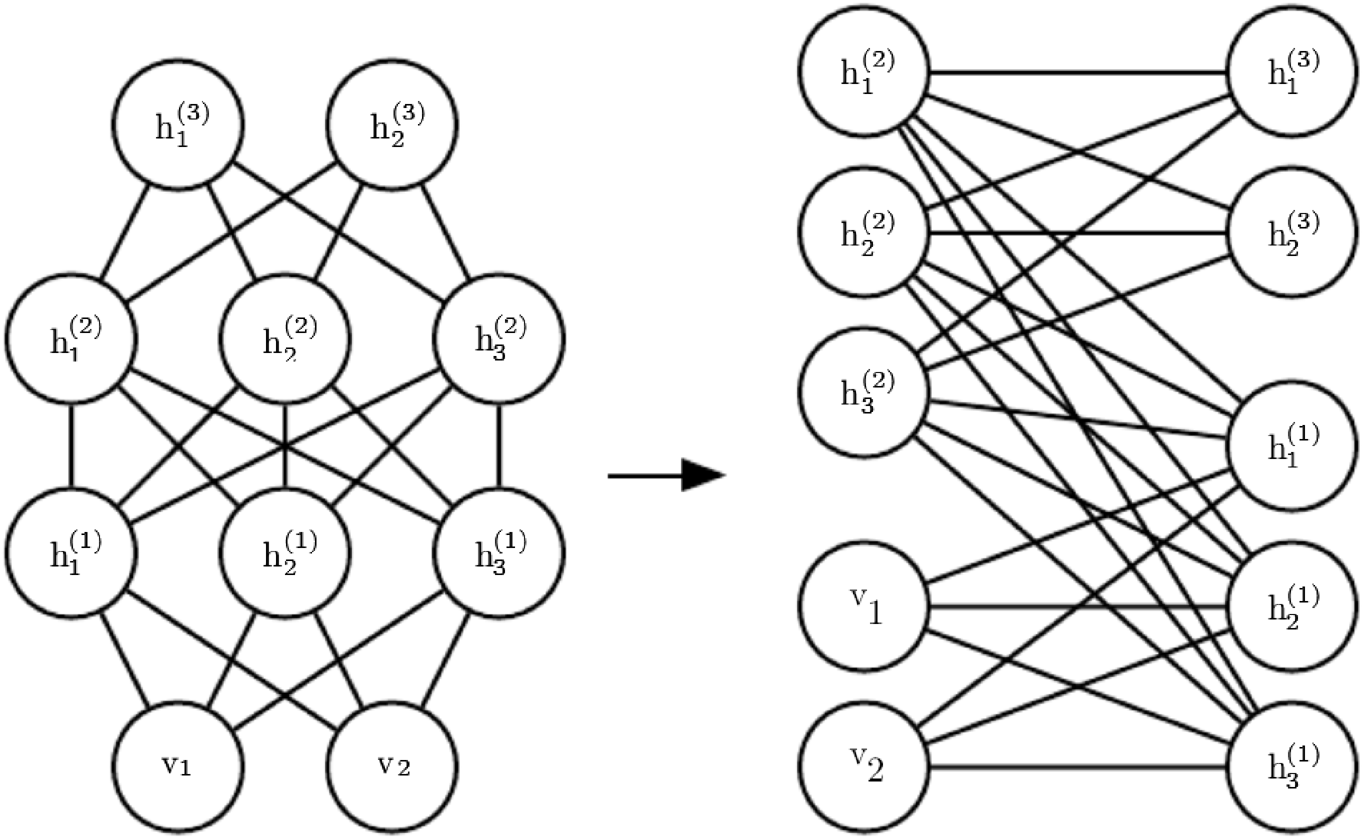
$$\begin{aligned} & E(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}; \boldsymbol{\theta}) \\ &= -\boldsymbol{v}^T \boldsymbol{W}^{(1)} \boldsymbol{h}^{(1)} - \boldsymbol{h}^{(1)T} \boldsymbol{W}^{(2)} \boldsymbol{h}^{(2)} - \boldsymbol{h}^{(2)T} \boldsymbol{W}^{(3)} \boldsymbol{h}^{(3)} \end{aligned}$$

and

$$\boldsymbol{\theta} = \{\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}, \boldsymbol{W}^{(3)}\}$$

- Note that bias terms are omitted for simplicity

- Graphical model for DBM, where odd layers can be separated from even layers to reveal a bipartite structure



- As a result, variables in odd layers are conditionally independent given even layers and vice versa; this enables block Gibbs sampling

- Likewise, it is seen that variables in a layer are conditionally independent given the neighbouring layers
- In the case of two hidden layers, we have

$$p(v_i = 1|\boldsymbol{h}^{(1)}) = \sigma(\boldsymbol{W}^{(1)}_{i,:}\boldsymbol{h}^{(1)})$$

$$p(h^{(1)}_i = 1|\boldsymbol{v}, \boldsymbol{h}^{(2)}) = \sigma(\boldsymbol{v}^T\boldsymbol{W}^{(1)}_{:,i} + \boldsymbol{W}^{(2)}_{i,:}\boldsymbol{h}^{(2)})$$

$$p(h^{(2)}_i = 1|\boldsymbol{h}^{(1)}) = \sigma(\boldsymbol{h}^{(1)T}\boldsymbol{W}^{(2)}_{:,i})$$

- However, the posterior distribution of all hidden layers given the visible layer does not factorize because of interactions between layers

$$p(\boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}|\boldsymbol{v}) \neq \prod_j p(h^{(1)}_j|\boldsymbol{v}) \prod_k p(h^{(2)}_k|\boldsymbol{v})$$

- Approximate inference needs to be sought

DBM Mean Field Inference

- To construct a factorial $Q(\boldsymbol{h}|\boldsymbol{v})$ for approximating $p(\boldsymbol{h}|\boldsymbol{v})$

$$p(\boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}|\boldsymbol{v}) \approx Q(\boldsymbol{h}|\boldsymbol{v}) = \prod_j q(h_j^{(1)}|\boldsymbol{v}) \prod_k q(h_k^{(2)}|\boldsymbol{v})$$

- In the present case, all hidden variables $h_j^{(1)}, h_k^{(2)}$ are binary; these $q(h|\boldsymbol{v})$ must have a functional form of the Bernoulli distribution, i.e.

$$q(h_j^{(1)}|\boldsymbol{v}) = (\hat{h}_j^{(1)})^{h_j^{(1)}}(1 - \hat{h}_j^{(1)})^{(1-h_j^{(1)})}, \forall i$$

$$q(h_k^{(2)}|\boldsymbol{v}) = (\hat{h}_k^{(2)})^{h_k^{(2)}}(1 - \hat{h}_k^{(2)})^{(1-h_k^{(2)})}, \forall k$$

where $\hat{h}_j^{(1)}, \hat{h}_k^{(2)} \in [0, 1]$ are the corresponding parameters

- Carrying out the expectation (needs some work)

$$\tilde{q}_j(h_j|\boldsymbol{v}) = \exp(E_{q_{-j}}(\log p(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \boldsymbol{\theta})))$$

yields the following fixed-point update equations

$$\hat{h}_j^{(1)} = \sigma\left(\sum_i v_i W_{i,j}^{(1)} + \sum_k W_{j,k}^{(2)} \hat{h}_k^{(2)}\right), \forall j$$

$$\hat{h}_k^{(2)} = \sigma\left(\sum_j W_{j,k}^{(2)} \hat{h}_j^{(1)}\right), \forall k$$

DBM Parameter Learning

- DBM learning has to confront both the intractable inference $p(\boldsymbol{h}|\boldsymbol{v})$ and the intractable partition function $Z(\boldsymbol{\theta})$
- Combined variational inference, learning, and MCMC is necessary
- The objective then becomes to find $\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)}$ that minimize

$$\mathcal{L}(Q, \boldsymbol{\theta}) = \sum_i \sum_j v_i W_{i,j}^{(1)} \hat{h}_j^{(1)} + \sum_j \sum_k \hat{h}_j^{(1)} W_{j,k}^{(2)} \hat{h}_k^{(2)} - \log Z(\boldsymbol{\theta}) + H(Q)$$

  which can be done via gradient descent

$$\boldsymbol{\theta}' = \boldsymbol{\theta} - \varepsilon \nabla_{\boldsymbol{\theta}} \mathcal{L}(Q, \boldsymbol{\theta})$$

  (study Algorithm 20.1)

- In general, layer-wise pre-training is needed to arrive at a good model

---

Set ϵ, the step size, to a small positive number
Set k, the number of Gibbs steps, high enough to allow a Markov chain of $p(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \boldsymbol{\theta} + \epsilon\Delta_{\boldsymbol{\theta}})$ to burn in, starting from samples from $p(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \boldsymbol{\theta})$.
Initialize three matrices, $\tilde{\boldsymbol{V}}$, $\tilde{\boldsymbol{H}}^{(1)}$ and $\tilde{\boldsymbol{H}}^{(2)}$ each with m rows set to random values (e.g., from Bernoulli distributions, possibly with marginals matched to the model's marginals).
while not converged (learning loop) **do**
  Sample a minibatch of m examples from the training data and arrange them as the rows of a design matrix $\boldsymbol{V}$.
  Initialize matrices $\hat{\boldsymbol{H}}^{(1)}$ and $\hat{\boldsymbol{H}}^{(2)}$, possibly to the model's marginals.
  while not converged (mean field inference loop) **do**
    $\hat{\boldsymbol{H}}^{(1)} \leftarrow \sigma\left(\boldsymbol{V}\boldsymbol{W}^{(1)} + \hat{\boldsymbol{H}}^{(2)}\boldsymbol{W}^{(2)\top}\right)$.
    $\hat{\boldsymbol{H}}^{(2)} \leftarrow \sigma\left(\hat{\boldsymbol{H}}^{(1)}\boldsymbol{W}^{(2)}\right)$.
  end while
  $\Delta_{\boldsymbol{W}^{(1)}} \leftarrow \frac{1}{m}\boldsymbol{V}^\top\hat{\boldsymbol{H}}^{(1)}$
  $\Delta_{\boldsymbol{W}^{(2)}} \leftarrow \frac{1}{m}\hat{\boldsymbol{H}}^{(1)\,\top}\hat{\boldsymbol{H}}^{(2)}$
  for $l = 1$ to k (Gibbs sampling) **do**
    Gibbs block 1:
    $\forall i, j, \tilde{V}_{i,j}$ sampled from $P(\tilde{V}_{i,j} = 1) = \sigma\left(\boldsymbol{W}_{j,:}^{(1)}\left(\tilde{\boldsymbol{H}}_{i,:}^{(1)}\right)^\top\right)$.
    $\forall i, j, \tilde{H}_{i,j}^{(2)}$ sampled from $P(\tilde{H}_{i,j}^{(2)} = 1) = \sigma\left(\tilde{\boldsymbol{H}}_{i,:}^{(1)}\boldsymbol{W}_{:,j}^{(2)}\right)$.
    Gibbs block 2:
    $\forall i, j, \tilde{H}_{i,j}^{(1)}$ sampled from $P(\tilde{H}_{i,j}^{(1)} = 1) = \sigma\left(\tilde{\boldsymbol{V}}_{i,:}\boldsymbol{W}_{:,j}^{(1)} + \tilde{\boldsymbol{H}}_{i,:}^{(2)}\boldsymbol{W}_{j,:}^{(2)\top}\right)$.
  end for
  $\Delta_{\boldsymbol{W}^{(1)}} \leftarrow \Delta_{\boldsymbol{W}^{(1)}} - \frac{1}{m}\boldsymbol{V}^\top\tilde{\boldsymbol{H}}^{(1)}$
  $\Delta_{\boldsymbol{W}^{(2)}} \leftarrow \Delta_{\boldsymbol{W}^{(2)}} - \frac{1}{m}\tilde{\boldsymbol{H}}^{(1)\top}\tilde{\boldsymbol{H}}^{(2)}$
  $\boldsymbol{W}^{(1)} \leftarrow \boldsymbol{W}^{(1)} + \epsilon\Delta_{\boldsymbol{W}^{(1)}}$ (this is a cartoon illustration, in practice use a more effective algorithm, such as momentum with a decaying learning rate)
  $\boldsymbol{W}^{(2)} \leftarrow \boldsymbol{W}^{(2)} + \epsilon\Delta_{\boldsymbol{W}^{(2)}}$
end while

Topics Not Covered

- Optimization for training deep models (Chapter 8)
- Representation learning (Chapter 15)
- Back-prop through random operations (REINFORCE, Chapter 20)
- BM for real-valued data (Chapter 20)
- Generative Stochastic Networks (Chapter 20)
- Deep Belief Networks (Chapter 20)
- Other generative models (Chapter 20)