Variants and Combinations of Basic Models

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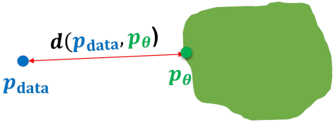
Lecture 12

Summary

$\mathbf{x}^{(j)} \sim p_{\text{data}}$
$j = 1, 2, \ldots, |\mathcal{D}|$



$\theta \in \mathcal{M}$

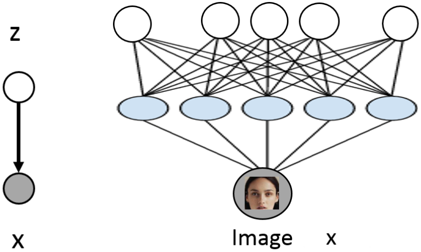
Model family

Story so far

- Representation: Latent variable vs. fully observed
- Objective function and optimization algorithm: Many divergences and distances optimized via likelihood-free (two sample test) or likelihood based methods
- Each have Pros and Cons

Plan for today: Combining models

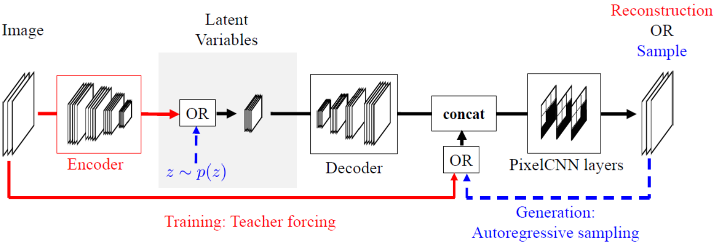
Variational Autoencoder



A mixture of an infinite number of Gaussians:

1. $\mathbf{z} \sim \mathcal{N}(0, I)$
2. $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}\left(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z})\right)$ where μ_θ,Σ_θ are neural networks
3. $p(\mathbf{x} \mid \mathbf{z})$ and $p(\mathbf{z})$ usually simple, e.g., Gaussians or conditionally independent Bernoulli vars (i.e., pixel values chosen independently given $\mathbf{z}$)
4. **Idea**: increase complexity using an autoregressive model

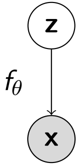
PixelVAE (Gulrajani et al.,2017)



Gulrajani et. al, 2017

- $\mathbf{z}$ is a feature map with the same resolution as the image $\mathbf{x}$
- Autoregressive structure: $p(\mathbf{x} \mid \mathbf{z}) = \prod_i p(x_i \mid x_1, \cdots, x_{i-1}, \mathbf{z})$
    - $p(\mathbf{x} \mid \mathbf{z})$ is a PixelCNN
    - Prior $p(\mathbf{z})$ can also be autoregressive
    - Can be hierarchical: $p(\mathbf{x} \mid \mathbf{z}_1)p(\mathbf{z}_1 \mid \mathbf{z}_2)$
- State-of-the art log-likelihood on some datasets; learns features (unlike PixelCNN); computationally cheaper than PixelCNN (shallower)

Autoregressive flow

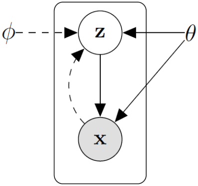


- Flow model, the marginal likelihood $p(\mathbf{x})$ is given by

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

  where $p_Z(\mathbf{z})$ is typically simple (e.g., a Gaussian). More complex prior?
- Prior $p_Z(\mathbf{z})$ can be autoregressive $p_Z(\mathbf{z}) = \prod_i p(z_i \mid z_1, \cdots, z_{i-1})$.
- Autoregressive models are flows. Just another MAF layer.
- See also neural autoregressive flows (Huang et al., ICML-18)

VAE + Flow Model

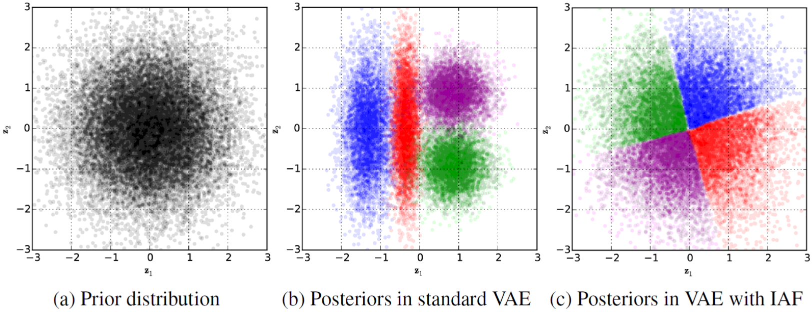


$$\log p(\mathbf{x};\theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x};\phi)\log p(\mathbf{z},\mathbf{x};\theta) + H(q(\mathbf{z}|\mathbf{x};\phi)) = \underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}}$$

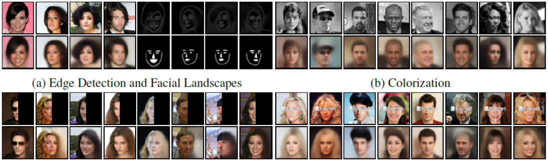
$$= \mathcal{L}(\mathbf{x};\theta,\phi) + \underbrace{D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))}_{\text{Gap between true log-likelihood and ELBO}}$$

- $q(\mathbf{z}|\mathbf{x};\phi)$ is often too simple (Gaussian) compared to the true posterior $p(\mathbf{z}|\mathbf{x};\theta)$, hence ELBO bound is loose
- **Idea:** Make posterior more flexible: $\mathbf{z}' \sim q(\mathbf{z}'|\mathbf{x};\phi)$, $\mathbf{z} = f_{\phi'}(\mathbf{z})$ for an invertible $f_{\phi'}$ (Rezende and Mohamed, 2015; Kingma et al., 2016)
- Still easy to sample from, and can evaluate density.

VAE + Flow Model



Posterior approximation is more flexible, hence we can get tighter ELBO (closer to true log-likelihood).

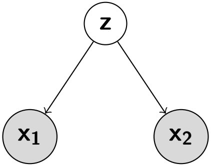


(a) Edge Detection and Facial Landscapes (b) Colorization

(c) Fill in the Blank (d) Removing Watermarks

Wu and Goodman, 2018

- **Goal:** Learn a joint distribution over the two domains $p(x_1, x_2)$, e.g., color and gray-scale images Can use a VAE style model:

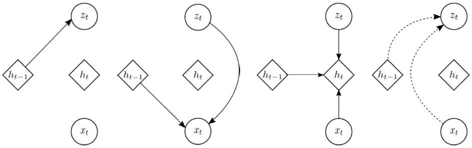


- Learn $p_\theta(x_1, x_2)$, use inference nets $q_\phi(z \mid x_1)$, $q_\phi(z \mid x_2)$, $q_\phi(z \mid x_1, x_2)$. Conceptually similar to semi-supervised VAE in HW2.

Variational RNN

- **Goal:** Learn a joint distribution over a sequence $p(x_1, \cdots, x_T)$
- VAE for sequential data, using latent variables $z_1, \cdots, z_T$. Instead of training separate VAEs $z_i \to x_i$, train a joint model:

$$p(x_{\leq T}, z_{\leq T}) = \prod_{t=1}^{T} p(x_t \mid z_{\leq t}, x_{<t}) p(z_t \mid z_{<t}, x_{<t})$$

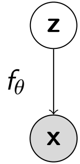


(a) Prior (b) Generation (c) Recurrence (d) Inference

Chung et al, 2016

- Use RNNs to model the conditionals (similar to PixelRNN)
- Use RNNs for inference $p(z_{\leq T} | x_{\leq T}) = \prod_{t=1}^{T} q(z_t \mid z_{<t}, x_{\leq t})$
- Train like VAE to maximize ELBO. Conceptually similar to PixelVAE.

Combining losses

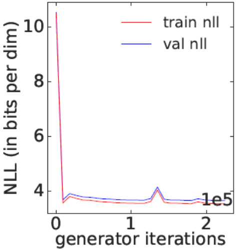


- Flow model, the marginal likelihood $p(\mathbf{x})$ is given by

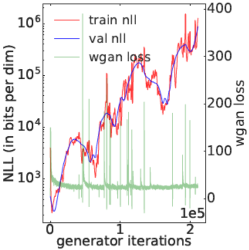
$$p_X(\mathbf{x};\theta) = p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

- Can also be thought of as the generator of a GAN
- Should we train by $\min_\theta D_{KL}(p_{data}, p_\theta)$ or $\min_\theta JSD(p_{data}, p_\theta)$?

FlowGAN



(a) MLE

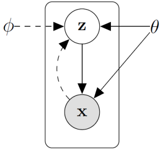


(b) ADV

Although $D_{KL}(p_{data}, p_\theta) = 0$ if and only if $JSD(p_{data}, p_\theta) = 0$, optimizing one does not necessarily optimize the other. If $\mathbf{z}, \mathbf{x}$ have same dimensions, can optimize $\min_\theta KL(p_{data}, p_\theta) + \lambda JSD(p_{data}, p_\theta)$

Objective	Inception Score	Test NLL (in bits/dim)
MLE	2.92	**3.54**
ADV	**5.76**	8.53
Hybrid ($\lambda = 1$)	3.90	4.21

Adversarial Autoencoder (VAE + GAN)



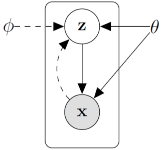
$$\log p(\mathbf{x};\theta) = \underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}} + D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))$$

$$\underbrace{E_{\mathbf{x}\sim p_{data}}[\mathcal{L}(\mathbf{x};\theta,\phi)]}_{\approx\text{training obj.}} = E_{\mathbf{x}\sim p_{data}}[\log p(\mathbf{x};\theta) - D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))]$$

$$\overset{\text{up to const.}}{\equiv} -\underbrace{D_{KL}(p_{data}(\mathbf{x}) \| p(\mathbf{x};\theta))}_{\text{equiv. to MLE}} - E_{\mathbf{x}\sim p_{data}}[D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))]$$

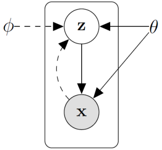
- Note: regularized maximum likelihood estimation
- Can add in a GAN objective $-JSD(p_{data}, p(\mathbf{x};\theta))$ to get sharper samples, i.e., discriminator attempting to distinguish VAE samples from real ones.

An alternative interpretation



$$
\begin{aligned}
\underbrace{E_{\mathbf{x}\sim p_{data}}[\mathcal{L}(\mathbf{x};\theta,\phi)]}_{\approx\text{training obj.}} &= E_{\mathbf{x}\sim p_{data}}\left[\log p(\mathbf{x};\theta) - D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))\right] \\
&\overset{\text{up to const.}}{\equiv} -D_{KL}(p_{data}(\mathbf{x})\|p(\mathbf{x};\theta)) - E_{\mathbf{x}\sim p_{data}}\left[D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))\right] \\
&= -\sum_{\mathbf{x}} p_{data}(\mathbf{x})\left(\log\frac{p_{data}(\mathbf{x})}{p(\mathbf{x};\theta)} + \sum_{\mathbf{z}} q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{q(\mathbf{z}\mid\mathbf{x};\phi)}{p(\mathbf{z}|\mathbf{x};\theta)}\right) \\
&= -\sum_{\mathbf{x}} p_{data}(\mathbf{x})\left(\sum_{\mathbf{z}} q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{q(\mathbf{z}\mid\mathbf{x};\phi)p_{data}(\mathbf{x})}{p(\mathbf{z}|\mathbf{x};\theta)p(\mathbf{x};\theta)}\right) \\
&= -\sum_{\mathbf{x},\mathbf{z}} p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)} \\
&= -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)}\,\|\,\underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)})
\end{aligned}
$$

An alternative interpretation

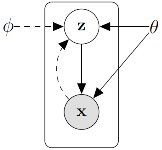


$$E_{\mathbf{x}\sim p_{data}}[\underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}}] \equiv -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \| \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)})$$

- Optimizing ELBO is the same as matching the inference distribution $q(\mathbf{z},\mathbf{x};\phi)$ to the generative distribution $p(\mathbf{z},\mathbf{x};\theta) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z};\theta)$
- **Intuition**: $p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta) = p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)$ if
  1. $p_{data}(\mathbf{x}) = p(\mathbf{x};\theta)$
  2. $q(\mathbf{z}\mid\mathbf{x};\phi) = p(\mathbf{z}|\mathbf{x};\theta)$ for all $\mathbf{x}$
  3. Hence we get the VAE objective:
     $-D_{KL}(p_{data}(\mathbf{x})\|p(\mathbf{x};\theta)) - E_{\mathbf{x}\sim p_{data}}[D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))]$
- Many other variants are possible! VAE + GAN:

$$-JSD(p_{data}(\mathbf{x})\|p(\mathbf{x};\theta)) - D_{KL}(p_{data}(\mathbf{x})\|p(\mathbf{x};\theta)) - E_{\mathbf{x}\sim p_{data}}[D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))]$$

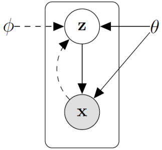
Adversarial Autoencoder (VAE + GAN)



$$E_{\mathbf{x}\sim p_{data}}\underbrace{[\mathcal{L}(\mathbf{x};\theta,\phi)]}_{\text{ELBO}} \equiv -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \,\|\, \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)})$$

- Optimizing ELBO is the same as matching the inference distribution $q(\mathbf{z},\mathbf{x};\phi)$ to the generative distribution $p(\mathbf{z},\mathbf{x};\theta)$
- **Symmetry:** Using alternative factorization: $p(\mathbf{z})p(\mathbf{x}|\mathbf{z};\theta) = q(\mathbf{z};\phi)q(\mathbf{x}\mid\mathbf{z};\phi)$ if
  1. $q(\mathbf{z};\phi) = p(\mathbf{z})$
  2. $q(\mathbf{x}\mid\mathbf{z};\phi) = p(\mathbf{x}|\mathbf{z};\theta)$ for all $\mathbf{z}$
  3. We get an *equivalent* form of the VAE objective: $-D_{KL}(q(\mathbf{z};\phi)\|p(\mathbf{z})) - E_{\mathbf{z}\sim q(\mathbf{z};\phi)}[D_{KL}(q(\mathbf{x}\mid\mathbf{z};\phi)\|p(\mathbf{x}|\mathbf{z};\theta))]$
- Other variants are possible. For example, can add $-JSD(q(\mathbf{z};\phi)\|p(\mathbf{z}))$ to match features in latent space (Zhao et al., 2017; Makhzani et al, 2018)

Information Preference



$$E_{\mathbf{x} \sim p_{data}}[\underbrace{\mathcal{L}(\mathbf{x}; \theta, \phi)}_{\text{ELBO}}] \equiv -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z} \mid \mathbf{x}; \phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \,\|\, \underbrace{p(\mathbf{x}; \theta)p(\mathbf{z}|\mathbf{x}; \theta)}_{p(\mathbf{z},\mathbf{x};\theta)})$$

- ELBO is optimized as long as $q(\mathbf{z}, \mathbf{x}; \phi) = p(\mathbf{z}, \mathbf{x}; \theta)$. Many solutions are possible! For example,
  1. $p(\mathbf{z}, \mathbf{x}; \theta) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}; \theta) = p(\mathbf{z})p_{data}(\mathbf{x})$
  2. $q(\mathbf{z}, \mathbf{x}; \phi) = p_{data}(\mathbf{x})q(\mathbf{z}|\mathbf{x}; \phi) = p_{data}(\mathbf{x})p(\mathbf{z})$
  3. Note $\mathbf{z}$ and $\mathbf{z}$ are independent. $\mathbf{z}$ carries no information about $\mathbf{x}$. This happens in practice when $p(\mathbf{x}|\mathbf{z}; \theta)$ is too flexible, like PixelCNN.
- **Issue:** Many more variables than constraints

Information Maximizing

- Explicitly add a mutual information term to the objective

$$-D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z} \mid \mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \parallel \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)}) + \alpha MI(\mathbf{x},\mathbf{z})$$

- MI intuitively measures how far $\mathbf{x}$ and $\mathbf{z}$ are from being independent

$$MI(\mathbf{x},\mathbf{z}) = D_{KL}\left(p(\mathbf{z},\mathbf{x};\theta) \| p(\mathbf{z})p(\mathbf{x};\theta)\right)$$

- InfoGAN (Chen et al, 2016) used to learn meaningful (disentangled?) representations of the data

$$MI(\mathbf{x},\mathbf{z}) - E_{\mathbf{x}\sim p_\theta}[D_{KL}(p_\theta(\mathbf{z}|\mathbf{x})\|q_\phi(\mathbf{z}|\mathbf{x}))] - JSD(p_{data}(\mathbf{x})\|p_\theta(\mathbf{x}))$$

(a) Azimuth (pose) (b) Elevation

(c) Lighting (d) Wide or Narrow

β-VAE

Model proposed to learn disentangled features (Higgins, 2016)

$$-E_{q_\phi(\mathbf{x},\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] + \beta E_{\mathbf{x}\sim p_{data}}\left[D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))\right]$$

It is a VAE with scaled up KL divergence term. This is equivalent (up to constants) to the following objective:

$$(\beta-1)MI(\mathbf{x};\mathbf{z}) + \beta D_{KL}(q_\phi(\mathbf{z})\|p(\mathbf{z}))) + E_{q_\phi(\mathbf{z})}[D_{KL}(q_\phi(\mathbf{x}|\mathbf{z})\|p_\theta(\mathbf{x}|\mathbf{z}))]$$

See *The Information Autoencoding Family: A Lagrangian Perspective on Latent Variable Generative Models* for more examples.

Conclusion

- We have covered several useful building blocks: autoregressive, latent variable models, flow models, GANs.
- Can be combined in many ways to achieve different tradeoffs: many of the models we have seen today were published in top ML conferences in the last couple of years
- Lots of room for exploring alternatives in your projects!
- Which one is best? Evaluation is tricky. Still largely empirical