Deep Generative Models

Lecture 8

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Recap of previous lecture

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z})) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}],$$

ELBO surgery

$$\frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) = \underbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Optimal prior

$$KL(q(\mathbf{z})||p(\mathbf{z})) = 0 \quad \Leftrightarrow \quad p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i).$$

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

Recap of previous lecture

Optimal prior

$$KL(q(\mathbf{z})||p(\mathbf{z})) = 0 \quad \Leftrightarrow \quad p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i).$$

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.

VampPrior

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K}\sum_{k=1}^{K} q(\mathbf{z}|\mathbf{u}_k),$$

where $\boldsymbol{\lambda} = \{\mathbf{u}_1, \dots, \mathbf{u}_K\}$ are trainable pseudo-inputs.

Flow-based VAE prior

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\boldsymbol{\epsilon}) + \log \det \left| \frac{d\boldsymbol{\epsilon}}{d\mathbf{z}} \right| = \log p(\boldsymbol{\epsilon}) + \log \det \left| \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right|$$

Tomczak J. M., Welling M. VAE with a VampPrior, 2017
Chen X. et al. Variational Lossy Autoencoder, 2016

Flows in VAE posterior

Apply a sequence of transformations to the random variable

$$\mathbf{z}_0 \sim q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

Let $q(\mathbf{z}|\mathbf{x}, \phi)$ (VAE encoder) be a base distribution for a flow model.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \det \left| \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right|$$

$$\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda}) = g^{-1}(\mathbf{z}, \boldsymbol{\lambda})$$

Here $f(\mathbf{z}, \boldsymbol{\lambda})$ is a flow model (e.g. stack of planar/coupling layers) parameterized by $\boldsymbol{\lambda}$.
Let use $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$ as a variational distribution. Here ϕ – encoder parameters, $\boldsymbol{\lambda}$ – flow parameters.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows-based VAE posterior

- Encoder outputs base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- Flow model $\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda})$ transforms the base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$ to the distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$.
- Distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$ is used as a variational distribution for ELBO maximization.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \det \left| \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right|$$

ELBO with flow-based VAE posterior

$$\begin{aligned} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \bigl[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})\bigr] \\ &= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) - KL(q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})||p(\mathbf{z}^*)). \end{aligned}$$

The second term in ELBO is reverse KL divergence. Planar flows was originally proposed for variational inference in VAE.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows-based VAE posterior

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \det \left| \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right|$$

ELBO objective

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \bigl[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})\bigr] =$$

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \bigl[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})\bigr]\bigr|_{\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda})} =$$

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right) \right| \right].$$

- Obtain samples $\mathbf{z}$ from the encoder $q(\mathbf{z}|\mathbf{x}, \phi)$.
- Apply flow model $\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda})$.
- Compute likelihood for $\mathbf{z}^*$ using the decoder, base distribution for $\mathbf{z}^*$ and the Jacobian.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Inverse autoregressive flow (IAF)

$$\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \quad \Rightarrow \quad x_i = \tilde{\sigma}_i(\mathbf{z}_{1:i-1}) \cdot z_i + \tilde{\mu}_i(\mathbf{z}_{1:i-1}).$$

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad \Rightarrow \quad z_i = (x_i - \tilde{\mu}_i(\mathbf{z}_{1:i-1})) \cdot \frac{1}{\tilde{\sigma}_i(\mathbf{z}_{1:i-1})}.$$

Reverse KL for flow model

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| - \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) \right]$$

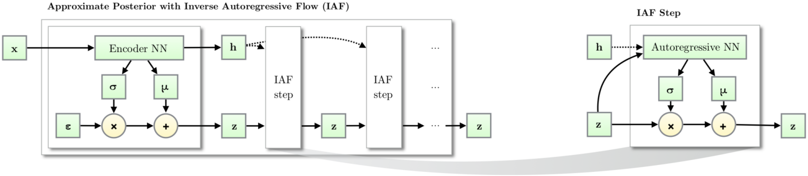
- We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.
- Inverse autoregressive flow is a natural choice for using flows in VAE:

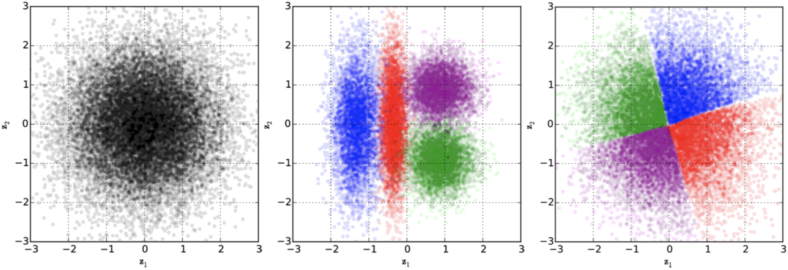
$$\mathbf{z} = \boldsymbol{\sigma}(\mathbf{x}) \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}|\mathbf{x}, \phi).$$

$$\mathbf{z}_k = \tilde{\boldsymbol{\sigma}}_k(\mathbf{z}_{k-1}) \odot \mathbf{z}_{k-1} + \tilde{\boldsymbol{\mu}}_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k|\mathbf{x}, \phi, \{\boldsymbol{\lambda}_j\}_{j=1}^k).$$

Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Inverse autoregressive flow (IAF)





(a) Prior distribution (b) Posteriors in standard VAE (c) Posteriors in VAE with IAF

Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Flows-based VAE prior vs posterior

Theorem

VAE with the flow-based prior for latent code $\mathbf{z}$ is equivalent to using flow-based posterior for latent code $\boldsymbol{\epsilon}$.

Proof

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \underbrace{KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}|\boldsymbol{\lambda}))}_{\text{flow-based prior}} \\
&= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \underbrace{KL(q(\mathbf{z}|\mathbf{x}, \phi, \boldsymbol{\lambda}) || p(\mathbf{z}))}_{\text{flow-based posterior}}
\end{aligned}
$$

(Here we use Flow KL duality theorem from Lecture 4)

Flows in VAE posterior

$$
\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}, \mathbf{z}^* | \boldsymbol{\theta}) - \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right) \right| \right].
$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Flows-based VAE prior vs posterior

- IAF posterior decoder path: $p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})$, $\mathbf{z} \sim p(\mathbf{z})$.
- AF prior decoder path: $p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})$, $\mathbf{z} = g(\boldsymbol{\epsilon},\boldsymbol{\lambda})$, $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$.

The AF prior and the IAF posterior have the same computation cost, so using the AF prior makes the model more expressive at no training time cost.

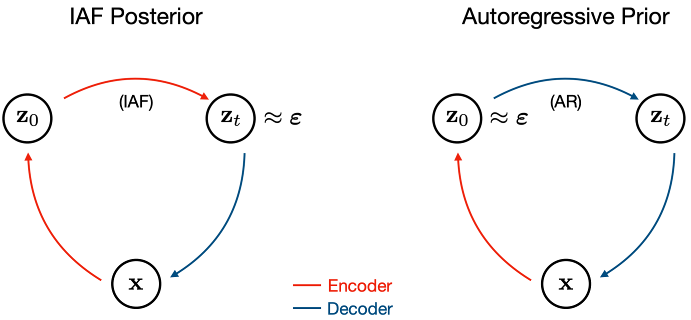


image credit: https://courses.cs.washington.edu/courses/cse599i/20au

Dequantization

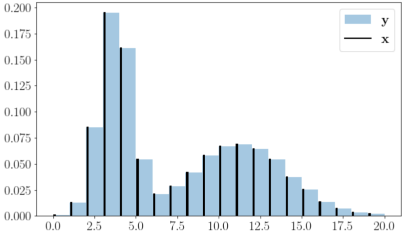
- Images are discrete data, pixels lie in the $\{0, 255\}$ integer domain (the model is $P(\mathbf{x}|\boldsymbol{\theta}) = \text{Categorical}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Flow is a continuous model (it works with continuous data $\mathbf{x}$).

By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.
How to convert a discrete data distribution to a continuous one?

Uniform dequantization

$$\mathbf{x} \sim \text{Categorical}(\boldsymbol{\pi})$$
$$\mathbf{u} \sim U[0, 1]$$

$$\mathbf{y} = \mathbf{x} + \mathbf{u} \sim \text{Continuous}$$



Theis L., Oord A., Bethge M. A note on the evaluation of generative models. 2015

Uniform dequantization

Statement

Fitting continuous model $p(\mathbf{y}|\boldsymbol{\theta})$ on uniformly dequantized data $\mathbf{y} = \mathbf{x} + \mathbf{u}$, $\mathbf{u} \sim U[0,1]$ is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

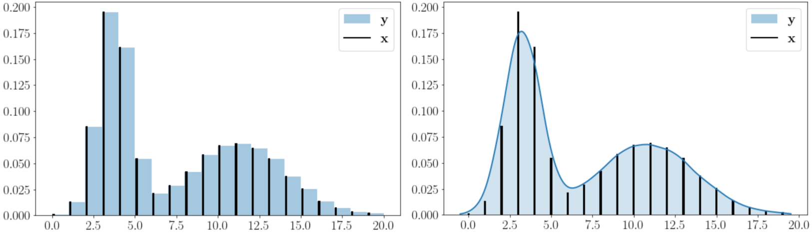
$$P(\mathbf{x}|\boldsymbol{\theta}) = \int_{U[0,1]} p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

Proof

$$\begin{aligned}
\mathbb{E}_\pi \log p(\mathbf{y}|\boldsymbol{\theta}) = \int \pi(\mathbf{y}) \log p(\mathbf{y}|\boldsymbol{\theta}) d\mathbf{y} = \\
&= \sum \pi(\mathbf{x}) \int_{U[0,1]} \log p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \leq \\
&\leq \sum \pi(\mathbf{x}) \log \int_{U[0,1]} p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} = \\
&= \sum \pi(\mathbf{x}) \log P(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_\pi \log P(\mathbf{x}|\boldsymbol{\theta}).
\end{aligned}$$

Theis L., Oord A., Bethge M. A note on the evaluation of generative models. 2015

Variational dequantization



- $p(\mathbf{y}|\boldsymbol{\theta})$ assign unifrom density to unit hypercubes $\mathbf{x} + U[0, 1]$ (left fig).
- Neural network density models are smooth function approximators (right fig).
- Smooth dequantization is more natural.

How to perform the smooth dequantization?

Flow++

Variational dequantization

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{x})$ and treat it as an approximate posterior.

Variational lower bound

$$\log P(\mathbf{x}|\boldsymbol{\theta}) = \left[\log \int q(\mathbf{u}|\mathbf{x}) \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u}\right] \geq$$
$$\geq \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} = \mathcal{L}(q, \boldsymbol{\theta}).$$

Uniform dequantization bound

$$\log P(\mathbf{x}|\boldsymbol{\theta}) = \log \int_{U[0,1]} p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \geq \int_{U[0,1]} \log p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}.$$

Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0,1]$).

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Flow++

Variational lower bound

$$\mathcal{L}(q, \boldsymbol{\theta}) = \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u}.$$

Let $\mathbf{u} = h(\boldsymbol{\epsilon}, \boldsymbol{\phi})$ is a flow model with base distribution $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon}) = \mathcal{N}(0, \mathbf{I})$:

$$q(\mathbf{u}|\mathbf{x}) = p(h^{-1}(\mathbf{u}, \boldsymbol{\phi})) \cdot \left| \det \frac{\partial h^{-1}(\mathbf{u}, \boldsymbol{\phi})}{\partial \mathbf{u}} \right|.$$

Flow-based variational dequantization

$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{x} + h(\boldsymbol{\epsilon}, \boldsymbol{\phi})|\boldsymbol{\theta})}{p(\boldsymbol{\epsilon}) \cdot \left| \det \frac{\partial h(\boldsymbol{\epsilon}, \boldsymbol{\phi})}{\partial \boldsymbol{\epsilon}} \right|^{-1}} \right) d\boldsymbol{\epsilon}.$$

If $p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Flow++

Flow-based variational dequantization

$$\log P(\mathbf{x}|\theta) \geq \int p(\epsilon) \log \left(\frac{p(\mathbf{x} + h(\epsilon, \phi))}{p(\epsilon) \cdot \left| \det \frac{\partial h(\epsilon, \phi)}{\partial \epsilon} \right|^{-1}} \right) d\epsilon.$$

Table 1. Unconditional image modeling results in bits/dim

Model family	Model	CIFAR10	ImageNet 32x32	ImageNet 64x64
Non-autoregressive	RealNVP (Dinh et al., 2016)	3.49	4.28	–
	Glow (Kingma & Dhariwal, 2018)	3.35	4.09	3.81
	IAF-VAE (Kingma et al., 2016)	3.11	–	–
	Flow++ (ours)	**3.08**	**3.86**	**3.69**
Autoregressive	Multiscale PixelCNN (Reed et al., 2017)	–	3.95	3.70
	PixelCNN (van den Oord et al., 2016b)	3.14	–	–
	PixelRNN (van den Oord et al., 2016b)	3.00	3.86	3.63
	Gated PixelCNN (van den Oord et al., 2016c)	3.03	3.83	3.57
	PixelCNN++ (Salimans et al., 2017)	2.92	–	–
	Image Transformer (Parmar et al., 2018)	2.90	3.77	–
	PixelSNAIL (Chen et al., 2017)	2.85	3.80	3.52

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

VAE limitations

- Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\mathbf{x})).$$

- Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

- Poor probabilistic model (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{z})).$$

- Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

Disentangled representations

Unsupervised representation learning

Learning an interpretable factorised representation of the independent data generative factors of the world without supervision.

Disentanglement informal definition

A disentangled representation can be defined as one where single latent units are sensitive to changes in single generative factors, while being relatively invariant to changes in other factors.

Example

Model trained on a dataset of 3D objects might learn independent latent units sensitive to single independent data generative factors, such as object identity, position, scale, lighting or colour.

Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

Disentanglement learning

Generative process

- $\pi(\mathbf{x}|\mathbf{v}, \mathbf{w}) = \mathrm{Sim}(\mathbf{v}, \mathbf{w})$ – true world simulator;
- $\mathbf{v}$ – conditionally independent factors: $\pi(\mathbf{v}|\mathbf{x}) = \prod_{j=1}^{d} \pi(v_j|\mathbf{x})$;
- $\mathbf{w}$ – conditionally dependent factors.

Goal

Construct an unsupervised deep generative model

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \pi(\mathbf{x}|\mathbf{v}, \mathbf{w}).$$

- Ensure that the inferred latent factors $q(\mathbf{z}|\mathbf{x})$ capture the factors $\mathbf{v}$ in a disentangled manner.
- The conditionally dependent factors $\mathbf{w}$ can remain entangled in a separate subset of $\mathbf{z}$ that is not used for representing $\mathbf{v}$.

Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

β-VAE

ELBO objective

$$\mathcal{L}(q, \boldsymbol{\theta}, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})).$$

What do we get at $\beta = 1$?

Constrained optimization

$$\max_{q, \boldsymbol{\theta}} \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}), \quad \text{subject to } KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) < \epsilon.$$

Hypothesis

We are able to learn disentangled representations of the independent factors $\mathbf{v}$ by setting a stronger constraint with $\beta > 1$.

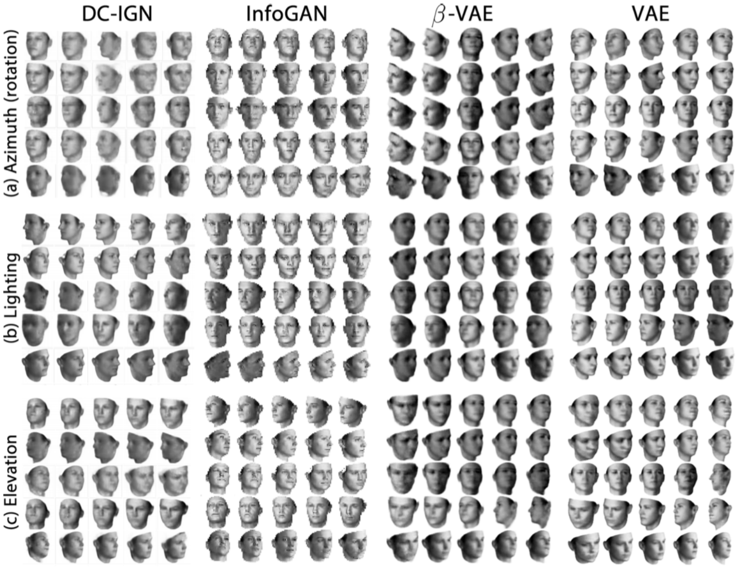
Note: It leads to poorer reconstructions and a loss of high frequency details.

Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

β-VAE

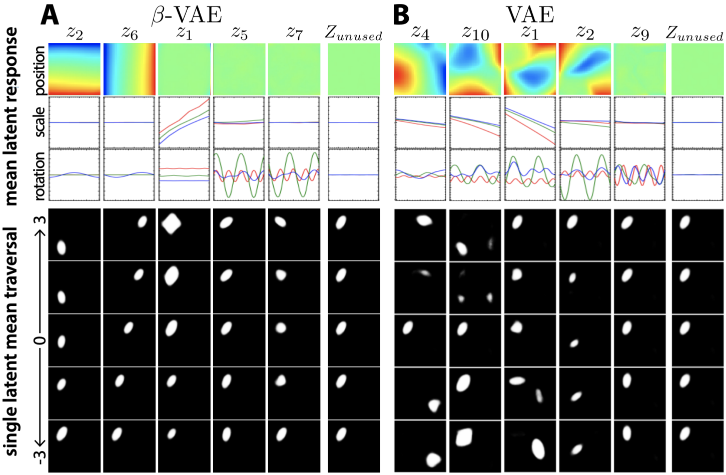
Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

β-VAE



Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

β-VAE



Higgins I. et al. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework, 2017

β-VAE

ELBO

$$\mathcal{L}(q, \boldsymbol{\theta}, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})).$$

ELBO surgery

$$\frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}, \beta) = \underbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \beta \cdot \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \beta \cdot \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Minimization of MI

- It is not necessary and not desirable for disentanglement.
- It hurts reconstruction.

Burgess C. P. et al. Understanding disentangling in β-VAE, 2018

DIP-VAE

Disentangled aggregated variational posterior

$$q(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}) = \prod_{j=1}^{d} q(z_j)$$

DIP-VAE Objective

$$\mathcal{L}_{\text{DIP}}(q, \boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) - \lambda \cdot KL(q(\mathbf{z})||p(\mathbf{z})) =$$

$$= \frac{1}{n}\sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z}))\right] - \lambda \cdot KL(q(\mathbf{z})||p(\mathbf{z})) =$$

$$= \underbrace{\frac{1}{n}\sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \boldsymbol{\theta})\right]}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - (1 + \lambda) \cdot \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Kumar A., Sattigeri P., Balakrishnan A. Variational Inference of Disentangled Latent Concepts from Unlabeled Observations, 2017

DIP-VAE

$$\mathcal{L}_{\text{DIP}}(q, \boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) - \lambda \cdot \underbrace{KL(q(\mathbf{z}) || p(\mathbf{z}))}_{\text{intractable}}$$

Let match the moments of $q(\mathbf{z})$ and $p(\mathbf{z})$:

$$\text{cov}_{q(\mathbf{z})}(\mathbf{z}) = \mathbb{E}_{q(\mathbf{z})} \left[(\mathbf{z} - \mathbb{E}_{q(\mathbf{z})}(\mathbf{z}))(\mathbf{z} - \mathbb{E}_{q(\mathbf{z})}(\mathbf{z}))^T \right]$$

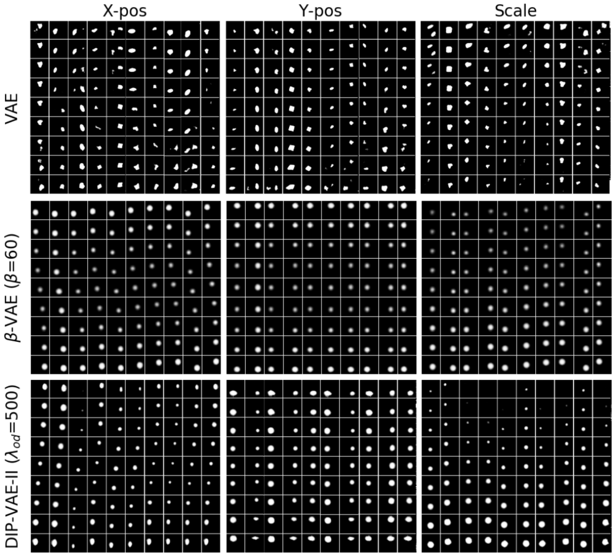
DIP-VAE regularizes $\text{cov}_{q(\mathbf{z})}(\mathbf{z})$ to be close to the identity matrix.

Objective

$$\max_{q, \boldsymbol{\theta}} \Big[\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) - \\ - \lambda_1 \sum_{i \neq j} \left[\text{cov}_{q(\mathbf{z})}(\mathbf{z}) \right]_{ij}^2 - \lambda_2 \sum_i \left(\left[\text{cov}_{q(\mathbf{z})}(\mathbf{z}) \right]_{ii} - 1 \right)^2 \Big]$$

Kumar A., Sattigeri P., Balakrishnan A. Variational Inference of Disentangled Latent Concepts from Unlabeled Observations, 2017

DIP-VAE



Kumar A., Sattigeri P., Balakrishnan A. Variational Inference of Disentangled Latent Concepts from Unlabeled Observations, 2017

Challenging Disentanglement Assumptions

Whether unsupervised disentanglement learning is even possible for arbitrary generative models?

Theorem

For $d > 1$, let $\mathbf{z} \sim P$ denote any distribution which admits a density $p(\mathbf{z}) = \prod_{i=1}^{d} p(z_i)$. Then, there exists an infinite family of bijective functions $f : \mathrm{supp}(\mathbf{z}) \to \mathrm{supp}(\mathbf{z})$ such that

- $\frac{\partial f_i(\mathbf{z})}{\partial z_j} \neq 0$ almost everywhere for all i and j (i.e., $\mathbf{z}$ and $f(\mathbf{z})$ are completely entangled);
- and $P(\mathbf{z} \leq \mathbf{u}) = P(f(\mathbf{z}) \leq \mathbf{u})$ for all $\mathbf{u} \in \mathrm{supp}(\mathbf{z})$ (i.e., they have the same marginal distribution).

Theorem claims that unsupervised disentanglement learning is impossible for arbitrary generative models with a factorized prior.

Locatello F. et al. Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations, 2018

Challenging Disentanglement Assumptions

Assume we have $p(\mathbf{z})$ and some $p(\mathbf{x}|\mathbf{z})$ defining a generative model. Consider any unsupervised disentanglement method and assume that it finds a representation that is perfectly disentangled with respect to $\mathbf{z}$ in the generative model.

- Theorem claims that $\exists\ \hat{\mathbf{z}} = f(\mathbf{z})$ where $\hat{\mathbf{z}}$ is completely entangled with respect to $\mathbf{z}$.
- Since the (unsupervised) disentanglement method only has access to observations $\mathbf{x}$, it hence cannot distinguish between the two equivalent generative models and thus has to be entangled to at least one of them

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} = \int p(\mathbf{x}|\hat{\mathbf{z}})p(\hat{\mathbf{z}})d\hat{\mathbf{z}}.$$

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Proof (1)

1. Consider the function $g : \text{supp}(\mathbf{z}) \to [0,1]^d$:

$$g_i(\mathbf{u}) = P(z_i \leq u_i), \quad i = 1, \ldots, d.$$

   - g is bijective (since $p(\mathbf{z}) = \prod_{i=1}^{d} p(z_i)$).
   - $\frac{\partial g_i(\mathbf{u})}{\partial u_i} \neq 0$, for all i and $\frac{\partial g_i(\mathbf{u})}{\partial u_j} = 0$ for all $i \neq j$.
   - $g(\mathbf{z})$ is an independent d-dimensional uniform distribution.

2. Consider $h : (0,1]^d \to \mathbb{R}^d$

$$h_i(\mathbf{u}) = \psi^{-1}(u_i), \quad i = 1, \ldots, d.$$

   Here ψ denotes the CDF of a standard normal distribution.

   - h is bijective.
   - $\frac{\partial h_i(\mathbf{u})}{\partial u_i} \neq 0$, for all i and $\frac{\partial h_i(\mathbf{u})}{\partial u_j} = 0$ for all $i \neq j$.
   - $h(g(\mathbf{z}))$ is a d-dimensional standard normal distribution.

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Proof (2)

Let $\mathbf{A} \in \mathbb{R}^{d \times d}$ be an arbitrary orthogonal matrix with $A_{ij} \neq 0$ for all i, j. The family of such matrices is infinite.

- $\mathbf{A}$ is orthogonal, it is invertible and thus defines a bijective linear operator.
- $\mathbf{A}h(g(\mathbf{z})) \in \mathbb{R}^d$ is hence an independent, multivariate standard normal distribution.
- $h^{-1}(\mathbf{A}h(g(\mathbf{z}))) \in \mathbb{R}^d$ is an independent d-dimensional uniform distribution.

Define $f : \text{supp}(\mathbf{z}) \to \text{supp}(\mathbf{z})$:

$$f(\mathbf{u}) = g^{-1}(h^{-1}(\mathbf{A}h(g(\mathbf{z})))).$$

By definition $f(\mathbf{z})$ has the same marginal distribution as $\mathbf{z}$: $P(\mathbf{z} \leq \mathbf{u}) = P(f(\mathbf{z}) \leq \mathbf{u})$ and $\frac{\partial f_i(\mathbf{z})}{\partial z_j} \neq 0$.

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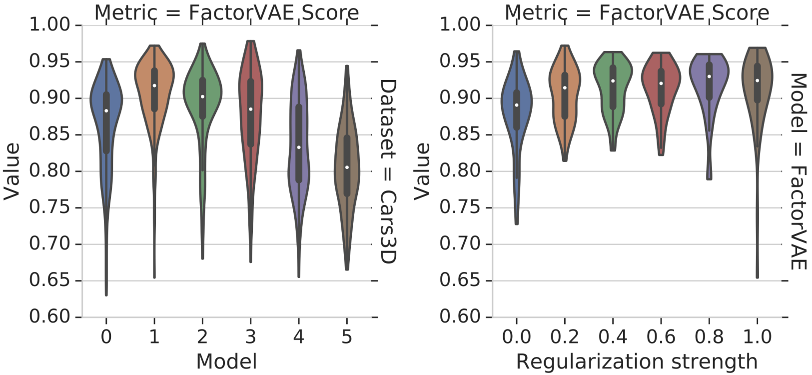
Challenging Disentanglement Assumptions

Importance of different models and hyperparameters for disentanglement



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Challenging Disentanglement Assumptions

Agreement of different disentanglement metrics

Dataset = Noisy-dSprites

	(A)	(B)	(C)	(D)	(E)	(F)
BetaVAE Score (A)	100	80	44	41	46	37
FactorVAE Score (B)	80	100	49	52	25	38
MIG (C)	44	49	100	76	6	42
DCI Disentanglement (D)	41	52	76	100	-8	38
Modularity (E)	46	25	6	-8	100	13
SAP (F)	37	38	42	38	13	100

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Summary

- Uniform dequantization is the simplest form of dequantization.
- Variational dequantization is a more natural type that was proposed in Flow++ model.
- Disentanglement learning tries to make latent components more informative.
- β-VAE makes the latent components more independent, but the reconstructions get poorer.