Deep Generative Models
Lecture supp

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ELBO gradient (E-step, $\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta})$)

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \mathbb{E}_q \log p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\theta}) - KL(q(\mathbf{Z}|\mathbf{X}, \phi)||p(\mathbf{Z})) \to \max_{\boldsymbol{\phi},\boldsymbol{\theta}}.$$

Difference from M-step: density function $q(\mathbf{z}|\mathbf{x}, \phi)$ depends on the parameters ϕ, it is impossible to use Monte-Carlo estimation:

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int \nabla_{\boldsymbol{\phi}} q(\mathbf{Z}|\mathbf{X}, \boldsymbol{\phi}) \log p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\theta}) d\mathbf{Z} - \nabla_{\boldsymbol{\phi}} KL$$

Log-derivative trick

$$\nabla_\xi q(\eta|\xi) = q(\eta|\xi) \left(\frac{\nabla_\xi q(\eta|\xi)}{q(\eta|\xi)} \right) = q(\eta|\xi) \nabla_\xi \log q(\eta|\xi).$$

$$\nabla_{\boldsymbol{\phi}} q(\mathbf{Z}|\mathbf{X}, \boldsymbol{\phi}) = q(\mathbf{Z}|\mathbf{X}, \boldsymbol{\phi}) \nabla_{\boldsymbol{\phi}} \log q(\mathbf{Z}|\mathbf{X}, \boldsymbol{\phi}).$$

ELBO gradient (E-step, $\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta})$)

$$\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta}) = \int \nabla_\phi q(\mathbf{Z}|\mathbf{X}, \phi) \log p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\theta}) d\mathbf{Z} - \nabla_\phi KL =$$

$$= \int q(\mathbf{Z}|\mathbf{X}, \phi) \left[\nabla_\phi \log q(\mathbf{Z}|\mathbf{X}, \phi) \log p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\theta})\right] d\mathbf{Z} - \nabla_\phi KL$$

After applying log-reparametrization trick, we are able to use Monte-Carlo estimation:

$$\nabla_\phi \mathcal{L}(\phi, \boldsymbol{\theta}) \approx n \nabla_\phi \log q(\mathbf{z}_i^*|\mathbf{x}_i, \phi) \log p(\mathbf{x}_i|\mathbf{z}_i^*, \boldsymbol{\theta}) - \nabla_\phi KL,$$

$$\mathbf{z}_i^* \sim q(\mathbf{z}_i|\mathbf{x}_i, \phi).$$

Problem

Unstable solution with huge variance.

Solution

Reparametrization trick

IWAE, 2015

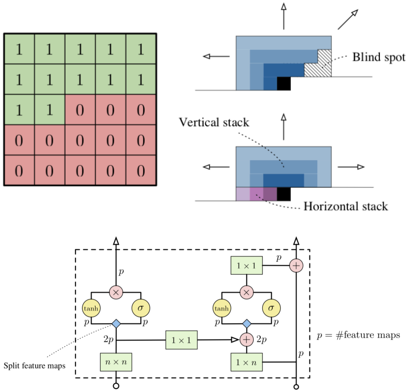
How to determine whether all VAE latent variables are informative?

$$A_i = \mathrm{cov}_{\mathbf{x}} \left(\mathbb{E}_{q(z_i|\mathbf{x})}[z_i] \right) > 0.01 \quad \Leftrightarrow \quad z_i \text{ is active}$$

		MNIST				OMNIGLOT			
		VAE		IWAE		VAE		IWAE	
# stoch. layers	k	NLL	active units	NLL	active units	NLL	active units	NLL	active units
1	1	86.76	19	86.76	19	108.11	28	108.11	28
	5	86.47	20	85.54	22	107.62	28	106.12	34
	50	86.35	20	84.78	25	107.80	28	104.67	41
2	1	85.33	16+5	85.33	16+5	107.58	28+4	107.56	30+5
	5	85.01	17+5	83.89	21+5	106.31	30+5	104.79	38+6
	50	84.78	17+5	82.90	26+7	106.30	30+5	103.38	44+7

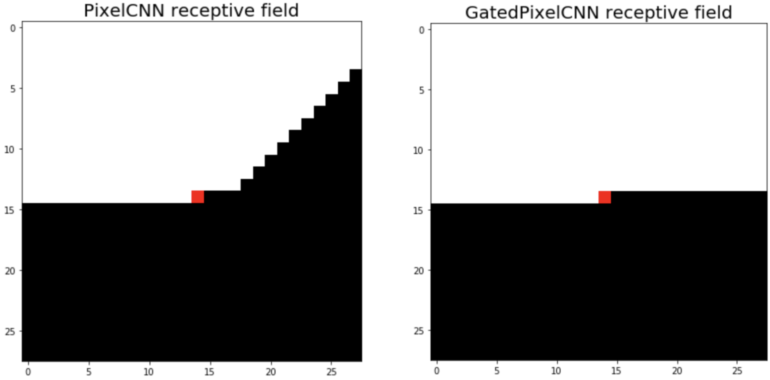
https://arxiv.org/pdf/1509.00519.pdf

GatedPixelCNN (2016)



Van den Oord A. et al. Conditional image generation with pixelcnn decoders
https://arxiv.org/pdf/1606.05328.pdf

GatedPixelCNN (2016)



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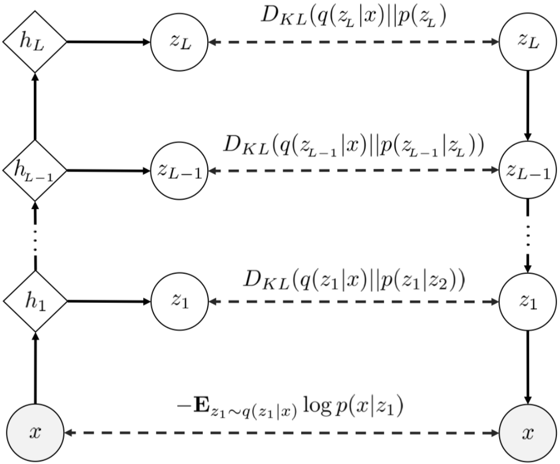
Extensions

- **PixelCNN++**: *Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications*
  https://arxiv.org/pdf/1701.05517.pdf
  (mixture of logistics instead of softmax);
- **PixelSNAIL**: *An Improved Autoregressive Generative Model*
  https://arxiv.org/pdf/1712.09763.pdf
  (self-attention to learn optimal autoregression ordering).

PixelVAE, 2016

Hierarchical VAE



https://arxiv.org/pdf/1611.05013.pdf

PixelVAE, 2016

Hierarchical decomposition

$$p(\mathbf{z}_1, \dots, \mathbf{z}_L) = p(\mathbf{z}_L) p(\mathbf{z}_{L-1}|\mathbf{z}_L) \dots p(\mathbf{z}_1, \mathbf{z}_2);$$
$$q(\mathbf{z}_1, \dots, \mathbf{z}_L|\mathbf{x}) = q(\mathbf{z}_1|\mathbf{x}) \dots q(\mathbf{z}_L|\mathbf{x}).$$

ELBO

$$\begin{aligned}
\mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \boldsymbol{\theta}) - KL(q(\mathbf{z}_1, \dots, \mathbf{z}_L|\mathbf{x})||p(\mathbf{z}_1, \dots, \mathbf{z}_L)) \\
&= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \boldsymbol{\theta}) - \int \prod_{j=1}^{L} q(\mathbf{z}_j|\mathbf{x}) \sum_{i=1}^{L} \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_1 \dots d\mathbf{z}_L \\
&= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \boldsymbol{\theta}) - \sum_{i=1}^{L} \int \prod_{j=1}^{L} q(\mathbf{z}_j|\mathbf{x}) \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_1 \dots d\mathbf{z}_L \\
&= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \boldsymbol{\theta}) - \sum_{i=1}^{L} \int q(\mathbf{z}_{i+1}|\mathbf{x}) q(\mathbf{z}_i|\mathbf{x}) \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_i d\mathbf{z}_{i+1} \\
&= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \boldsymbol{\theta}) - \sum_{i=1}^{L} \mathbb{E}_{q(\mathbf{z}_{i+1}|\mathbf{x})} \left[KL(q(\mathbf{z}_i|\mathbf{x})||p(\mathbf{z}_i|\mathbf{z}_{i+1})) \right]
\end{aligned}$$

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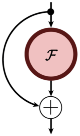
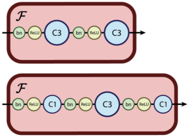
https://arxiv.org/pdf/1611.05013.pdf

RevNets, 2017

- Modern neural networks are trained via backpropagation.
- Residual networks are state of the art in image classification.
- Backpropagation requires storing the network activations.





Problem

Storing the activations imposes an increasing memory burden. GPUs have limited memory capacity, leading to constraints often exceeded by state-of-the-art architectures (with thousand layers).

Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

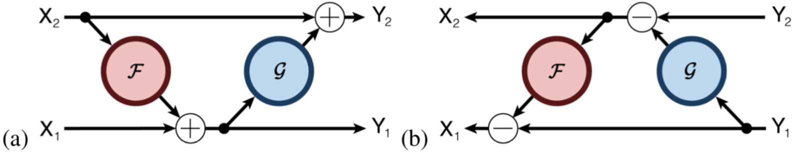
RevNets, 2017

NICE

$$\begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = \mathbf{x}_2 + \mathcal{F}(\mathbf{x}_1, \boldsymbol{\theta}); \end{cases} \quad \Leftrightarrow \quad \begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 - \mathcal{F}(\mathbf{z}_1, \boldsymbol{\theta}). \end{cases}$$

RevNet

$$\begin{cases} \mathbf{y}_1 = \mathbf{x}_1 + \mathcal{F}(\mathbf{x}_2, \boldsymbol{\theta}); \\ \mathbf{y}_2 = \mathbf{x}_2 + \mathcal{G}(\mathbf{y}_1, \boldsymbol{\theta}); \end{cases} \quad \Leftrightarrow \quad \begin{cases} \mathbf{x}_2 = \mathbf{y}_2 - \mathcal{F}(\mathbf{y}_1, \boldsymbol{\theta}); \\ \mathbf{x}_1 = \mathbf{y}_1 - \mathcal{G}(\mathbf{x}_2, \boldsymbol{\theta}). \end{cases}$$



Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

RevNets, 2017

Architecture	CIFAR-10 [15]		CIFAR-100 [15]	
	ResNet	RevNet	ResNet	RevNet
32 (38)	**7.14%**	7.24%	29.95%	**28.96%**
110	**5.74%**	5.76%	26.44%	**25.40%**
164	5.24%	**5.17%**	**23.37%**	23.69%

- If the network contains non-reversible blocks (poolings, strides), activations for these blocks should be stored.
- To avoid storing activations in the modern frameworks, the backward pass should be manually redefined.

Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

i-RevNet, 2018

Hypothesis

The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

- It is difficult to recover images from their hidden representations.
- Information bottleneck principle: an optimal representation must reduce the MI between an input and its representation to reduce uninformative variability + maximize the MI between the output and its representation to preserve each class from collapsing onto other classes.

Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

i-RevNet, 2018

Hypothesis

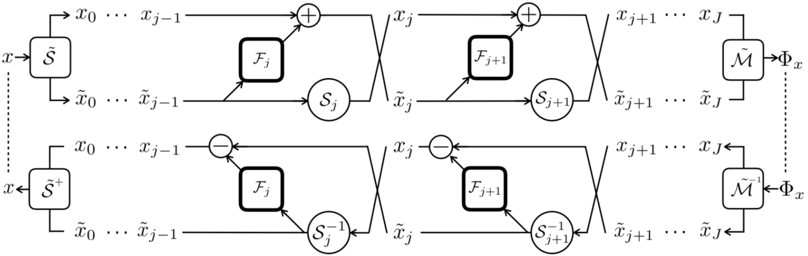
The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

Idea

Build a cascade of homeomorphic layers (i-RevNet), a network that can be fully inverted up to the final projection onto the classes, i.e. no information is discarded.

Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

i-RevNet, 2018



Architecture	Injective	Bijective	Top-1 error	Parameters
ResNet	-	-	24.7	26M
RevNet	-	-	25.2	28M
i-RevNet (a)	yes	-	24.7	181M
i-RevNet (b)	yes	yes	26.7	29M

Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

InfoGAN

GAN objective

$$\min_G \max_D V(G, D)$$

$$V(G, D) = \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z})))$$

Latent vector $\mathbf{z}$ is not imposed to be disentangled.
InfoGAN decomposes input vector:

- $\mathbf{z}$ – incompressible noise;
- $\mathbf{c}$ – structured latent code $p(\mathbf{c}) = \prod_{j=1}^{d} p(c_j)$.

Information-theoretic regularization

$$\max I(\mathbf{c}, G(\mathbf{z}, \mathbf{c}))$$

Information in the latent code $\mathbf{c}$ should not be lost in the generation process.

Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016

InfoGAN

Objective

$$\min_G \max_D V(G, D) - \lambda I(\mathbf{c}, G(\mathbf{z}, \mathbf{c}))$$

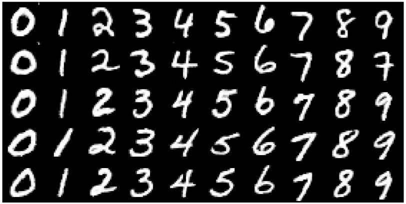
Variational Information Maximization

$$\begin{aligned}
I(\mathbf{c}, G(\mathbf{z}, \mathbf{c})) = H(\mathbf{c}) - H(\mathbf{c}|G(\mathbf{z}, \mathbf{c})) = \\
= H(\mathbf{c}) + \mathbb{E}_{\mathbf{x}\sim G(\mathbf{z},\mathbf{c})}\left[\mathbb{E}_{\mathbf{c}'\sim p(\mathbf{c}|\mathbf{x})} \log p(\mathbf{c}'|\mathbf{x})\right] = \\
= H(\mathbf{c}) + \mathbb{E}_{\mathbf{x}\sim G(\mathbf{z},\mathbf{c})} KL(p(\mathbf{c}'|\mathbf{x})||q(\mathbf{z}'|\mathbf{x})) + \\
+ \mathbb{E}_{\mathbf{x}\sim G(\mathbf{z},\mathbf{c})}\mathbb{E}_{\mathbf{c}'\sim p(\mathbf{c}|\mathbf{x})} \log q(\mathbf{c}'|\mathbf{x}) \geq \\
\geq H(\mathbf{c}) + \mathbb{E}_{\mathbf{x}\sim G(\mathbf{z},\mathbf{c})}\mathbb{E}_{\mathbf{c}'\sim p(\mathbf{c}|\mathbf{x})} \log q(\mathbf{c}'|\mathbf{x}) = \\
H(\mathbf{c}) + \mathbb{E}_{\mathbf{c}\sim p(\mathbf{c})}\mathbb{E}_{\mathbf{x}\sim G(\mathbf{z},\mathbf{c})} \log q(\mathbf{c}|\mathbf{x})
\end{aligned}$$

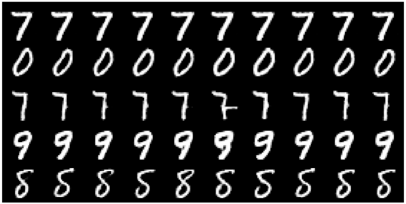
Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016

InfoGAN

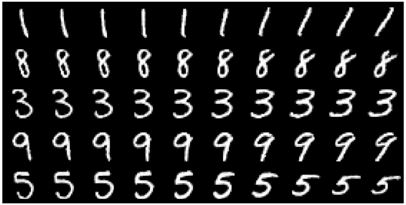
Latent codes on MNIST



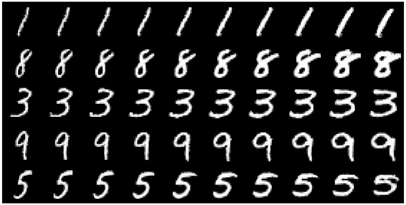
(a) Varying c_1 on InfoGAN (Digit type)



(b) Varying c_1 on regular GAN (No clear meaning)



(c) Varying c_2 from -2 to 2 on InfoGAN (Rotation)

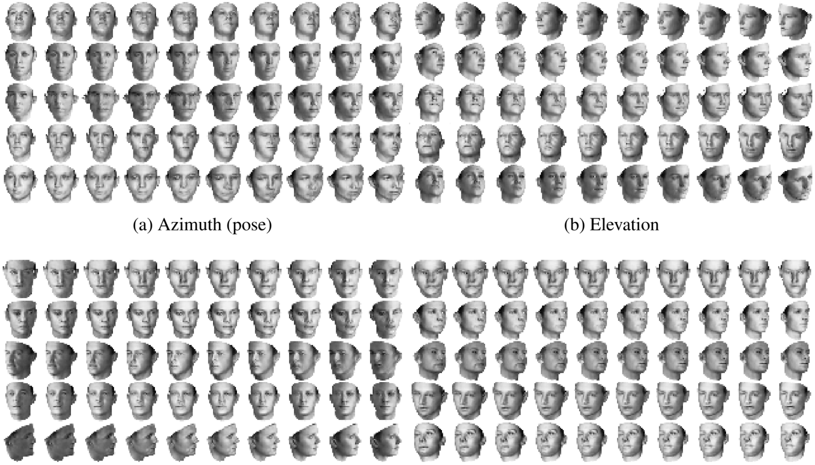


(d) Varying c_3 from -2 to 2 on InfoGAN (Width)

Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016

InfoGAN

Latent codes on 3D Faces



(a) Azimuth (pose) (b) Elevation

(c) Lighting (d) Wide or Narrow

Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016