Deep Generative Models

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Introduction

Deep Generative Models
- Early Forms of DGMs
- DGMs Training Procedure
- Modern DGMs
- A Unified View of DGMs

Applications
- Generative Adversarial Networks (GANs)
- Normalizing Flow (NF)
- Integrating Domain Knowledge into Deep Learning

Introduction

Motivation

This lecture is about a unifying theoretical perspective of DGMs. The reason why we are interested:

- Trending: most popular research topic nowadays (CVPR, ICML, NeurIPS, etc.)
- Promising: style transfer/fusion, music/image/text generations, etc.

Definition

Generative vs. Discriminative models:

- $\mathbb{P}(X, Y)$ vs. $\mathbb{P}(Y|X)$;
- Estimate distribution (G) instead of just boundaries (D);
- etc.

Deep: multiple layers of hidden variables.

Course Materials

Prof. Eric Xing's lecture 12 & 13. [1]

- Lecture scribe: 12 & 13
- Lecture slides: 12 & 13
- Lecture record: 12 & 13

Prerequisites:

- Variational Inferences (Lecture 7&8 in Prof. Xing's lecture, in our reading group presented by Yewen.)

[1] www.cs.cmu.edu/ epxing/Class/10708-20/lectures.html

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Deep Generative Models

Sigmoid Belief Nets [2]

A kind of Hierarchical Bayesian Model. We estimate the hidden values and the parameters to approximate the observations.

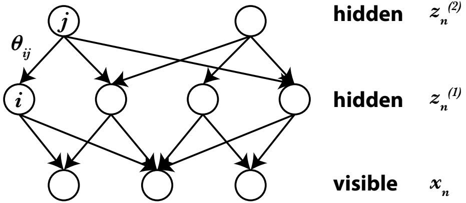

Figure: SBNs: lower layers are connect to upper layers via sigmoid functions. Use θ_k to denote all parameters connected to $x_{k,n}$; θ_i for that connected to $z_{i,n}^{(1)}$ from $z_{*,n}^{(2)}$. Then:
$p(x_{k,n} = 1|\theta_k, z_n^{(1)}) = \sigma(\theta_k^T z_n^{(1)})$; $p(z_{i,n}^{(1)} = 1|\theta_i, z_n^{(2)}) = \sigma(\theta_i^T z_n^{(2)})$.

[2] Neal, 1992

A dual, alternative process that unifies **inference** and **generative** process:

- run **generative** model on input $p_\theta(\mathbf{X})$, and also run **inference** model on hidden values $p_\phi(\mathbf{h})$.
- Use the **process** instead of a global math expression to define the model.
- inference and generative models may or may not be related.

$$\mathbf{X}_n = G_\theta(\mathbf{X}_{n-1})\,, \qquad \mathbf{X}_{n-1} = F_\phi(\mathbf{X}_n)$$

[3] Dayan et al.,1995

Predictability Minimization [4]

Defines a **training procedure**. Not “model” in a rigorous way.

- Using alternative loss-functions. Containing an **encoder** network and a **predictor** network.
- Use the **training procedure** instead of a global math expression to define the model.

Suppose the latent representation (code) is $\mathbf{y} \in \mathbb{R}^m$, $y_i \in [0, 1]$, then the predictor minimizes the prediction error on $\mathbf{y}$, while the encoder maximizes the prediction error (e.g. mean square error).

[4] Schmidhuber, Since 1991 (see also: a conclusion on ArXiV)

Restricted Boltzmann machines (RBMs) [Smolensky, 1986]

- Equivalent to an infinitely-deep sigmoid network.

Deep belief networks (DBNs) [Hinton et al., 2006]

- Inference in DBNs is problematic due to "*explaining away*" (e.g. one observation A, two potential causes B and C, symptom A makes both B and C become more likely, but once you pick a cause, then the other's probability goes back down [5]);
- Hybrid graphical model, some layers directed, some layers undirected.

Resurgence of deep generative models II

Deep Boltzmann Machines (DBMs) [Salakhutdinov & Hinton, 2009]

- Undirected model.

Variational autoencoders (VAEs) [Kingma & Welling, 2014] / Neural Variational Inference and Learning (NVIL) [Mnih & Gregor, 2014]

- The first modern actively-used DGMs.
- Old ideas (generative model $p_\theta(\mathbf{x}|\mathbf{z})$ and inference model $q_\phi(\mathbf{z}|\mathbf{x})$) but excellent executions, produce very nice results.
- Still, the two models can be very different.
- Trained in a variational way.

Generative adversarial networks (GANs) [Goodfellow et al,. 2014]

- Defining a procedure, again, not really a "model". Alternatively train G_θ and D_ϕ.

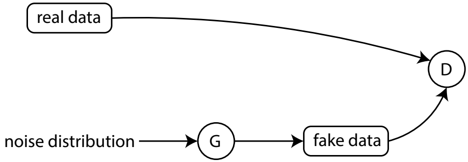

Figure: GAN:
$\min_G \max_D \mathbb{E}_{\mathbf{x}_{real}}\big(\log(D(\mathbf{x}_{real}))\big) + \mathbb{E}_{\mathbf{x}_{fake}}\big(\log(1 - D(G(\mathbf{x}_{fake})))\big)$

And countless ideas following them. We have a zoo of such models.

[5] Reference slides on "explaining away".

Synonyms in the Literature

Posterior Distribution / Inference model

- Variational approximation
- Recognition model
- Inference network (if parameterized as neural networks)
- Recognition network (if parameterized as neural networks)
- (Probabilistic) encoder

"The Model" (prior + conditional, or joint) / Generative model

- The (data) likelihood model
- Generative network (if parameterized as neural networks)
- Generator
- (Probabilistic) decoder

Training I

Training of early forms of DGMs typically uses EM framework.

- via sampling / data augmentation: directly infer hidden variable, given observations $p(\mathbf{z}|\mathbf{x})$

$$\mathbf{z} = \{\mathbf{z}_1, \mathbf{z}_2\}$$
$$\mathbf{z}_1^{new} \sim p(\mathbf{z}_1|\mathbf{z}_2, \mathbf{x})$$
$$\mathbf{z}_2^{new} \sim p(\mathbf{z}_2|\mathbf{z}_1^{new}, \mathbf{x})$$

- variational inference: generator parameters θ, variational inference model parameters ϕ, optimizing an variational lower bound:

$$log(p(\mathbf{x})) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))] + KL(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) := \mathcal{L}(\theta, \phi; \mathbf{x})$$

$$\max_{\theta,\phi} \mathcal{L}(\theta, \phi; \mathbf{x})$$

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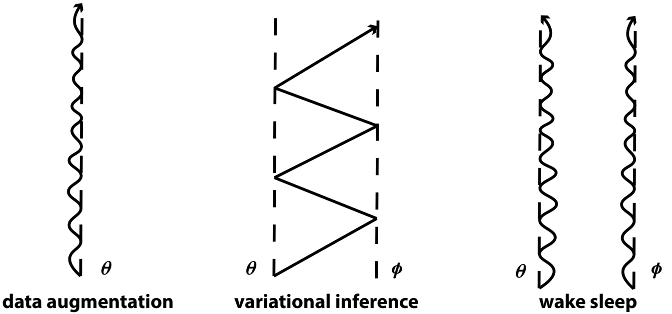


Figure: Illustration of the training methods' differences.

Training III

- wake sleep: the **loss**-functions become **different**

$$\text{Wake:} \quad \min_{\theta} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$$

$$\text{Sleep:} \quad \min_{\phi} \mathbb{E}_{p_\theta(\mathbf{x}|\mathbf{z})}[\log(q_\phi(\mathbf{z}|\mathbf{x}))]$$

Recap: Variational Inference

Consider a generative model $p_\theta(\mathbf{x}|\mathbf{z})$, and prior $p(\mathbf{z})$; we have joint distribution:

$$p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})$$

Assume variational distribution $q_\phi(\mathbf{z}|\mathbf{x})$;
Objective: Maximize lower bound for log likelihood.

$$log(p(\mathbf{x})) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))] + \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) := \mathcal{L}(\theta, \phi; \mathbf{x})$$

where KL refers to KL Divergence (p, q are distributions): [6]

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

There are **multiple ways** of expressing its objectives.

[6] references of KL.

Recap: Variational Inference

Maximizing the variational lower bound:

$$
\begin{aligned}
\mathcal{L}(\theta, \phi; \mathbf{x}) &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))] + \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \\
&= \log p(\mathbf{x}) - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))
\end{aligned}
$$

"E-Step": [7]

$$\max_\phi \mathcal{L}(\theta, \phi; \mathbf{x})$$

"M-Step":

$$\max_\theta \mathcal{L}(\theta, \phi; \mathbf{x})$$

Equivalently: minimize free energy.

$$\mathcal{F}(\theta, \phi; \mathbf{x}) = -\log p(\mathbf{x}) + \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$$

[7] To call it EM is misleading but there is a correspondence.

Wake Sleep I

Maximize data log-likelihood with two steps of loss relaxation.

Wake phase: $\min_\theta \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$

- Maximize the variational lower bound of log-likelihood, or minimizing free energy (original goal)

$$\mathcal{F}(\theta, \phi; \mathbf{x}) = -\log p(\mathbf{x}) + \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$$

- Correspond to variational **M step**).
- Get samples from $q_\phi(\mathbf{z}|\mathbf{x})$ through inference on hidden variables.

Sleep phase: $\min_\phi \mathbb{E}_{p_\theta(\mathbf{x}|\mathbf{z})}[\log(q_\phi(\mathbf{z}|\mathbf{x}))]$, simplified as $\min_\phi \mathbb{E}_{p_\theta(\mathbf{x},\mathbf{z})}[\log(q_\phi(\mathbf{z}|\mathbf{x}))]$ (for the ease of optimization).

$$\nabla_\phi \mathcal{F}(\theta, \phi; \mathbf{x}) = \cdots + \nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{z}|\mathbf{x}))] + \dots$$

includes the high variance term $\log p_\theta$, but could be estimated with the log-derivative trick:

$$\begin{aligned}\nabla_\phi \mathbb{E}_{q_\phi}[\log p_\theta] &= \int \nabla_\phi q_\phi \log p_\theta = \int q_\phi \log p_\theta \nabla_\phi \log q_\phi \\ &= \mathbb{E}_{q_\phi}[\log p_\theta \nabla_\phi \log q_\phi]\end{aligned}$$

estimated by Monte Carlo ($\log p_\theta(\mathbf{x}, \mathbf{z}_i)$ can be arbitrarily large):

$$\nabla_\phi \mathbb{E}_{q_\phi}[\log p_\theta] \approx \mathbb{E}_{\mathbf{z}_i \sim q_\phi}[\log p_\theta(\mathbf{x}, \mathbf{z}_i) \nabla_\phi q_\phi(\mathbf{z}_i|\mathbf{x})]$$

Wake Sleep III

- Minimize a different objective (reversed KLD) wrt ϕ to ease the optimization:

$$\mathcal{F}'(\theta, \phi; \mathbf{x}) = -\log p(\mathbf{x}) + \mathrm{KL}(p_\theta(\mathbf{z}|\mathbf{x})||q_\phi(\mathbf{z}|\mathbf{x}))$$

- Correspond to the variational **E step**.
- Why changing objective: original objective is suffering from high variance caused by the gradient of the original KL term, and therefore it is generally intractable.
- "Dreaming" up samples from $p_\theta(\mathbf{x}|\mathbf{z})$ through top-down pass.
- Doing something "wrong" but not "too wrong".

Variational Inference v.s. Wake Sleep

Variational Inference

- Distribution $q_\phi(\mathbf{z}|\mathbf{x})$
- M Step:
  $\min_\theta \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$
  - $\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\nabla_\theta \log(p_\theta(\mathbf{x}|\mathbf{z}))]$
- E Step:
  $\min_\phi \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$
  - $\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$
  - High variance, need variance-reduce in practice
  - Learning with real samples of $\mathbf{x}$.
- Single objective, guaranteed to converge

Wake Sleep

- Inference model $q_\phi(\mathbf{z}|\mathbf{x})$
- Wake:
  $\min_\theta \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$
  - $\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\nabla_\theta \log(p_\theta(\mathbf{x}|\mathbf{z}))]$
- Sleep:
  $\min_\phi \mathrm{KL}(p_\theta(\mathbf{z}|\mathbf{x})||q_\phi(\mathbf{z}|\mathbf{x}))$
  - $\mathbb{E}_{p_\theta(\mathbf{z},\mathbf{x})}[\nabla_\phi \log(q_\phi(\mathbf{z},\mathbf{x}))]$
  - Low variance
  - Learning with generated samples of $\mathbf{x}$.
- Two objective, not guaranteed to converge

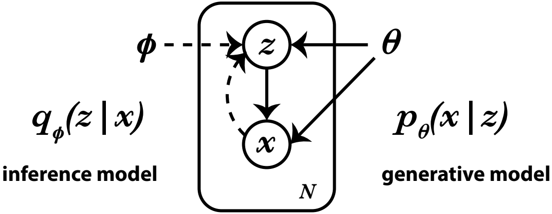


Figure: Key Ideas: Inference model and Generative model. Prior $p(\mathbf{z})$, joint distribution $p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})$. Use variational inference with an inference model, enjoy similar applicability with wake-sleep algorithm. [Kingma & Welling, 2014]

Variational lower bound:

$$\mathcal{L}(\theta, \phi; \mathbf{x}) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}, \mathbf{z})] - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

Recall that for a variational inference model we suffer from large variance in sleep / E phase:

$$\nabla_\phi \mathcal{F}(\theta, \phi; \mathbf{x}) = \cdots + \nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{z}|\mathbf{x}))] + \ldots$$

This time the variance is reduced via **reparameterization trick**. (Alternatives: use control variates as in reinforcement learning.)

Reparameterization trick in gradient estimation of the inference model:

1. Assume a trivial noise distribution (e.g. standard Gaussian): $\epsilon \sim p(\epsilon)$
2. Do a deterministic transformation:

$$\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x}) \iff \mathbf{z} = g_\phi(\epsilon, \mathbf{x})$$

3. Reparameterized expression e.g.:

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}, \mathbf{z}))] = \mathbb{E}_{\epsilon \sim p(\epsilon)}[\nabla_\phi \log p_\theta(\mathbf{x}, \mathbf{z}_\phi(\epsilon))]$$

has empirically lower variance of the gradient estimate.

Variational autoencoders (VAEs) IV

Figure: Celebrity faces generated (Radford 2015). VAEs tend to generate **blurred** images due to the mode covering behavior.

Mode-covering behavior has something to do with the KL divergence: reference.

Defining a procedure involving a generator G_θ and a discriminator D_ϕ.

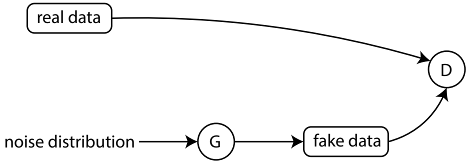


Figure: [Goodfellow et al,. 2014] GAN:
$\min_G \max_D \mathbb{E}_{\mathbf{x}_{real}}\big(\log(D(\mathbf{x}_{real}))\big) + \mathbb{E}_{\mathbf{x}_{fake}}\big(\log(1 - D(G(\mathbf{x}_{fake})))\big)$

D (discriminator, output 1 for real data and 0 for fake data) is trained first and then **G** in each iteration. While training **D** we minimize:

$$\ell_D = -\mathbb{E}_{\mathbf{x}_{real}}\big(\log(D(\mathbf{x}_{real}))\big) - \mathbb{E}_{\mathbf{x}_{fake}}\big(\log(1 - D(G(\mathbf{x}_{fake})))\big)$$

and while training **G** we minimize:

$$\ell_G = \log(1 - D(G(\mathbf{x}_{fake})))$$

where $\mathbf{x}_{real}$ are sampled from real data $\mathbf{x}_{real} \sim p_{data}(\mathbf{x})$ and $\mathbf{x}_{fake}$ is sampled from a noise distribution $\mathbf{x}_{fake} \sim p_{noise}(\mathbf{x})$.

Learning goal is to achieve equilibrium of the game, optimal state:

- Generated distribution is identical to the real distribution.
- $D(\mathbf{x}) = \frac{1}{2}$

Generative Adversarial Nets (GANs) IV

Figure: Generated bedrooms (Radford et al., 2016). GANs tend to generate **sharp** images but very **narrow** (focusing on a few areas e.g. the bed).

Necessity of a Unified View

Analogy: from *Alchemy* to *modern Chemistry*.

- Basic elements are concluded in a unified way;
- Rules are found accordingly;
- No need to try countless times until getting some "Hail Mary results" with luck.

Paper: On Unifying Deep Generative Models [Z Hu, Z YANG, R Salakhutdinov, E Xing]

- GANs: achieve an equilibrium between generator and discriminator
- VAEs: maximize lower bound of the data likelihood

Is there a way of making DGMs expressions a little bit similar with each other?

- GAN objective in variational-EM format;
- VAE's new formulation (and comparision to GAN);
- Linking GAN and VAE to Wake-Sleep.

GAN Objective New Form

To model a distribution:
$\mathbf{x} \sim p_\theta(\mathbf{x}|y) \iff \mathbf{x} = G_\theta(\mathbf{z}), \mathbf{z} \sim p(\mathbf{z}|y=0)$ where

$$p_\theta(\mathbf{x}|y) = \begin{cases} p_{g_\theta}(\mathbf{x}) & y = 0 \\ p_{\text{data}}(\mathbf{x}) & y = 1 \end{cases}$$

Conventional formulation ($\mathbf{z} \sim p_{noise}(\mathbf{z})$):

$$\min_{\theta} \max_{\phi} \mathbb{E}_{\mathbf{x}\sim p_{data}(\mathbf{x})}[\log(D_\phi(\mathbf{x}))] + \mathbb{E}_{\mathbf{x}\sim G_\theta(\mathbf{z})}[\log(1 - D_\phi(\mathbf{x}))]$$

$$\begin{cases} \max_\phi \mathcal{L}_\phi = \mathbb{E}_{\mathbf{x}\sim p_{data}(\mathbf{x})}[\log(D_\phi(\mathbf{x}))] + \mathbb{E}_{\mathbf{x}\sim G_\theta(\mathbf{z})}[\log(1 - D_\phi(\mathbf{x}))] \\ \max_\theta \mathcal{L}_\theta = \mathbb{E}_{\mathbf{x}\sim G_\theta(\mathbf{z})}[\log(D_\phi(\mathbf{x}))] \end{cases}$$

The new form:

$$\begin{cases} \max_\phi \mathcal{L}_\phi = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi(y|\mathbf{x}))] \\ \max_\theta \mathcal{L}_\theta = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi(1 - y|\mathbf{x}))] \end{cases}$$

where $q_\phi(1 - y|\mathbf{x}))$ can also be denoted as $q^r_\phi(y|\mathbf{x}))$.

GAN in variational-EM Format

Variational EM

$$\mathcal{L}(\theta,\phi;\mathbf{x}) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))] + KL(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

$$\max_\theta \mathcal{L}(\theta,\phi;\mathbf{x}), \qquad \max_\phi \mathcal{L}(\theta,\phi;\mathbf{x})$$

- Single objective
- Generative model: $p_\theta(\mathbf{x}|\mathbf{z})$
- Inference model: $q_\phi(\mathbf{z}|\mathbf{x})$
- The reconstruction term $\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$ is similar to GANs' objectives.

GANs

$$\max_\phi \mathcal{L}_\phi = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi(y|\mathbf{x}))]$$

$$\max_\theta \mathcal{L}_\theta = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi(1-y|\mathbf{x}))]$$

- Two objectives
- Interpret $q_\phi(y|\mathbf{x})$ as the generative model
- Interpret $p_\theta(\mathbf{x}|y)$ as the inference model
- Doesn't exist prior regularization of $p(\mathbf{z})$.

GAN: Minimizing KLD

Recall that in maximizing the variational lower bound:

$$\begin{aligned}\mathcal{L}(\theta, \phi; \mathbf{x}) &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))] + KL(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \\ &= \log p(\mathbf{x}) - KL(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))\end{aligned}$$

That is, we minimized the KLD from the inference model to the posterior:

$$-\log p(\mathbf{x}) + KL(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x}))$$

Starting from an initial point (θ_0, ϕ_0), let $p(y)$ be a uniform prior distribution, and

$$p_{\theta=\theta_0}(\mathbf{x}) = \mathbb{E}_{p(y)}[p_{\theta=\theta_0}(\mathbf{x}|y)]$$
$$q^r(\mathbf{x}|y) \propto q^r(y|\mathbf{x})p_{\theta=\theta_0}(\mathbf{x})$$

Lemma (update rule for θ [8])

$$\begin{aligned}&\nabla_\theta \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q^r_{\phi=\phi_0}(y|\mathbf{x}))]\Big|_{\theta=\theta_0}\\ =&\nabla_\theta\Big(\mathbb{E}_{p(y)}[\mathrm{KL}(p_\theta(\mathbf{x}|y)||q^r(\mathbf{x}|y))] - \mathrm{JSD}(p_\theta(\mathbf{x}|y=0)||p_\theta(\mathbf{x}|y=1))\Big)\Big|_{\theta=\theta_0}\end{aligned}$$

[8] JSD = Jensen-Shannon divergence, KL = KL divergence.

GAN: Minimizing KLD

Lemma (update rule for θ)

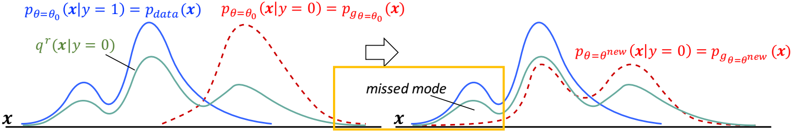
$$
\begin{aligned}
&\nabla_\theta \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q^r_{\phi=\phi_0}(y|\mathbf{x}))]\Big|_{\theta=\theta_0} \\
=&\nabla_\theta \Big(\mathbb{E}_{p(y)}[\mathrm{KL}(p_\theta(\mathbf{x}|y)||q^r(\mathbf{x}|y))] - \mathrm{JSD}(p_\theta(\mathbf{x}|y=0)||p_\theta(\mathbf{x}|y=1))\Big)\Big|_{\theta=\theta_0}
\end{aligned}
$$

Connection to variational inference:

- See $\mathbf{x}$ as latent variables, y as visible;
- $p_{\theta=\theta_0}(\mathbf{x})$ as prior distribution, $q^r(\mathbf{x}|y)$ as posterior distribution, $p_\theta(\mathbf{x}|y)$ as variational distribution.

GAN: Minimizing KLD — "sharpness of images" [9]

GANs: minimizing KLD



- Missing mode phenomena of GANs
  - Asymmetry of KLD
    - Concentrates $p_\theta(\boldsymbol{x}|y=0)$ to large modes of $q^r(\boldsymbol{x}|y)$
      $\Rightarrow p_{g_\theta}(\boldsymbol{x})$ misses modes of $p_{data}(\boldsymbol{x})$
  - Symmetry of JSD
    - Does not affect the behavior of mode missing

$$\mathrm{KL}\left(p_{g_\theta}(x) \,||\, q^r(x|y=0)\right) = \int p_{g_\theta}(x) \log \frac{p_{g_\theta}(x)}{q^r(x|y=0)} dx$$

- **Large positive contribution to the KLD in the regions of x space where $q^r(x|y=0)$ is small, unless $p_{g_\theta}(x)$ is also small**
- **$\Rightarrow p_{g_\theta}(x)$ tends to avoid regions where $q^r(x|y=0)$ is small**

Figure: Blue: prior distribution of real data, Green: posterior distribution of the synthetic data, Red: variational distribution of synthetic data.

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[9] You won't pop up unless you have adequate samples.

VAE New Formulation

VAE: maximizing the variational lower bound:

$$\mathcal{L}(\theta, \phi; \mathbf{x}) = \mathbb{E}_{p_{data}(\mathbf{x})}\left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}, \mathbf{z})] - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))\right]$$

To align VAE with GAN, we introduce the real/fake indicator y and adversarial discriminator.

Beside $\mathbf{x}$ the code / observation / example /etc., and $\mathbf{z}$ the hidden state / latent representation, we introduce y, together with a perfect discriminator $q_*(y|\mathbf{x})$.

$$q_*(y = 1|\mathbf{x}) = 1 \text{ if } \mathbf{x} \text{ is real}$$
$$q_*(y = 0|\mathbf{x}) = 1 \text{ if } \mathbf{x} \text{ is generated}$$

and also a generative distribution: [10]

$$p_\theta(\mathbf{x}|\mathbf{z}, y) = \begin{cases} p_\theta(\mathbf{x}|\mathbf{z}) & y = 0 \\ p_{data}(\mathbf{x}) & y = 1 \end{cases}$$

[10] This format is similar to InfoGAN.

Also, let the posterior $p_\theta(\mathbf{z}, y|\mathbf{x}) \propto p_\theta(\mathbf{z}, y|\mathbf{x})p(\mathbf{z}|y)p(y)$: [11]

Lemma (New Objective of VAE at (θ_0, ϕ_0))

$$\begin{aligned}\mathcal{L}(\theta,\phi;\mathbf{x}) =&\mathbb{E}_{p_{data}(\mathbf{x})}\left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x},\mathbf{z})] - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))\right]\\ =&2\mathbb{E}_{p_{\theta_0}(\mathbf{x})}\left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x},y)q^r_*(y|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z},y)]\right.\\ &\left.- \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x},y)q^r_*(y|\mathbf{x})||p(\mathbf{z}|y)p(y))\right]\\ =&2\mathbb{E}_{p_{\theta_0}(\mathbf{x})}\left[- \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x},y)q^r_*(y|\mathbf{x})||p(\mathbf{z},y|\mathbf{x}))\right]\end{aligned}$$

[11] $p(\cdot)$ are fixed priors.

The KLD to minimize for VAE is:

$$\mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}, y)q_*^r(y|\mathbf{x})||p(\mathbf{z}, y|\mathbf{x}))$$

Recall that in the new form of GAN, the KLD to minimize:

$$\mathrm{KL}(p_\theta(\mathbf{x}|y)||q^r(\mathbf{x}|y))$$

There is a major difference here: GANs KL term does $\min_\theta(P_\theta||Q)$ and VAEs does $\min_\theta(Q||P_\theta)$. [12]

- GANs: $\min_\theta(P_\theta||Q)$ tends to missing mode, ignoring regions with small values of p_{data};
- VAEs: $\min_\theta(Q||P_\theta)$ tends to cover regions with small values of p_{data}.

[12] KLD Asymmetry inspires combination of GANs and VAEs.

Linking VAE to Wake-Sleep

Recall Wake Sleep: two loss-functions are used.

$$\text{Wake:} \quad \min_{\theta} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})p_{data}(\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$$

$$\text{Sleep:} \quad \min_{\phi} \mathbb{E}_{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}[\log(q_\phi(\mathbf{z}|\mathbf{x}))]$$

Recall VAEs objective to minimize:

$$\mathcal{L}(\theta, \phi; \mathbf{x}) = \mathbb{E}_{p_{data}(\mathbf{x})}\left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}, \mathbf{z})] - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))\right]$$

VAE only needs the wake phase, does not need the sleep phase, and thus doesn't need the reverse-KLD trick. Stick to minimizing the wake phase KLD w.r.t. θ, ϕ.

Linking GAN to Wake-Sleep

Wake Sleep: two loss-functions are used.

$$\text{Wake:}\quad \min_{\theta} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})p_{data}(\mathbf{x})}[\log(p_\theta(\mathbf{x}|\mathbf{z}))]$$

$$\text{Sleep:}\quad \min_{\phi} \mathbb{E}_{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}[\log(q_\phi(\mathbf{z}|\mathbf{x}))]$$

Recall GANs objective:

$$\max_{\phi} \mathcal{L}_\phi = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi(y|\mathbf{x}))]$$

$$\max_{\theta} \mathcal{L}_\theta = \mathbb{E}_{p_\theta(\mathbf{x}|y)p(y)}[\log(q_\phi^r(y|\mathbf{x}))]$$

GAN is directly extending sleep phase, only difference is $q_\theta \to q_\theta^r$. Stick to minimizing the sleep-phase KLD.

DGMs have a long history, and is a big family.

Unification of the different DGMs is possible & useful.

- GANs and VAEs are essentially minimizing KLD in opposite directions and extend two phases of classic wake sleep algorithm, respectively;
- The general formulation is useful for analyzing a broad class of existing DGM models, and can inspire new models and algorithms.

Applications

GAN Progress

- It is trending because of its outstanding performance.
- Vanilla GAN [Goodfellow et al,. 2014] objective:

$$\min_{\theta} \mathrm{JSD}(P_{\mathrm{data}} || P_{g_\theta})$$

  - Note: this expression is symbolic, not executable.
- Unifying version [Hu et al. 2017] objective:

$$\min_{\theta} \mathrm{KL}(P_{\theta} || Q)$$

Wasserstein GAN (WGAN): Motivation

Shortcoming of KLD: for $\mathrm{KL}(P||Q)$ if P and Q have neglectable overlap, then the KLD is degenerated, meaningless. Sometimes it becomes undefined or infinite, messing up the loss. [13]

In practice: if our data is a low-dimensional manifold of a high dimensional space, there can be a **negligible** intersection between the model's manifold and the true data manifold.

[13] Similar shortcoming applies to JSD.

Shortcoming of KLD: for $\mathrm{KL}(P||Q)$ if P and Q have neglectable overlap, then the KLD is degenerated, meaningless. Sometimes it becomes undefined or infinite, messing up the loss. [13]

In practice: if our data is a low-dimensional manifold of a high dimensional space, there can be a **negligible** intersection between the model's manifold and the true data manifold.

The loss function is re-defined via **Wasserstein Distance**.

- Well-defined in math, a.k.a Earth Mover's Distance;
- Minimum transportation cost for making pile of dirt in shape of one probability distribution to the other.

[13] Similar shortcoming applies to JSD.

Wasserstein GAN (WGAN) [14]

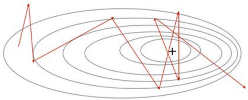
Wasserstein GAN (WGAN)

- Objective

$$W(p_{data}, p_g) = \frac{1}{K} \sup_{||D||_L \leq K} \mathrm{E}_{x \sim p_{data}}[D(x)] - \mathrm{E}_{x \sim p_g}[D(x)]$$

- $||D||_L \leq K$: K- Lipschitz continuous
- Use gradient-clipping to ensure D has the Lipschitz continuity

Without gradient clipping   With gradient clipping



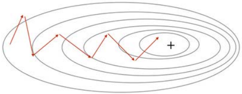


Figure: Lipschitz continuous: intuitively limited in how fast it can change, previously learned with convex optimization.

[14] [Arjovsky et al., 2017]

Progressive GAN [15]

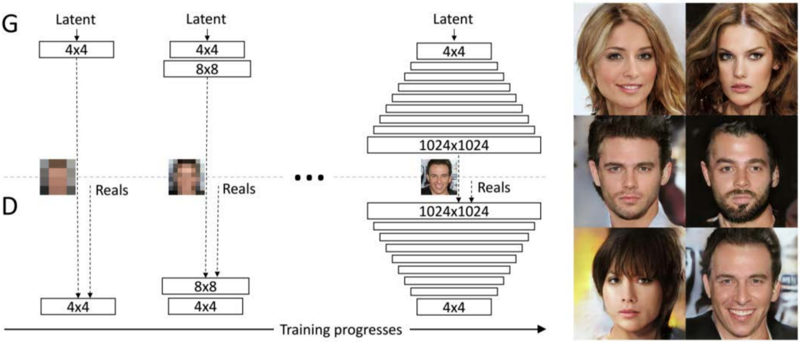


Figure: Ideas: Begin with very low-resolution images and very shallow G, D. As training goes on, add additional layers to G & D, and use higher resolution images. By-passing the size bottleneck by not having to train the whole network at once.

[15] [Karras et al., 2018]

BigGAN [16]

GANs benefit dramatically from scaling.

They put efforts in scaling up GANs.

- $2-4$ times more parameters to improve expressiveness;
- $8\times$ larger batch size to avoid overfitting;
- Simple architecture changes that improve scalability.

[16] [Brock et al., 2018]

Normalizing Flow (NF): Basic Concepts

Idea: to amplify / transform an originally very simple model into something more complex / powerful; to transform a simple distribution into an arbitrarily complex one.

Method: applying a sequence of invertible transformation functions. [17]

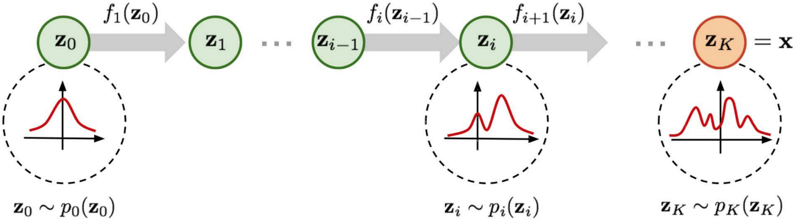


Figure: Figure from Prof. Xing's lecture slides, Figure courtesy: Lilian Weng.

[17] Libraries do that all the time, e.g. Uniform → Gaussian.

Normalizing Flow (NF): Single Transform

Starting from $\mathbf{z} \sim p(\mathbf{z})$, given transformation function f, generating $\mathbf{x} = f(\mathbf{z})$.

- To do inference we need $\mathbf{z} = f^{-1}(\mathbf{x})$, thus need f to be invertible.
- To compute density we have:

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

  and there are tricks of making the **Jacobian determinant** $\det \frac{\mathrm{d}f^{-1}}{\mathrm{d}\mathbf{x}}$ easy to compute, e.g. making $\frac{\mathrm{d}f^{-1}}{\mathrm{d}\mathbf{x}}$ a triangular matrix.

Normalizing Flow (NF): Sequence

$$
\begin{aligned}
&\mathbf{z}_0 \sim p(\mathbf{z}_0) \\
&\mathbf{x} = \mathbf{z}_K = f_K \circ f_{K-1} \circ \cdots \circ f_1(\mathbf{z}_0) \\
\text{inference: } &\mathbf{z}_i = f_i^{-1}(\mathbf{z}_{i-1}) \\
\text{density: } &p(\mathbf{z}_i) = p(\mathbf{z}_{i-1}) \left| \det \frac{\mathrm{d}\mathbf{z}_{i-1}}{\mathrm{d}\mathbf{z}_i} \right|
\end{aligned}
$$

While training, we maximize the log likelihood:

$$
\log p(\mathbf{x}) = \log p(\mathbf{z}_0) + \sum_{i=1}^{K} \log \left| \det \frac{\mathrm{d}\mathbf{z}_{i-1}}{\mathrm{d}\mathbf{z}_i} \right|
$$

Making the **Jacobian determinant** easy to compute by choosing $\frac{\mathrm{d}f_i^{-1}}{\mathrm{d}\mathbf{z}_i}$ to be triangular matrix.

NF example: GLOW [18]

One step of flow in the Glow model go passes the layers:

- activation normalization;
- invertible 1×1 convolutional;
- affine coupling.

Small building block of potentially big architectures.

Not as powerful as GAN, but cheap, easy to compute.

[18] [Kingma and Dhariwal., 2018]

Integrating Domain Knowledge into Deep Learning

Motivation: Deep Learning has some disadvantages by itself.

- Heavily rely on massive labeled data;
- Uninterpretable;
- Hard to encode human intention and domain knowledge.

Human learning:

- Learn from concrete examples (similar to deep learning models)
- Learn from abstract knowledge (definitions, logic rules, etc)

Consider a statistical model $\mathbf{x} \sim p_\theta(\mathbf{x})$, it could be conditional model, generative model, discriminative model, etc.

Consider a constraint function $f_\phi(\mathbf{x}) \in \mathbb{R}$.

- The higher $f_\phi(\mathbf{x})$ is, the better quality $\mathbf{x}$ has w.r.t. knowledge.

Image example:

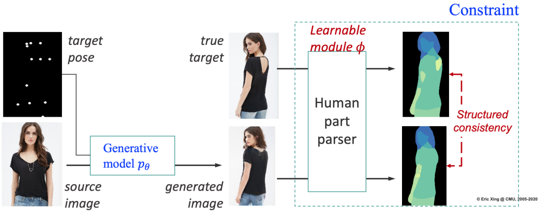


Figure: An example of using real pose as knowledge.

Sentiment classification example:

- "This was a terrific movie, but the director could have done better."
- Logical Rules: Sentence S with structure A-but-B $\Rightarrow$ sentiment of B dominates.

One way to impose the constraint is to maximize $\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]$, which means, adding a regularization term to the objective:

$$\min_\theta \mathcal{L}(\theta) - \alpha \mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]$$

It is **difficult** to compute $\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]$. Because when we compute the derivative $\frac{\mathrm{d}\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]}{\mathrm{d}\theta}$, we use the log probability trick (always the case when deriving expectation over distribution). In the end we'll have a term that is the log probability itself (and something else) — that term will explode, high variance, extremely unstable. (Recall: Wake-Sleep's Sleep phase.)

A variational approximation [19] to ease the computation of $\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]$ is to use $q(\mathbf{x})$ to approximate $p_\theta(\mathbf{x})$.

$$\mathcal{L}(\theta, q) = \mathrm{KL}(q(\mathbf{x}) || p_\theta(\mathbf{x})) - \lambda \mathbb{E}_q[f_\phi(\mathbf{x})]$$

It introduces variational distribution q:

- Impose constraint f_ϕ on q;
- Encourage q to stay close to p_θ.

The objective of data-driven and knowledge-driven combination:

$$\min_{\theta, q} \mathcal{L}(\theta) - \alpha \mathcal{L}(\theta, q)$$

[19] Called a Posterior Regularization [Ganchev et al., 2010].

Learning with Constraints

$$\min_{\theta, q} \mathcal{L}(\theta) - \alpha \mathcal{L}(\theta, q)$$

$$\mathcal{L}(\theta, q) = \mathrm{KL}(q(\mathbf{x}) || p_\theta(\mathbf{x})) - \lambda \mathbb{E}_q [f_\phi(\mathbf{x})]$$

One way to learn via EM algorithm:

- E-Step: $q^*(\mathbf{x}) = p_\theta(\mathbf{x}) \exp\{\lambda_\phi(\mathbf{x})\}/Z$
  - This approach is known as a soft constraint. Higher value of λ_ϕ, higher probability under q.
- M-Step: $\min_\theta \mathcal{L}(\theta) - \mathbb{E}_{q^*}[\log p_\theta(\mathbf{x})]$

Logical Rule Constraints [20]

Consider a supervised learning: $p_\theta(\mathbf{y}|\mathbf{x})$ and Input-Target space $(\mathbf{X}, \mathbf{Y})$, with first-order logic rules: (r, λ)

- $r(\mathbf{X}, \mathbf{Y}) \in [0, 1]$ could be soft;
- λ is the confidence level of the rule.

Given l rules:

- E-Step: $q^*(\mathbf{y}|\mathbf{x}) = p_\theta(\mathbf{x}) \exp \left\{ \sum_l \lambda_l r_l(\mathbf{y}|\mathbf{x}) \right\} / Z$
  - Current version of p_θ with all rule constraints.
- M-Step: $\min_\theta \mathcal{L}(\theta) - \mathbb{E}_{q^*}[\log p_\theta(\mathbf{y}|\mathbf{x})]$

Similar efforts were made by Hinton: Knowledge Distillation.

[20] [Hu et al., 2016]

Knowledge Distillation [21]

Student network: $p_\theta(\mathbf{y}|\mathbf{x})$ (difficult to learn)

- Typically contains only takes labeled data.

Teacher network: $q^*(\mathbf{y}|\mathbf{x})$

- Auxiliary, variational approximation, etc.
- Designed to be ensemble, take labeled data, but could possibly take unlabeled data as well.

Match **soft** predictions (not just 0 or 1) of the teacher network and student network.

- Train the teachers in one step, train the student to imitate the outputs of teacher network in another step.
- Will eventually get student closer to some / one / average of the teachers.

[21] [Hinton et al., 2015; Bucilu et al., 2006]

Rule Knowledge Distillation [22]

Teacher network is rule-regularized. Recall the previous E-Step:

$$p^*(\mathbf{y}|\mathbf{x}) = p_\theta(\mathbf{x}) \exp\left\{\sum_l \lambda_l r_l(\mathbf{y}|\mathbf{x})\right\}/Z$$

The results from teacher network are soft, including both p_θ and logic rules constraints: $\mathbf{s}_n^{(t)}$ (n is the sample index, t is the current iteration).

There is also a ground truth label: $\mathbf{y}_n$. Student output is $\sigma_\theta(\mathbf{x}_n)$.

At iteration t ($\pi \in [0, 1]$ is a balancing parameter):

$$\theta^{(t+1)} = \arg\min_{\theta \in \Theta} \frac{1}{N} \sum_{n=1}^{N} (1 - \pi)\ell(\mathbf{y}_n, \sigma_\theta(\mathbf{x}_n)) + \pi\ell(\mathbf{s}_n^{(t)}, \sigma_\theta(\mathbf{x}_n))$$

[22] [Hu et al., 2016]

More on learning rules / constraints:

- Teacher / student network structures.
- Learn the confidence value λ_l of each rule. [Hu et al., 2016b]
- More generally, optimize parameters of the constraint $f_\phi(\mathbf{x})$. [Hu et al., 2018]
- Teachers can reach beyond the scope of logical rules. Possible to make the reward function of reinforcement learning as a type of teaching function.
  - From this perspective, reinforcement learning becomes an instance of knowledge-driven machine learning.
  - See keyword: **variational reinforcement learning**.

Generative Adversarial Networks (GANs)

- Wasserstein GAN: new learning objectives
- Progressive GAN: new training schedule
- BigGAN: scaling up GAN models

Normalizing Flow (NF)

- Chained transformation functions
- Exact latent inference, density evaluation, sampling

Integrating Domain Knowledge into Deep Learning

- Domain knowledge as constraint
- Learning rules / constraints