Deep generative modeling

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Plan for this lecture

1. Introduction and motivation
2. Generative adversarial networks
3. Variational autoencoders
4. Autoregressive models
Success stories of deep learning in recent years

- Convolutional neural networks
- For stationary signals such as audio, images, and video
- Applications: Object detection, semantic segmentation, image retrieval, pose estimation, ...
Success stories of deep learning in recent years

- Convolutional neural networks
- For stationary signals such as audio, images, and video
- Applications: Object detection, semantic segmentation, image retrieval, pose estimation, ...
Success stories of deep learning in recent years

▶ Recurrent neural networks

▶ For variable length sequence data, e.g. in natural language

▶ Applications: Machine translation, image captioning, speech recognition, ...

Example from Ilya Sutskever
It’s all about the features
It’s all about the features

- Conventional vision / audio processing approach
  1. Features (engineered): SIFT, MFCC, …
  2. Pooling (unsupervised): bag-of-words, Fisher vectors, …
  3. Recognition (supervised): linear/kernel classifier, …

Image from [Chatfield et al., 2011]
It’s all about the features

- Deep learning blurs boundary feature / classifier
  - Stacks simple non-linear transformations
  - Learns progressively more abstract representation
  - Starts from raw input signal, e.g. image pixels
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- End-to-end training to minimize a task-specific loss

- Supervised learning from lots of labeled data
Motivations for unsupervised (deep) learning

1. Improve supervised learning from few samples
   ▶ Unlabeled data often abundantly available
   ▶ Learn representations/features from unlabeled data

2. Generative models for image and other complex data
   ▶ Unconditional: sandbox research problem (?)
   ▶ Conditional structured prediction: in-painting, colorization, text-to-image, video forecasting, etc.

Image colorization [Royer et al., 2017]
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Image colorization [Royer et al., 2017]
(Un)supervised learning and un(conditional) models
(Un)supervised learning and un(conditional) models

- **Supervised learning**: model conditional distribution $p_\theta(y|x)$
  - For example: $x$ an image, $y$ a class label
  \[
  \max_\theta \sum_{(x,y) \sim \mathcal{D}} \ln p_\theta(y|x) \tag{1}
  \]
  - $\mathcal{D}$: data generating distribution
  - $\theta$: model parameters
(Un)supervised learning and un(conditional) models

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- $\mathcal{D}$: data generating distribution
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- **Unsupervised learning**: model unconditional distribution $p(x)$
  - For example: $x$ an image

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\max_\theta \sum_{x \sim \mathcal{D}} \ln p_\theta(x)
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Self-supervised learning

- Learning conditional models $p(y|x)$ from unlabeled data
Self-supervised learning

- Learning conditional models $p(y|x)$ from unlabeled data
- Prediction of structural data properties
  - Skip-gram language models (word2vec) [Mikolov et al., 2013]

![Skip-gram diagram]

Skip-gram
Self-supervised learning

- Learning conditional models $p(y|x)$ from unlabeled data
- Prediction of structural data properties
  - Skip-gram language models (word2vec) [Mikolov et al., 2013]
  - Relative position of image patches [Doersch et al., 2015]
Self-supervised learning

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  - Relative ordering of video frames [Fernando et al., 2017]

```
X = (w(t-2), w(t-1), w(t+1), w(t+2)); Y = 3
```
Self-supervised learning

- Learning **conditional models** $p(y|x)$ from unlabeled data

- Prediction of structural data properties
  - Skip-gram language models (word2vec) [Mikolov et al., 2013]
  - Relative position of image patches [Doersch et al., 2015]
  - Relative ordering of video frames [Fernando et al., 2017]
  - Image inpainting [Pathak et al., 2016]
  - ...
Self-supervised learning to prime supervised learning

- Supervised pre-training of network on proxy-task
- Fine-tune on final task with limited training data

Example: features for action recognition
[Fernando et al., 2017]

- Unsupervised representation learning
- Does not allow to sample data from model
Self-supervised learning to prime supervised learning

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<tr>
<th>Method</th>
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<tbody>
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- Unsupervised **representation learning**

- Does not allow to sample data from model
Generative models

- Unconditional density model $p_\theta(x)$
- Parameters estimated from unlabeled data
- Possible to draw samples from model

Samples from ImageNet dataset (left) and GAN model (right), figure from OpenAI
My first generative model

- Gaussian mixture model

\[
p(z = k) = \pi_k \quad (3)
\]
\[
p(x | z = k) = \mathcal{N}(x; \mu_k, \sigma I_D) \quad (4)
\]

\[
p(x) = \sum_z p(z)p(x | z) \quad (5)
\]

Figure from [Bishop, 2006]
My first generative model

- Gaussian mixture model

\[ p(z = k) = \pi_k \]  \hspace{1cm} (3)

\[ p(x|z = k) = \mathcal{N}(x; \mu_k, \sigma I_D) \]  \hspace{1cm} (4)

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- Estimation: Expectation-Maximization (EM) algorithm

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- Estimation: Expectation-Maximization (EM) algorithm

- Sampling: pick component from prior distribution \( p(z) \),
  then draw sample from conditional distribution \( p(x | z) \)
My second generative model

- Probabilistic Principal Component Analysis
  [Roweis, 1997, Tipping and Bishop, 1999]

\[
p(z) = \mathcal{N}(z; 0, I_d) \quad (6)
\]

\[
p(x|z) = \mathcal{N}(x; \mu + Wz, \sigma I_D) \quad (7)
\]

\[
p(x) = \int_z p(z)p(x|z) \quad (8)
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Figure from [Bishop, 2006]
My second generative model

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- Estimation: SVD or EM algorithm

Figure from [Bishop, 2006]
My second generative model

- **Probabilistic Principal Component Analysis**
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- Estimation: SVD or EM algorithm

- Sampling: pick point in subspace from prior \( p(z) \), then draw sample from conditional distribution \( p(x|z) \)

Figure from [Bishop, 2006]
Linear latent variable models

- Linear transformation of latent variable
  - PCA: $z$ from unit Gaussian
  - GMM: $z$ random 1-hot vector

$$\hat{x} = Wz + \mu \quad (9)$$
Linear latent variable models

- **Linear transformation** of latent variable
  - PCA: $z$ from unit Gaussian
  - GMM: $z$ random 1-hot vector

$$\hat{x} = Wz + \mu \quad (9)$$

- Gaussian noise makes support non-degenerate in data space

$$p(x|\hat{x}) = \mathcal{N}(x; \hat{x}, \sigma I_D) \quad (10)$$
Linear latent variable models

- **Linear transformation** of latent variable
  - PCA: $z$ from unit Gaussian
  - GMM: $z$ random 1-hot vector

\[ \hat{x} = Wz + \mu \quad (9) \]

- Gaussian noise makes support non-degenerate in data space

\[ p(x|\hat{x}) = \mathcal{N}(x; \hat{x}, \sigma I_D) \quad (10) \]

- Negative log-likelihood gives $\ell_2$ “reconstruction” loss of PCA and k-means

\[ -\ln p(x|\hat{x}) = ||x - \hat{x}||_2^2 \quad (11) \]
Non-linear latent variable models

- Simple distribution $p(z)$ on latent variable $z$, e.g. standard Gaussian
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- Non-linear function $x = f_\theta(z)$ maps latent variable to data space, for example deep neural net

Figure from Aaron Courville
Non-linear latent variable models

- Simple distribution $p(z)$ on latent variable $z$, e.g. standard Gaussian

- Non-linear function $x = f_\theta(z)$ maps latent variable to data space, for example deep neural net

- Induces complex marginal distribution $p_\theta(x)$

Figure from Aaron Courville
Learning deep latent variable models

- Marginal distribution on $x$ obtained by integrating out $z$

\[
p(z) = \mathcal{N}(z; 0, I),
\]

\[
p_\theta(x) = \int z p(z)p(x|f_\theta(z)).
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Learning deep latent variable models

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- Evaluation of $p_\theta(x)$ intractable due to integral involving non-linear deep net $f_\theta(\cdot)$
Learning deep latent variable models

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Learning deep latent variable models

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1. Approximate integral: Variational autoencoders (VAE)
Learning deep latent variable models

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- Two approaches to learn deep latent variable models
  1. Approximate integral: Variational autoencoders (VAE)
  2. Avoid integral: Generative adversarial networks (GAN)
Part I

Generative adversarial networks
Generative adversarial networks [Goodfellow et al., 2014]

- Sample $p(z)$, map it using deep net to $x = G_\theta(z)$
Generative adversarial networks [Goodfellow et al., 2014]

- Sample $p(z)$, map it using deep net to $x = G_\theta(z)$
- Instead of evaluating $p_\theta(x)$, use classifier $D_\phi$
  - $D_\phi(x) \in [0, 1]$ probability $x$ is real vs. synth. image
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Figure from Kevin McGuinness
Discriminator architecture for images

- Recognition CNN model, with sigmoid output layer
- Binary classification output: real / synthetic

Figure from Kevin McGuinness
Generator architecture for images

- Unit Gaussian prior on $z$, typically $10^2$ to $10^3$ dimensions
Generator architecture for images

▸ Unit Gaussian prior on $z$, typically $10^2$ to $10^3$ dimensions

▸ Up-convolutional deep network (reverse recognition CNN)
  ▸ Replace pooling layers that reduce resolution with upsampling layers (nearest neighbor, bi-linear, or learned)
Generator architecture for images

- Unit Gaussian prior on $z$, typically $10^2$ to $10^3$ dimensions

- Up-convolutional deep network (reverse recognition CNN)
  - Replace pooling layers that reduce resolution with upsampling layers (nearest neighbor, bi-linear, or learned)
  - Low-resolution layers induce long-range correlations
  - High-resolution layers induce short-range correlations

Figure from OpenAI
Training GANs

- **Discriminator**: maximize classification for a given generator
- **Generator**: degrade classification of a given discriminator
Training GANs

- **Discriminator**: maximize classification for a given generator
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- **Samples z** pass through two differentiable modules
Training GANs

- **Discriminator**: maximize classification for a given generator
- **Generator**: degrade classification of a given discriminator
- Samples $z$ pass through two differentiable modules
- **Discriminator** acts as **trainable loss function**
GAN learning process

$p_D(\text{data})$

Data distribution

Model distribution

Poorly fit model
GAN learning process

\[ p_D(\text{data}) \]

Data distribution

Model distribution

Poorly fit model

After updating D
GAN learning process

$p_D(\text{data})$  Data distribution

Model distribution

$x$

Poorly fit model  After updating $D$  After updating $G$
GAN learning process

$p_D(\text{data})$

Data distribution

Model distribution

Poorly fit model

After updating D

After updating G

Mixed strategy equilibrium
GAN Optimization problem

- Objective function $V(\phi, \theta)$: performance of discriminator

$$V(\phi, \theta) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\ln D_\phi(x)] + \mathbb{E}_{z \sim p(z)}[\ln (1 - D_\phi(G_\theta(z)))]$$
GAN Optimization problem

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$$\min_{\theta} \max_{\phi} V(\phi, \theta)$$
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- Assuming infinite data and model capacity, and reaching optimal discriminator at each iteration
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  1. Unique global optimum for $G$ at data distribution
GAN Optimization problem

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- Assuming infinite data and model capacity, and reaching optimal discriminator at each iteration
  1. Unique global optimum for G at data distribution
  2. Convergence to optimum guaranteed
Optimal discriminator

For fixed generator $G$, the optimal discriminator $D$ is the Bayes classifier

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

Proof: Given generator $f$, the optimal discriminator maximizes

$$V(D, G) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\ln D(x)] + \mathbb{E}_{z \sim p(z)}[\ln(1 - D(G(z)))].$$

$$= \int p_{\text{data}}(x) \ln D(x) + p_G(x) \ln(1 - D(x)) \, dx.$$

For any $(a, b) \in \mathbb{R}^2 \setminus \{0, 0\}$ the function $a \ln(y) + b \ln(1 - y)$ achieves its maximum in $[0, 1]$ at $y = a/(a + b)$. Discriminator only needs to be defined in support of training data and $p_G(x)$. 

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Link with Jensen-Shannon divergence

- Plugging in the optimal discriminator we obtain

\[ \max_D V(D, G) = - \ln 4 + 2 D_{JS}(p_{data}||p_G) \]
Link with Jensen-Shannon divergence

- Plugging in the optimal discriminator we obtain

$$\max_D V(D, G) = -\ln 4 + 2D_{JS}(p_{\text{data}} || p_G)$$

with Jensen-Shannon divergence

$$D_{JS}(p||q) = \frac{1}{2} D_{KL} \left( p \left\| \frac{p + q}{2} \right\| \right) + \frac{1}{2} D_{KL} \left( q \left\| \frac{p + q}{2} \right\| \right)$$
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- Unique global minimum obtained for $p_{\text{data}} = p_G$
Link with Jensen-Shannon divergence

- Plugging in the optimal discriminator we obtain

$$\max_D V(D, G) = -\ln 4 + 2D_{JS}(p_{data} \mid\mid p_G)$$

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- Unique global minimum obtained for $p_{data} = p_G$

- If $D$ is set to optimum at each iteration, then convexity shows that gradient descent on $p_G$ recovers the global optimum
Training GANs in practice

\[ V(\phi, \theta) = \mathbb{E}_{x \sim p_{data}(x)}[\ln D_\phi(x)] + \mathbb{E}_{z \sim p(z)}[\ln(1 - D_\phi(f_\theta(z)))] \]

- Replace expectations with sample average in mini-batch
Training GANs in practice

\[ V(\phi, \theta) = \mathbb{E}_{x \sim p_{data}(x)}[\ln D_\phi(x)] + \mathbb{E}_{z \sim p(z)}[\ln(1 - D_\phi(f_\theta(z)))] \]

- Replace expectations with sample average in mini-batch
- Parallel stochastic gradient descent on \( \phi \) and \( \theta \)
Samples model learned on face images [Radford et al., 2016]
GAN generalizes beyond training data

- Sample along linear trajectory in latent space $z_1 \rightarrow z_2$
- Smooth transitions suggest generalization, sharp transitions would suggest literal memorization

Examples taken from [Radford et al., 2016], trained on LSUN bedroom dataset
GAN generalizes beyond training data

- Sample along linear trajectory in latent space $z_1 \rightarrow z_2$

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Vector arithmetic on latent variables

- Word2vec word embedding shows semantic regularities [Mikolov et al., 2013]

\[ (\mathbf{z}_{\text{king}} - \mathbf{z}_{\text{man}}) + \mathbf{z}_{\text{woman}} \approx \mathbf{z}_{\text{queen}} \]  

(15)
Vector arithmetic on latent variables

- Word2vec word embedding shows semantic regularities [Mikolov et al., 2013]

$$ (z_{king} - z_{man}) + z_{woman} \approx z_{queen} $$

- Consider GAN trained on human faces, average $z$ vectors over three samples for stability
Why is GAN training is difficult in practice?

- Recall divergence measures between distributions
- Kullback-Leibler divergence: maximum likelihood training
  
  \[
  D_{KL}(p||q) = \int x p(x) \left[ \ln q(x) - \ln p(x) \right]
  \] (16)

- Jensen-Shannon divergence: idealized GAN training
  
  \[
  D_{JS}(p||q) = \frac{1}{2} D_{KL}(p||\frac{p+q}{2}) + \frac{1}{2} D_{KL}(q||\frac{p+q}{2})
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Why is GAN training is difficult in practice?

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Why is GAN training difficult in practice?

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    $$D_{KL}(p||q) = \int_x p(x) \left[ \ln q(x) - \ln p(x) \right]$$
    
    (16)

- Jensen-Shannon divergence: idealized GAN training
  - Symmetric KL to mixture of $p$ and $q$
    
    $$D_{JS}(p||q) = \frac{1}{2} D_{KL} \left( p \bigg\| \frac{p+q}{2} \right) + \frac{1}{2} D_{KL} \left( q \bigg\| \frac{p+q}{2} \right)$$
    
    (17)
Why is GAN training is difficult in practice?

[Arjovsky et al., 2017]
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   - Direction of KL term leads to mode dropping
Wasserstein or “earth-mover” distance

- Consider joint distribution $\gamma(x, y)$
  with marginals $p(x) = \gamma(x)$ and $q(y) = \gamma(y)$

- Conditional $\gamma(y|x)$ “moves mass” to transform $p(\cdot)$ into $q(\cdot)$
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- Cost associated with a given transformation

\[
T(\gamma) = \int_{x,y} \gamma(x, y) \|x - y\| = \int_x p(x) \int_y \gamma(y|x) \|x - y\|
\]
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$$ T(\gamma) = \int_{x,y} \gamma(x, y) ||x - y|| = \int_x p(x) \int_y \gamma(y|x) ||x - y|| $$

- Wasserstein distance is the cost of optimal transformation

$$ D_{\text{WS}}(p\|q) = \inf_{\gamma \in \Gamma(p,q)} T(\gamma) \quad (18) $$
Distributions with low dimensional support

- Simple example: support on lines in $\mathbb{R}^2$
  - $p_0$ uniform on $x_2 \in [0, 1]$ for $x_1 = 0$
  - $p_\theta$ uniform on $x_2 \in [0, 1]$ for $x_1 = \theta$

$D_{KL}(p_0 || p_\theta) = \infty$

$D_{JS}(p_0 || p_\theta) = \ln 2$

$D_{WS}(p_0 || p_\theta) = |\theta|$

Wasserstein based on proximity of support

JS and KL based on overlap of support

In general measure zero overlap with low dim. supports

GAN has support with dimension of latent variable $z$
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Wasserstein GAN

- Dual formulation of Wasserstein distance

\[
D_{WS}(p_{\text{data}} \| p_G) = \frac{1}{k} \max_{\|D\|_L \leq k} \mathbb{E}_{p_{\text{data}}} [D(x)] - \mathbb{E}_{p_z} [D(G(z))]
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Experimental comparison GAN and WGAN

- GAN loss unstable, and actually increases over iterations!
- WGAN loss decreases in a stable manner
- WGAN gives better correlation loss and sample quality
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Latent variable inference in GANs [Donahue et al., 2017]

- Vanilla GAN lacks a mechanism to infer $z$ from $x$
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- **Generator**: maps latent variable $z$ to data point $x$
Latent variable inference in GANs [Donahue et al., 2017]

- Vanilla GAN lacks a mechanism to infer \( z \) from \( x \)

- **Generator**: maps latent variable \( z \) to data point \( x \)

- **Encoder**: infers latent representation \( z \) from data point \( x \)
Induced joint distributions over \((x, z)\)
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- **Generator:**
  \[ p_G(x, z) = p_z(z) \delta (x - G(z)) \]
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  \[ p_E(x, z) = p_{\text{data}}(x) \delta(z - E(x)) \]
Induced joint distributions over \((x, z)\)

- **Generator:** \(p_G(x, z) = p_z(z) \delta(x - G(z))\)
- **Encoder:** \(p_E(x, z) = p_{\text{data}}(x) \delta(z - E(x))\)
- **Discriminator:** pair \((x, z)\) completed by generator or encoder?
Bidirectional GANs [Donahue et al., 2017]

\[ V(D, E, G) = \mathbb{E}_{p_{\text{data}}} [\ln D(x, E(x))] + \mathbb{E}_{p(z)} [\ln(1 - D(G(z), z))] \]

\[
\min_{G,E} \max_{D} V(D, E, G)
\]
Bidirectional GANs [Donahue et al., 2017]

\[
V(D, E, G) = \mathbb{E}_{p_{data}}[\ln D(x, E(x))] + \mathbb{E}_{p(z)}[\ln(1 - D(G(z), z))]
\]

\[
\min_G \max_E \max_D V(D, E, G)
\]

- For optimal discriminator objective equals JS divergence

\[
\max_D V(D, E, G) = 2D_{JS}(p_E(x, z)\|p_G(x, z)) - \ln 4
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Bidirectional GANs [Donahue et al., 2017]

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- For optimal discriminator objective equals JS divergence

\[
\max_D V(D, E, G) = 2D_{JS} (p_E(x, z) \mid \mid p_G(x, z)) - \ln 4
\]

- At optimum \( G \) and \( E \) are each others inverse
BiGAN samples, ImageNet $64 \times 64$

$G(z)$
BiGAN samples, ImageNet $64 \times 64$

$G(z)$

$x$

$G(E(x))$

$x$

$G(E(x))$
BiGAN: feature transfer to PASCAL VOC’07

<table>
<thead>
<tr>
<th>trained layers</th>
<th>Classification (% mAP)</th>
<th>FRCN Detection (% mAP)</th>
<th>FCN Segmentation (% mIU)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>fc8</td>
<td>fc6-8</td>
<td>all</td>
</tr>
<tr>
<td>sup. ImageNet</td>
<td>37.0</td>
<td>78.8</td>
<td>78.3</td>
</tr>
<tr>
<td>self-sup.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Agrawal et al. (2015)</td>
<td>31.2</td>
<td>31.0</td>
<td>54.2</td>
</tr>
<tr>
<td>Pathak et al. (2016)</td>
<td>30.5</td>
<td>34.6</td>
<td>56.5</td>
</tr>
<tr>
<td>Wang &amp; Gupta (2015)</td>
<td>28.4</td>
<td>55.6</td>
<td>63.1</td>
</tr>
<tr>
<td>Doersch et al. (2015)</td>
<td>44.7</td>
<td>55.1</td>
<td>65.3</td>
</tr>
<tr>
<td>unsup. $k$-means (Krähenbühl et al. 2016)</td>
<td>32.0</td>
<td>39.2</td>
<td>56.6</td>
</tr>
<tr>
<td>Discriminator ($D$)</td>
<td>30.7</td>
<td>40.5</td>
<td>56.4</td>
</tr>
<tr>
<td>Latent Regressor (LR)</td>
<td>36.9</td>
<td>47.9</td>
<td>57.1</td>
</tr>
<tr>
<td>Joint LR</td>
<td>37.1</td>
<td>47.9</td>
<td>56.5</td>
</tr>
<tr>
<td>Autoencoder ($\ell_2$)</td>
<td>24.8</td>
<td>16.0</td>
<td>53.8</td>
</tr>
<tr>
<td>BiGAN (ours)</td>
<td>37.5</td>
<td>48.7</td>
<td>58.9</td>
</tr>
<tr>
<td>BiGAN, 112 $\times$ 112 $E$ (ours)</td>
<td>40.7</td>
<td>52.3</td>
<td>60.1</td>
</tr>
</tbody>
</table>

- Encoder network used to pre-train/initialize recognition net
- Similar performance of BiGAN and self-supervised methods
  - Self-sup: CNN trained using image structure as supervision
  - Discriminator: uses GAN discriminator layers as features
  - Latent regressor: trains network to invert GAN (jointly)
Unpaired image-to-image translation [Zhu et al., 2017]

- Learn 2-way mapping between different image domains
Unpaired image-to-image translation [Zhu et al., 2017]

- Learn 2-way mapping between different image domains
- Without using supervised aligned training samples
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1. Discriminator ensures realistic samples in each domain
Unpaired image-to-image translation [Zhu et al., 2017]

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1. Discriminator ensures realistic samples in each domain
2. Cycle-consistency loss ensures alignment
Some successful examples

horse → zebra
Some successful examples

- Without using any supervised/aligned examples!
Some successful examples

- Without using any supervised/aligned examples!
Some successful examples

- Without using any supervised/aligned examples!

- horse → zebra

- winter Yosemite → summer Yosemite

- orange → apple
And a failure case
Part II

Variational Autoencoders
Autoencoders

- Learn latent representation $z$ via reconstruction of data $x$
Autoencoders

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- Neural network where output $\sim$ input
  - Encoder: maps data $x$ to latent code $z$
  - Decoder: maps latent code $z$ to reconstruction $\tilde{x}$
Autoencoders

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- Neural network where output $\sim$ input
  - Encoder: maps data $x$ to latent code $z$
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- Loss minimizes discrepancy between $x$ and $\tilde{x}$
Relation autoencoders and PCA [Baldi and Hornik, 1989]

- Autoencoder recovers PCA if
  1. Encoder and decoder are both linear
  2. Optimizing $\ell_2$ reconstruction loss

\[
\min_{V,W} \frac{1}{2N} \sum_{n=1}^{N} \|x_n - VWx_n\|^2
\]  

(19)
Deep non-linear autoencoders

- Stack many non-linear layers in encoder and decoder
Deep non-linear autoencoders

- Stack many non-linear layers in encoder and decoder
- Non-linear representation learning
Deep non-linear autoencoders

- Stack many non-linear layers in encoder and decoder
- Non-linear representation learning
- Does not provide a generative model that can be sampled
Autoencoding variational Bayes [Kingma and Welling, 2014]

- Decoder $f$ implements generative latent variable model
  - Maps latent code $z$ to observation $x$

\[
p_{\theta}(x|z) = \mathcal{N}(x; f^\mu_\theta(z), f^\sigma_\theta(z))
\]  

(20)
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p_\theta(x|z) = \mathcal{N}(x; f_\theta^\mu(z), f_\theta^\sigma(z)) \]  
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- Encoder $g$ compute approximate posterior distribution
  - Maps data $x$ to latent code $z$
    \[
    q_\phi(z|x) = \mathcal{N}(z; g_\phi^\mu(x), g_\phi^\sigma(x)) \]  
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Objective function: Evidence lower bound (ELBO)

- Quantity of interest: marginal likelihood or “evidence”

\[ p_\theta(x) = \int_z p(z)p_\theta(x|z) \]  

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\[ p_\theta(x) = \int_z p(z)p_\theta(x|z) \]  \hspace{1cm} (22)

- Bound using variational approximation of posterior \( p_\theta(z|x) \)

\[ F(\theta, q) \equiv \ln p_\theta(x) \quad D_{KL}(q(z)||p_\theta(z|x)) \leq \ln p_\theta(x) \]  \hspace{1cm} (23)
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- Bound tight if variational distribution matches real posterior
**EM algorithm performs coordinate ascent over ELBO**

- **Expectation step**: Fix parameters \( \theta \), optimize over \( q(z) \)
  - Bound is tight if we can set \( q(z) = p_\theta(z|x) \)

\[
F(\theta, q) \equiv \ln p_\theta(x) - D_{KL}(q(z) \| p_\theta(z|x)) \quad \text{fixed} \tag{25}
\]
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- **Maximization step**: Fix $q(z)$, optimize model parameters $\theta$
  - Log-marginal decomposed into log-prior and log-conditional

  $$F(\theta, q) = H(q) + \mathbb{E}_q[\ln p(z) + \ln p_\theta(x|z)] \quad (26)$$
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- Iterating EM steps monotonically increases evidence bound
  - Monotonically increases evidence with exact inference in E-step
Variational EM with inference net (amortized inference)

- Efficient feed-forward computation of approximate posterior
  
  \[ q_\phi(z|x) = \mathcal{N}(z; g^\mu_\phi(x), g^\sigma_\phi(x)) \]  
  
  (27)

- No iterative optimization of approx. posterior per data point
- Avoids initialization and tracking posterior across iterations

Figure from kvfrans@github
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- Avoids initialization and tracking posterior across iterations

- ELBO becomes function of inference net and generative net
  
  \[ F(\theta, \phi) = \mathbb{E}_{q_\phi} [\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z)) \]  

![Diagram of variational autoencoder]
Computation ELBO for variational autoencoder

\[ F(\theta, \phi) = \mathbb{E}_{q_{\phi}}[\ln p_{\theta}(x|z)] - D_{KL}(q_{\phi}(z|x)||p(z)) \]  

(29)

- **Regularization term** keeps \( q \) from collapsing to single point \( z \)
Computation ELBO for variational autoencoder

\[ F(\theta, \phi) = \mathbb{E}_{q_\phi}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)||p(z)) \]  

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- **Regularization term** keeps \( q \) from collapsing to single point \( z \)
- Closed form if both terms are Gaussian, for \( p(z) = \mathcal{N}(z; 0, I) \)

\[ D_{KL}(q_\phi(z|x)||p(z)) = \frac{1}{2} \left[ 1 + \ln g_\phi(x) - g_\phi^\mu(x) - g_\phi^\sigma(x) \right] \]  

(30)
Computation ELBO for variational autoencoder

\[ F(\theta, \phi) = \mathbb{E}_{q_\phi} [\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x) || p(z)) \]  \hspace{1cm} (29)

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- Differentiable function of inference net parameters
Computation ELBO for variational autoencoder

\[ F(\theta, \phi) = \mathbb{E}_{q_\phi}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)\|p(z)) \]  \hspace{1cm} (31)

- **Reconstruction term**: to what extent can \( x \) be reconstructed from \( z \) following approximate posterior \( q(z|x) \)

\[ \text{Reconstruction} - \text{Regularization} \]

- **Reconstruction term**: to what extent can \( x \) be reconstructed from \( z \) following approximate posterior \( q(z|x) \)
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- Use sample approximation of intractable expectation

\[
\mathbb{E}_{q_\phi}[\ln p_\theta(x|z)] \approx \frac{1}{S} \sum_{s=1}^{S} \ln p_\theta(x|z_s) \tag{32}
\]
Computation ELBO for variational autoencoder

\[ F(\theta, \phi) = \mathbb{E}_{q_\phi}[\ln p_\theta(x|z)] - D_{KL}(q_\phi(z|x)||p(z)) \]

- **Reconstruction term**: to what extent can \( x \) be reconstructed from \( z \) following approximate posterior \( q(z|x) \)

- Use sample approximation of intractable expectation
  \[ z_s \sim q_\phi(z|x) \]

  \[ \mathbb{E}_{q_\phi}[\ln p_\theta(x|z)] \approx \frac{1}{S} \sum_{s=1}^{S} \ln p_\theta(x|z_s) \]  

- Estimator is non-differentiable due to sampling operator
Re-parametrization trick

- Side-step non-differentiable sampling operator by re-parametrizing samples $z_s \sim q_\phi(z|x) = \mathcal{N} \left( z; g_\phi^\mu(x), g_\phi^\sigma(x) \right)$
Re-parametrization trick

- Side-step non-differentiable sampling operator by re-parametrizing samples $z_s \sim q_\phi(z|x) = \mathcal{N}(z; g_\phi^\mu(x), g_\phi^\sigma(x))$

- Use inference net to modulate samples from a unit Gaussian

$$z_s = g_\phi^\mu(x) + g_\phi^\sigma(x) \odot \epsilon_s, \quad \epsilon_s \sim \mathcal{N}(\epsilon_s; 0, I) \quad (33)$$
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- Unbiased differentiable approximation of ELBO

$$F(\theta, \phi) \approx \frac{1}{S} \sum_{s=1}^{S} \ln p_\theta(x|g_\phi^\mu(x) + g_\phi^\sigma(x) \odot \epsilon_s) \tag{34}$$

$$-\frac{1}{2} \left[ 1 + \ln g_\phi^\sigma(x) - g_\phi^\mu(x) - g_\phi^\sigma(x) \right] \tag{35}$$
Re-parametrization trick in a cartoon

Figure from [Doersch, 2016]
Re-parametrization trick in a cartoon

Figure from [Doersch, 2016]
Autoencoding variational Bayes training algorithm

- For each data point $x$ in a mini-batch
  1. Sample one or multiple values $\{\epsilon_s\}$
  2. Use back-propagation to compute
     \[
     g_\theta = \nabla_\theta F(\theta, \phi, \{\epsilon_s\})
     \]
     \[
     g_\phi = \nabla_\phi F(\theta, \phi, \{\epsilon_s\})
     \]
  3. Gradient-based parameter update

Figure from Aaron Courville
Random samples from VAE and GAN

- Trained from 200k images in CelebA dataset

Figure from [Hou et al., 2016]
Random samples from VAE and GAN

- Trained from 200k images in CelebA dataset
- VAE samples appear overly smooth / blurred

Figure from [Hou et al., 2016]
Random samples from VAE and GAN

- Trained from 200k images in CelebA dataset
- VAE samples appear overly smooth / blurred
- GAN samples show more (imperfect) detail

Figure from [Hou et al., 2016]
Semi-supervised learning with VAE [Kingma et al., 2014]
Semi-supervised learning with VAE [Kingma et al., 2014]

- **Generative model**: Add class label $y$, latent variable $z$ models in-class variations

$$
p_{\pi}(y) = \text{Cat}(y; \pi) \quad p(z) = \mathcal{N}(z; 0, I)
$$
Semi-supervised learning with VAE [Kingma et al., 2014]

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\[
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p_\theta(x|y, z) = \mathcal{N}(x; \mu_\theta(y, z), \sigma^2_\theta(y, z))
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- **Inference network**
Semi-supervised learning with VAE [Kingma et al., 2014]

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  1. Posterior on class-label acts as classifier

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Semi-supervised learning with VAE [Kingma et al., 2014]

- **Generative model**: Add class label $y$, latent variable $z$ models in-class variations

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  $$

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Objective function for semi-supervised model

- Objective function has three terms

\[
\mathcal{J} = \alpha \sum_{(x,y) \sim \tilde{p}_l} \ln q_\phi(y|x)
\]

1. Discriminative term: trains classifier from labeled data
Objective function for semi-supervised model

- Objective function has three terms

\[ J = \alpha \sum_{(x,y) \sim \tilde{p}_l} \ln q_\phi(y|x) + \sum_{(x,y) \sim \tilde{p}_l} \mathcal{L}(x, y) \] (38)

1. Discriminative term: trains classifier from labeled data

2. Generative labeled data: infer latent variable \( z \)

\[ \mathcal{L}(x, y) = \mathbb{E}_{q_\phi(z|x,y)}[\ln p_\theta(x, y, z) - \ln q_\phi(z|x, y)] \leq \ln p(x, y) \]
Objective function for semi-supervised model

- Objective function has three terms

\[
J = \alpha \sum_{(x,y) \sim \tilde{p}_l} \ln q_{\phi}(y|x) + \sum_{(x,y) \sim \tilde{p}_l} \mathcal{L}(x,y) + \sum_{(x) \sim \tilde{p}_u} \mathcal{U}(x) \tag{38}
\]

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\mathcal{L}(x,y) = \mathbb{E}_{q_{\phi}(z|x,y)}[\ln p_{\theta}(x,y,z) - \ln q_{\phi}(z|x,y)] \leq \ln p(x,y)
\]

3. Generative unlabeled data: infer label \( y \) and latent variable \( z \)

\[
\mathcal{U}(x) = \mathbb{E}_{q_{\phi}(y,z|x)}[\ln p_{\theta}(x,y,z) - \ln q_{\phi}(y|x) - q_{\phi}(z|x,y)] \leq \ln p(x)
\]
Class-conditional image generation on MNIST

- Fix class label $y \in \{2, 3, 4\}$, vary latent variable $z \in \mathbb{R}^2$
Cross-class style transfer

- Fix latent variable $z$, vary class label $y \in \{1, \ldots, 9, 0\}$
- First column: images from the test set, infer $z$
- Others: images generated for each class using inferred $z$
Semi-supervised classification on MNIST

- M1+TSVM: use TSVM on learn representation with VAE
- M2: use presented semi-supervised VAE
- M1+M2: use M2 on representation learned by M1

Table 1: Benchmark results of semi-supervised classification on MNIST with few labels.

<table>
<thead>
<tr>
<th>N</th>
<th>NN</th>
<th>CNN</th>
<th>TSVM</th>
<th>CAE</th>
<th>MTC</th>
<th>AtlasRBF</th>
<th>M1+TSVM</th>
<th>M2</th>
<th>M1+M2</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>25.81</td>
<td>22.98</td>
<td>16.81</td>
<td>13.47</td>
<td>12.03</td>
<td>8.10 (± 0.95)</td>
<td>11.82 (± 0.25)</td>
<td>11.97 (± 1.71)</td>
<td><strong>3.33 (± 0.14)</strong></td>
</tr>
<tr>
<td>600</td>
<td>11.44</td>
<td>7.68</td>
<td>6.16</td>
<td>6.3</td>
<td>5.13</td>
<td>–</td>
<td>5.72 (± 0.049)</td>
<td>4.94 (± 0.13)</td>
<td><strong>2.59 (± 0.05)</strong></td>
</tr>
<tr>
<td>1000</td>
<td>10.7</td>
<td>6.45</td>
<td>5.38</td>
<td>4.77</td>
<td>3.64</td>
<td>3.68 (± 0.12)</td>
<td>4.24 (± 0.07)</td>
<td>3.60 (± 0.56)</td>
<td><strong>2.40 (± 0.02)</strong></td>
</tr>
<tr>
<td>3000</td>
<td>6.04</td>
<td>3.35</td>
<td>3.45</td>
<td>3.22</td>
<td>2.57</td>
<td>–</td>
<td>3.49 (± 0.04)</td>
<td>3.92 (± 0.63)</td>
<td><strong>2.18 (± 0.04)</strong></td>
</tr>
</tbody>
</table>
Improving variational autoencoders

ELBO uses KL divergence to bound the data log-likelihood:

\[
F(x, \theta, \phi) = \ln p(x) - D(q_{\phi}(z|x) || p(z|x))
\]

Generally true posterior is not Gaussian: loose bound

Encourages true posterior to match variational factored Gaussian produced by recognition net

Making progress
1. More accurate bound for given posterior
2. Enlarge the family of variational posteriors
3. Avoid approximate inference altogether
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Importance weighted autoencoders [Burda et al., 2016]

- Construct tighter lower bound using importance sampling

\[
F_k(x; \theta, \phi) = I \mathbb{E}_{z_1, \ldots, z_k \sim q(z|x)} \left[ \ln \frac{1}{k} \sum_{i=1}^{k} w(x, z_i) \right] \\
\leq I \mathbb{E}_{z_1, \ldots, z_k \sim q(z|x)} \left[ \ln \frac{1}{k} \sum_{i=1}^{k} w(x, z_i) \right] = \ln I \mathbb{E}_{z \sim q(z|x)} [w(x, z)] = \ln p(x)
\]

1. VAE lower bound recovered for \( k = 1 \)
2. More samples tighten the bound: \( F_k \leq F_{k+1} \leq \ln p(x) \)
3. If the weights are bounded, then \( F_k \to \ln p(x) \) as \( k \to \infty \)

- Use as objective to train models for \( k \approx 10 \)
- Use as likelihood estimator for (IW-)VAE with \( k \approx 10 \)
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$$\leq \ln \mathbb{E}_{z_1, \ldots, z_k \sim q_\phi(z|x)} \left[ \frac{1}{k} \sum_{i=1}^{k} w(x, z_i) \right]$$

$$= \ln \mathbb{E}_{z \sim q_\phi(z|x)} [w(x, z)]$$

$$= \ln p(x)$$
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$$= \ln \mathbb{E}_{z \sim q_\phi(z|x)} [w(x, z)]$$

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- Use as likelihood estimator for (IW-)VAE with $k \approx 10^3$
Training procedure importance weighted autoencoders

- Gradients of importance weighted lower bound

\[
\nabla F_k(x) = \mathbb{E}_{z_1:k \sim q_\phi(z|x)} \left[ \sum_{i=1}^{k} \tilde{w}_i \nabla \left( \ln p(x, z_i) - \ln q_\phi(z_i|x) \right) \right]
\]
Training procedure importance weighted autoencoders

- Gradients of importance weighted lower bound

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\]

- Similar to VAE, but samples weighted w.r.t. true posterior
  - Normalized importance weights \( \tilde{w}_i = w(x, z_i) / \sum_{j=1}^{k} w(x, z_j) \)
Training procedure importance weighted autoencoders

▶ Gradients of importance weighted lower bound

\[ \nabla F_k(x) = \mathbb{E}_{z_{1:k} \sim q_\phi(z|x)} \left[ \sum_{i=1}^{k} \tilde{w}_i \nabla \left( \ln p(x, z_i) - \ln q_\phi(z_i|x) \right) \right] \]

▶ Similar to VAE, but samples weighted w.r.t. true posterior

▶ Normalized importance weights \( \tilde{w}_i = w(x, z_i) / \sum_{j=1}^{k} w(x, z_j) \)

▶ Allows for more accurate models with complex posteriors

True posterior \( p(z|x) \) VAE (left) and IW-VAE (right)
Variational inference with normalizing flows

[Rezende and Mohamed, 2015]

- Variational inference (in VAE) uses limited class of posteriors
  - For example, Gaussian with diagonal covariance
  - Optimizing loose bound on data log-likelihood
Variational inference with normalizing flows

[Rezende and Mohamed, 2015]

- Variational inference (in VAE) uses limited class of posteriors
  - For example, Gaussian with diagonal covariance
  - Optimizing loose bound on data log-likelihood

- Improve posterior with series of invertible transformations

![Diagram of variational inference with normalizing flows]
Normalizing flows

- Let density "flow" through set of invertible transformations

\[ z_K = f_K \circ \cdots \circ f_2 \circ f_1(z_0), \]

\[ \ln q_K(z_K) = \ln q_0(z_0) - \sum_{k=1}^{K} \ln \left| \det \frac{\partial f_k}{\partial z_k} \right| \]
Normalizing flows

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\[ \ln q_K(z_K) = \ln q_0(z_0) - \sum_{k=1}^{K} \ln \left| \det \frac{\partial f_k}{\partial z_k} \right| \]

- Linear-time determinant for planar and radial flows

\[ f(z) = z + uh(w^\top z + b) \]
\[ f(z) = z + \beta h(\alpha, r) (z - z_0) \]
Normalizing flows

- Let density “flow” through set of invertible transformations
  \[
  z_K = f_K \circ \cdots \circ f_2 \circ f_1(z_0),
  \]
  \[
  \ln q_K(z_K) = \ln q_0(z_0) - \sum_{k=1}^{K} \ln \left| \det \frac{\partial f_k}{\partial z_k} \right|
  \]

- Linear-time determinant for planar and radial flows
  \[
  f(z) = z + uh(w^\top z + b)
  \]
  \[
  f(z) = z + \beta h(\alpha, r) (z - z_0)
  \]
**Autoregressive flow** [Kingma et al., 2016]

- Restrictive flows in [Rezende and Mohamed, 2015]
  - Planar flow similar to MLP with single hidden unit

- Use autoregressive transformations in flow
  - Rich and tractable class of transformations
  - Fewer transformations needed
Autoregressive flow [Kingma et al., 2016]

- Class of **affine transformations** with respect to $z$

\[ z_{t+1} = \mu_t + \sigma_t \odot z_t \]
Autoregressive flow [Kingma et al., 2016]

- Class of affine transformations with respect to $z$

$$z_{t+1} = \mu_t + \sigma_t \odot z_t$$

- Autoregressive computation of affine parameters

$$\mu_{t,i+1} = f(z_{t,1:i}) \quad \sigma_{t,i+1} = g(z_{t,1:i})$$
Autoregressive flow [Kingma et al., 2016]

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  z_{t+1} = \mu_t + \sigma_t \odot z_t
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- **Autoregressive computation** of affine parameters
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  \mu_{t,i+1} = f(z_{t,1:i}) \quad \sigma_{t,i+1} = g(z_{t,1:i})
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- Triangular Jacobian, log-determinant $\sum_{i=1}^{D} \log \sigma_{t,i}$
Autoregressive flow [Kingma et al., 2016]

- Class of **affine transformations** with respect to $z$

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- Triangular Jacobian, log-determinant $\sum_{i=1}^{D} \log \sigma_{t,i}$

- Parallel computations of $z_t, \mu_t, \sigma_t$ across dimensions
Autoregressive flow [Kingma et al., 2016]

- Class of **affine transformations** with respect to $z$

  $z_{t+1} = \mu_t + \sigma_t \odot z_t$

- **Autoregressive computation** of affine parameters

  $\mu_{t,i+1} = f(z_{t,1:i}) \quad \sigma_{t,i+1} = g(z_{t,1:i})$

- Triangular Jacobian, log-determinant $\sum_{i=1}^{D} \log \sigma_{t,i}$

- Parallel computations of $z_t, \mu_t, \sigma_t$ across dimensions

- Free to chose form of autoregressive dependency
Non-volume preserving (NVP) transformation [Dinh et al., 2017]

- Learn invertible function from latent to data space
Non-volume preserving (NVP) transformation [Dinh et al., 2017]

- Learn invertible function from latent to data space
- Latent and data space have same dimensionality
Non-volume preserving (NVP) transformation [Dinh et al., 2017]

- Learn invertible function from latent to data space
- Latent and data space have same dimensionality
- Unit Gaussian prior on latent variables

\[ x \sim \hat{p}_X \]
\[ z = f(x) \]

```
Inference
```

```
Generation
```

\[ z \sim p_Z \]
\[ x = f^{-1}(z) \]
Non-volume preserving (NVP) transformation [Dinh et al., 2017]

- Learn invertible function from latent to data space
- Latent and data space have same dimensionality
- Unit Gaussian prior on latent variables
- Tractable sampling and exact inference

\[
\begin{align*}
\text{Inference} & \quad x \sim \hat{p}_X \\
& \quad z = f(x)
\end{align*}
\]

\[
\begin{align*}
\text{Generation} & \quad z \sim p_Z \\
& \quad x = f^{-1}(z)
\end{align*}
\]
Change of variable formula for invertible function

- Ensuring efficient computation of $y = f(x)$ and determinant

$$p_X(x) = p_Y(f(x)) \times \left| \det \left( \frac{\partial f(x)}{\partial x} \right) \right|$$
Change of variable formula for invertible function

- Ensuring efficient computation of $y = f(x)$ and determinant

$$p_X(x) = p_Y(f(x)) \times \left| \det \left( \frac{\partial f(x)}{\partial x^T} \right) \right|$$

1. Partition variables in two groups

![Diagram showing variable partitioning and transformation]
Change of variable formula for invertible function

- Ensuring efficient computation of $y = f(x)$ and determinant

$$p_X(x) = p_Y(f(x)) \times \left| \det \left( \frac{\partial f(x)}{\partial x^T} \right) \right|$$

1. Partition variables in two groups
2. Keep one group unchanged

![Diagram showing the change of variable process](image)
Change of variable formula for invertible function

- Ensuring efficient computation of $y = f(x)$ and determinant

$$p_X(x) = p_Y(f(x)) \times \left| \det \left( \frac{\partial f(x)}{\partial x^\top} \right) \right|$$

1. Partition variables in two groups
2. Keep one group unchanged
3. Let one group transform the other via translation and scaling

$$y_1 = x_1$$
$$y_2 = t(x_1) + x_2 \odot \exp(s(x_1))$$
Properties: Efficient inversion

- Inverse transformation

\[
\begin{align*}
  x_1 &= y_1 \\
  x_2 &= (y_2 - t(x_1)) \odot \exp(-s(x_1))
\end{align*}
\]
Properties: Efficient inversion

- Inverse transformation

\[
x_1 = y_1 \tag{40}
\]
\[
x_2 = (y_2 - t(x_1)) \odot \exp(-s(x_1)) \tag{41}
\]

- No need to invert \( s(\cdot) \) and \( t(\cdot) \)
- Can use complex non-invertible functions, e.g. deep CNN

(a) Forward propagation  
(b) Inverse propagation
Properties: Efficient determinant computation

- Triangular structure of Jacobian
  \[
  \frac{\partial f(x)}{\partial x^\top} = \begin{bmatrix}
  I_d & 0 \\
  \frac{\partial y_2}{\partial x_1} \text{diag}(\exp(s(x_1))) & \text{diag}(\exp(s(x_1)))
  \end{bmatrix}
  \]

- Determinant given by product of Jacobian’s diagonal terms
  \[
  \ln \det \left( \frac{\partial f(x)}{\partial x^\top} \right) = 1^\top s(x_1)
  \]
Properties: Efficient determinant computation

- Triangular structure of Jacobian

\[
\frac{\partial f(x)}{\partial x^\top} = \begin{bmatrix} I_d & 0 \\ \frac{\partial y_2}{\partial x_1} & \text{diag}(\exp(s(x_1))) \end{bmatrix}
\]

- Determinant given by product of Jacobian’s diagonal terms

\[
\ln \det \left( \frac{\partial f(x)}{\partial x^\top} \right) = 1^\top s(x_1)
\]

- Log-likelihood easily computed, optimize using stochastic gradient decent

\[
\ln p_X(x) = \ln p_Y(f(x)) + 1^\top s(x_1)
\]
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
  - Input to CNN masked, masked application of CNN output
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
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- Stack multiple layers of transformations
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
  - Input to CNN masked, masked application of CNN output

- Stack multiple layers of transformations
  - Alternating the masking patterns
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
  - Input to CNN masked, masked application of CNN output

- Stack multiple layers of transformations
  - Alternating the masking patterns
  - Composing data transformations, summing log determinants
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
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  - Alternating the masking patterns
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- Feature abstraction hierarchy
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
  - Input to CNN masked, masked application of CNN output

- Stack multiple layers of transformations
  - Alternating the masking patterns
  - Composing data transformations, summing log determinants

- Feature abstraction hierarchy
  - Squeeze $2n \times 2n \times c$ map into $n \times n \times 4c$
Implementation

- Variable partitioning schemes
  - Checkerboard mask, channel-wise mask
  - Input to CNN masked, masked application of CNN output

- Stack multiple layers of transformations
  - Alternating the masking patterns
  - Composing data transformations, summing log determinants

- Feature abstraction hierarchy
  - Squeeze $2n \times 2n \times c$ map into $n \times n \times 4c$
  - Factor out half of latent variables at regular intervals
Illustration multi-scale feature hierarchy

- Images obtained after re-sampling part of latent variables
Illustration multi-scale feature hierarchy

- Images obtained after re-sampling part of latent variables
- From left to right: original, keeping $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{16}$

ImageNet $64 \times 64$
Illustration multi-scale feature hierarchy

- Images obtained after re-sampling part of latent variables
- From left to right: original, keeping $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{16}$

ImageNet $64 \times 64$

CelebA $64 \times 64$
Images & Samples NVP: CIFAR10 Dataset $32 \times 32$
Part III

Autoregressive density estimation
Autoregressive modeling

Consider generic factorization of joint probability

\[
p(x_{1:D}) = p(x_1) \prod_{i=2}^{D} p(x_i|\mathbf{x}_{<i}) \tag{42}
\]

with \( \mathbf{x}_{<i} = \mathbf{x}_1, \ldots, \mathbf{x}_{i-1} \)
Autoregressive modeling

- Consider generic factorization of joint probability

\[
p(x_{1:D}) = p(x_1) \prod_{i=2}^{D} p(x_i|x_{<i})
\]  \hspace{1cm} (42)

with \( x_{<i} = x_1, \ldots, x_{i-1} \)

- Use (deep) neural net to model dependencies in \( p(x_i|x_{<i}) \)
Autoregressive modeling

- Consider generic factorization of joint probability

\[
p(x_1:D) = p(x_1) \prod_{i=2}^{D} p(x_i|x_{<i})
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(42)

with \(x_{<i} = x_1, \ldots, x_{i-1}\)

- Use (deep) neural net to model dependencies in \(p(x_i|x_{<i})\)

- Tractable exact likelihood computations
  - No complex integral over latent variables in likelihood
Autoregressive modeling

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- Use (deep) neural net to model dependencies in \(p(x_i|x_{<i})\)

- Tractable exact likelihood computations
  - No complex integral over latent variables in likelihood

- Slow sequential sampling process
  - Cannot rely on latent variables to couple pixels
Neural Autoregressive Distribution Estimator (NADE)

[Larochelle and Murray, 2011]
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[Larochelle and Murray, 2011]

- Assume ordering on binary variables
- Estimate conditional distributions using 2-layer sigmoid network
Neural Autoregressive Distribution Estimator (NADE)

[Larochelle and Murray, 2011]

- Assume ordering on binary variables
- Estimate conditional distributions using 2-layer sigmoid network

\[
p(v_i = 1 | v_{<i}) = \sigma \left( b_i + a_i^\top h_i \right),
\]

\[
h_i = \sigma \left( c + \sum_{j<i} v_j w_j \right)
\]
Neural Autoregressive Distribution Estimator (NADE)
[Larochelle and Murray, 2011]

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- History \( v_{<i} \) compressed in \( h_i \)
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- Input-to-hidden parameters \( w_j \) shared
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[Larochelle and Murray, 2011]

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p(v_i = 1|v_{<i}) = \sigma \left( b_i + a_i^\top h_i \right),
\]

\[
h_i = \sigma \left( c + \sum_{j<i} v_j w_j \right)
\]

- History \(v_{<i}\) compressed in \(h_i\)
- Input-to-hidden parameters \(w_j\) shared
- Hidden-to-output parameters \(a_i\) not shared
NADE scales as $O(DH)$

- Nr. of parameters linear in data and hidden dimension
NADE scales as $O(DH)$

- Nr. of parameters linear in data and hidden dimension
- Computation of $\ln p(v)$ and gradient also linear
NADE scales as $O(DH)$

- Nr. of parameters linear in data and hidden dimension
- Computation of $\ln p(v)$ and gradient also linear
- Sequential sampling from $p(v)$
  - Incremental computation of history vector $\tilde{h}_{i+1} = \tilde{h}_i + v_i w_i$
  - Compute $p(v_i | v_{<i})$ using $\tilde{h}_i$, and sample $v_i$
NADE scales as $O(DH)$

- Nr. of parameters linear in data and hidden dimension
- Computation of $\ln p(v)$ and gradient also linear
- Sequential sampling from $p(v)$
  - Incremental computation of history vector $\tilde{h}_{i+1} = \tilde{h}_i + v_i w_i$
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Samples from NADE trained on MNIST digits
Masked Autoencoder for Distribution Estimation (MADE)
[Germain et al., 2015]
Masked Autoencoder for Distribution Estimation (MADE)
[Germain et al., 2015]

- Adapt autoencoders for distribution estimation

![Autoencoder Diagram]
Masked Autoencoder for Distribution Estimation (MADE)

[Germain et al., 2015]

- Adapt autoencoders for distribution estimation
- Output conditional distributions $p(x_i|x_{<i})$
Masked Autoencoder for Distribution Estimation (MADE)

[Germain et al., 2015]

- Adapt autoencoders for distribution estimation
- Output conditional distributions $p(x_i|x_{<i})$
- Mask connections to ensure proper conditionals
Masked Autoencoder for Distribution Estimation (MADE)

- Set max. input index $1 \leq m(k) < D$ for each hidden node
  - Mask connections to ensure consistency of $m(k)$
Masked Autoencoder for Distribution Estimation (MADE)

- Set max. input index $1 \leq m(k) < D$ for each hidden node
  - Mask connections to ensure consistency of $m(k)$

- Vary ordering and connectivity during training
  - Ensemble of models sharing parameters on connections

\[
p(x_1|x_2, x_3) \quad p(x_2) \quad p(x_3|x_2)
\]
Pixel Recurrent/Convolutional Neural Networks

[Oord et al., 2016b]

- Predict pixels one-by-one in row-major ordering
Pixel Recurrent/Convolutional Neural Networks

[Oord et al., 2016b]

- Predict pixels one-by-one in row-major ordering
- Translation invariant definition of conditionals $p(x_i | x_{<i})$
Pixel Recurrent/Convolutional Neural Networks

[Oord et al., 2016b]

- Predict pixels one-by-one in row-major ordering
- Translation invariant definition of conditionals $p(x_i | x_{<i})$
- Decouple number of pixels from number of parameters
Pixel RNN: Bi-directional LSTM

- Two sets of LSTM units, working down-right and down-left
  - Input up and left/right state
  - Input up and left/right pixels
Pixel RNN: Bi-directional LSTM

- Two sets of LSTM units, working down-right and down-left
  - Input up and left/right state
  - Input up and left/right pixels

- Receptive field
  - In each stream: all pixels above and to the right/left
  - Combined: all previous pixels
Pixel RNN: Bi-directional LSTM

▶ Two sets of LSTM units, working down-right and down-left
  ▶ Input up and left/right state
  ▶ Input up and left/right pixels

▶ Receptive field
  ▶ In each stream: all pixels above and to the right/left
  ▶ Combined: all previous pixels

▶ Slow sequential training process
  ▶ Due to sequential state updates
Pixel Convolutional Neural Networks

- Use limited context via CNN layers
  - Only local dependencies per layer
- Masked convolutions to ensure autoregressive property

- Layers increase receptive field
- Two stacks to fill blind spot: horizontal stack reads from vertical stack, not vice-versa
- Efficient parallel training, but sampling remains sequential and slow
- Extensions: WaveNet (audio) [Oord et al., 2016a], Video Pixel Networks [Kalchbrenner et al., 2017]
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- Extensions: WaveNet (audio) [Oord et al., 2016a], Video Pixel Networks [Kalchbrenner et al., 2017]
Class-conditional pixelCNN [Oord et al., 2016c]

- Samples single model trained across 1,000 ImageNet classes
Images generated by PixelCNNs trained on CIFAR10

[Oord et al., 2016b] (top) and [Salimans et al., 2017] (bottom)
Images generated by PixelCNNs trained on CIFAR10

[Oord et al., 2016b] (top) and [Salimans et al., 2017] (bottom)

- Models capture texture and details relatively well
- Lacking in global structure / long range dependencies
Hierarchical Pixel-CNN [Kolesnikov and Lampert, 2017]

- Introduce an intermediate “high-level” representation $\hat{x}$
  - Gray scale version, low resolution version, etc.
Hierarchical Pixel-CNN [Kolesnikov and Lampert, 2017]

- Introduce an intermediate “high-level” representation \( \hat{x} \)
  - Gray scale version, low resolution version, etc.

- Learn two-stage Pixel-CNN model
  - High-level model for \( \hat{x} \)
  - Conditional model on \( x \) for the details
Hierarchical Pixel-CNN [Kolesnikov and Lampert, 2017]

- Introduce an intermediate “high-level” representation $\hat{x}$
  - Gray scale version, low resolution version, etc.

- Learn two-stage Pixel-CNN model
  - High-level model for $\hat{x}$
  - Conditional model on $x$ for the details

- Train independently: $\ln p(x) \geq \ln p(\hat{x}) + \ln p(x|\hat{x})$
Hierarchical Pixel-CNN [Kolesnikov and Lampert, 2017]

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- Learn two-stage Pixel-CNN model
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  - Conditional model on \( x \) for the details

- Train independently: \( \ln p(x) \geq \ln p(\hat{x}) + \ln p(x|\hat{x}) \)

CIFAR images (left), gray version \( \hat{x} \) (middle), samples \( p(x|\hat{x}) \) (right)
Hierarchical Pixel-CNN [Kolesnikov and Lampert, 2017]

- Introduce an intermediate “high-level” representation $\hat{x}$
  - Gray scale version, low resolution version, etc.

- Learn two-stage Pixel-CNN model
  - High-level model for $\hat{x}$
  - Conditional model on $x$ for the details

- Train independently: $\ln p(x) \geq \ln p(\hat{x}) + \ln p(x|\hat{x})$

- Loss dominated by low-level model

CIFAR images (left), gray version $\hat{x}$ (middle), samples $p(x|\hat{x})$ (right)
Hierarchical Pixel-CNN

- Samples from 4-bit gray model, and conditional color model
Parallel multiscale autoregressive density estimation
[Reed et al., 2017]

- Address the inherently limited sampling efficiency of autoregressive models

\[ p(x_{1:N}) = \prod_{i=1}^{N} p(x_{i}|x_{<i}) \]
Parallel multiscale autoregressive density estimation
[Reed et al., 2017]

- Address the inherently limited sampling efficiency of autoregressive models

\[ p(x_{1:N}) = \prod_{i=1}^{N} p(x_i | x_{<i}) \]

- Sample image along a scale pyramid
  - Pixel-CNN for base resolution, e.g. \(4 \times 4\)
  - Autoregressive upsampling networks
Parallel multiscale autoregressive density estimation
[Reed et al., 2017]

▶ Address the inherently limited sampling efficiency of autoregressive models

\[ p(x_1:N) = \prod_{i=1}^{N} p(x_i|x_{<i}) \]

▶ Sample image along a scale pyramid
  ▶ Pixel-CNN for base resolution, e.g. 4×4
  ▶ Autoregressive upsampling networks

▶ Impose group structure among pixels
  ▶ Independent sampling within each group
  ▶ Autoregressive sampling across groups
Sampling pixels in groups

- Group pixels along position in $2 \times 2$ blocks
  - Group 1 given from previous resolution
  - Sample remaining pixels in three steps

![Diagram showing pixel grouping and sampling process](image)
Sampling pixels in groups

- Group pixels along position in $2 \times 2$ blocks
  - Group 1 given from previous resolution
  - Sample remaining pixels in three steps

Example network to predict group 2 from group 1
- Use CNN without pooling to predict/sample new columns
- Interleave pixel columns from group 1 and 2
Example results of upsampling real low-resolution images

- About $100 \times$ speed-up w.r.t. pixel-CNN sampling
Hybrid VAE autoregressive models

[Gulrajani et al., 2017b, Chen et al., 2017]
Hybrid VAE autoregressive models
[Gulrajani et al., 2017b, Chen et al., 2017]

- Variational autoencoder
  - Latent variable $z$ generates global dependencies
  - Pixels conditionally independent given code
Hybrid VAE autoregressive models

[Gulrajani et al., 2017b, Chen et al., 2017]

- Variational autoencoder
  - Latent variable $z$ generates global dependencies
  - Pixels conditionally independent given code

- Autoregressive PixelCNN
  - Needs many layers to induce long-range dependencies
  - Doesn’t learn latent representation
Hybrid PixelVAE model [Gulrajani et al., 2017b]

- Latent var. input to deterministic upsampling decoder $f(z)$
Hybrid PixelVAE model [Gulrajani et al., 2017b]

- Latent var. input to deterministic upsampling decoder $f(z)$
- Pixel-CNN layers induce local pixel dependencies
Hybrid PixelVAE model [Gulrajani et al., 2017b]

- Latent var. input to deterministic upsampling decoder $f(z)$
- Pixel-CNN layers induce local pixel dependencies

$$p(z) = \mathcal{N}(z; 0, I), \quad (43)$$

$$p(x) = \int_z p(z) \prod_i p(x_i | x_{<i}, f(z)) \quad (44)$$
Hierarchical PixelVAE model

- Multiple levels of latent variables at increasing resolutions

\[
F = \ln p(x) - \sum_{i=1}^{L} \mathbb{E}_{q(z_{i+1} | x)} \left[ D_{KL}(q(z_i | x) || p(z_i)) \right]
\]

\[
-E_{z_1 \sim q(z_1 | x)} \log p(x | z_1)
\]
Hierarchical PixelVAE model

- Multiple levels of latent variables at increasing resolutions
- Autoregressive distribution over latent variables in 2D grid
Hierarchical PixelVAE model

- Multiple levels of latent variables at increasing resolutions
- Autoregressive distribution over latent variables in 2D grid
- Extended VAE log-likelihood bound

\[
F = \ln p(x) - D_{KL}(q(z_{1:L}|x)\|p(z_{1:L}|x))
\]

\[
= \mathbb{E}_{q(z_1|x)}[\ln p(x|z_1)] - \sum_{i=1}^{L} \mathbb{E}_{q(z_{i+1})}[D_{KL}(q(z_i|x)\|p(z_i|z_{i+1}))]
\]

Reconstruction

Regularization
Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at $1 \times 1$
  - Latent variables at $8 \times 8$
  - PixelCNN at $64 \times 64$
Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at $1 \times 1$
  - Latent variables at $8 \times 8$
  - PixelCNN at $64 \times 64$

Re-sampling PixelCNN only
Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at $1 \times 1$
  - Latent variables at $8 \times 8$
  - PixelCNN at $64 \times 64$

Re-sampling PixelCNN only
Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at $1 \times 1$
  - Latent variables at $8 \times 8$
  - PixelCNN at $64 \times 64$

Re-sampling PixelCNN only
Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at $1 \times 1$
  - Latent variables at $8 \times 8$
  - PixelCNN at $64 \times 64$

- Hierarchical representation learning

Re-sampling PixelCNN only

Re-sampling $8 \times 8$ + PixelCNN
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