10417-617
Deep Learning: Fall 2020

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Lecture 16:
Variational autoencoders, evaluating representations

Recap: the simplest of representation learners

Sparse coding: learn features, s.t. each input can be written as a *sparse linear combination* of some of these features.

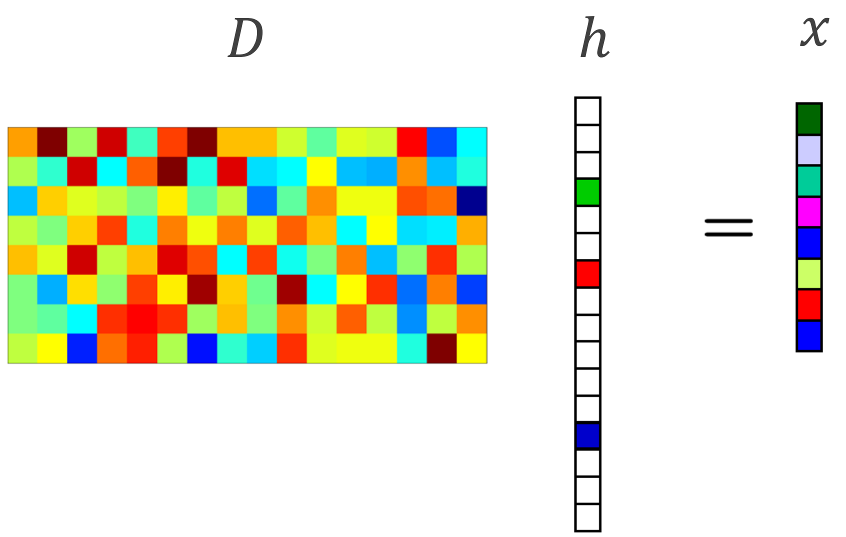
Originally made famous by *Olshausen and Field,* '96 as a model for how early visual processing works (edge detection etc.)

Autoencoders: learn encoding with some constraints (e.g. functional form, sparsity, denoising ability) from which the inputs can be approximately reconstructed.

Sparse coding

Goal: learn a *dictionary* D of features, s.t. each sample x is (approximately) writeable as a *sparse* (i.e. mostly zeros) linear combination of these features.

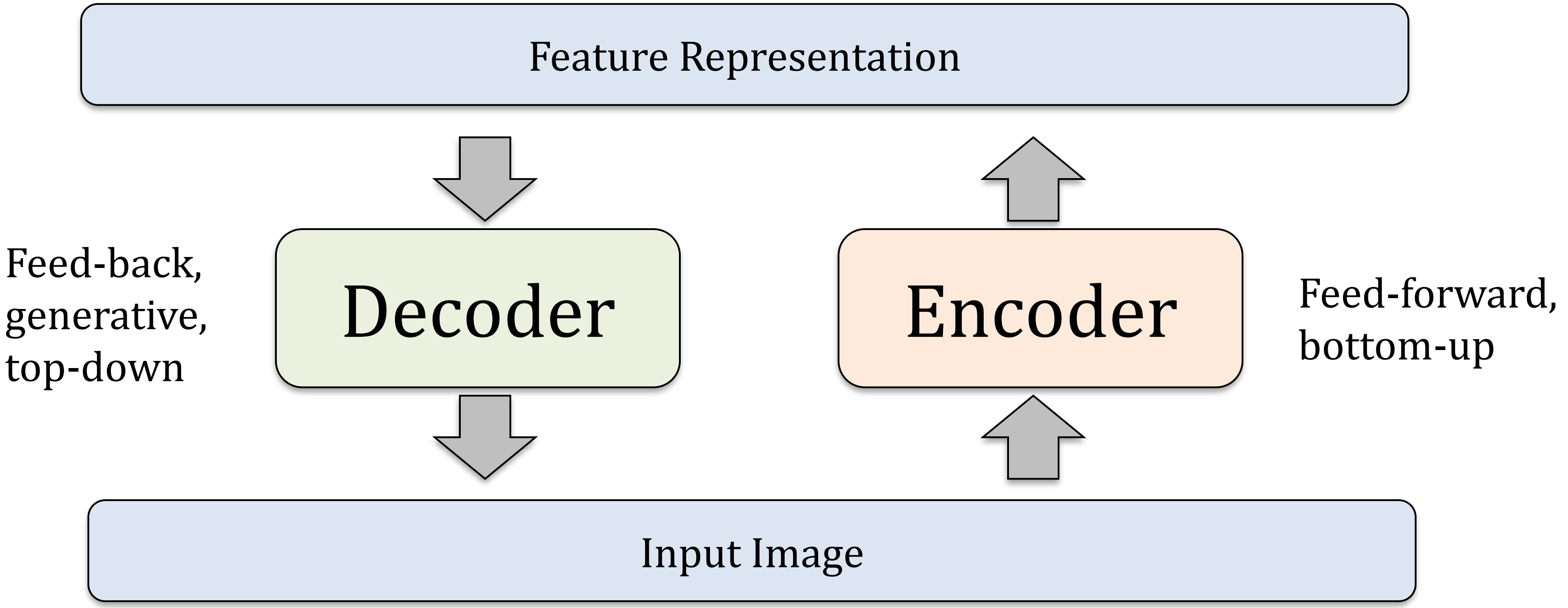
$$\forall x: \quad x \approx Dh, \qquad \|h\|_0 \text{ small}$$



h is the representation of sample x

Autoencoders

The idea behind autoencoders: learn features, s.t. input is reconstructable from them



- Details of what goes insider the encoder and decoder matter!
- Need *constraints* to **avoid learning an identity**.

Autoencoders

Some way to prevent identity:

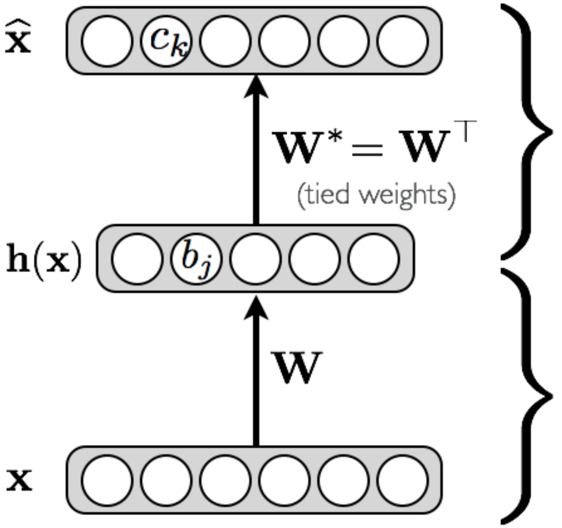
•*Weight tying* of encoder/decoder. (Often magical!)

•*Smaller dimension* for latent variables

•Enforce *sparsity* of the latent representation

•Encourage decoder to be robust to adding noise to x. (*Denoising autoencoder*)

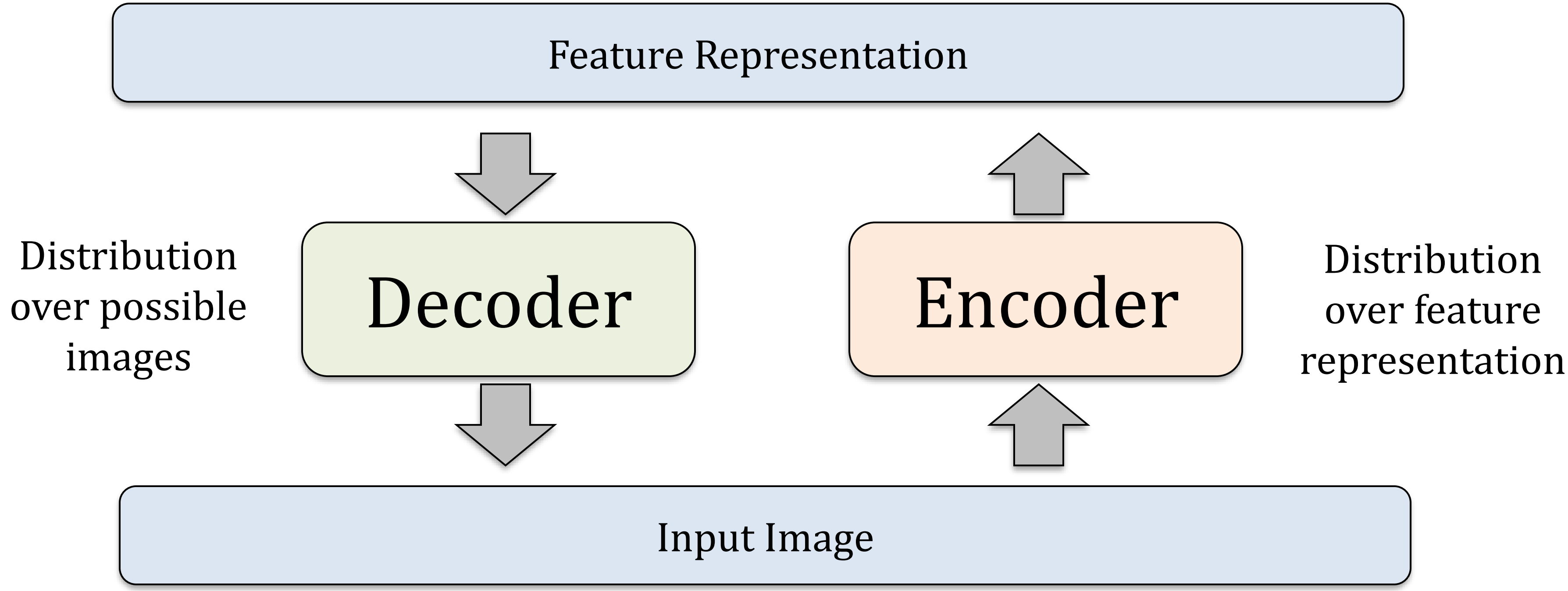
•Encode to distribution rather than pointmass. (*Variational autoencoder*)



Variational autoencoders

The idea: the encoder can output a *distribution*, rather than a *point mass*.

We will derive this via a variational approach.

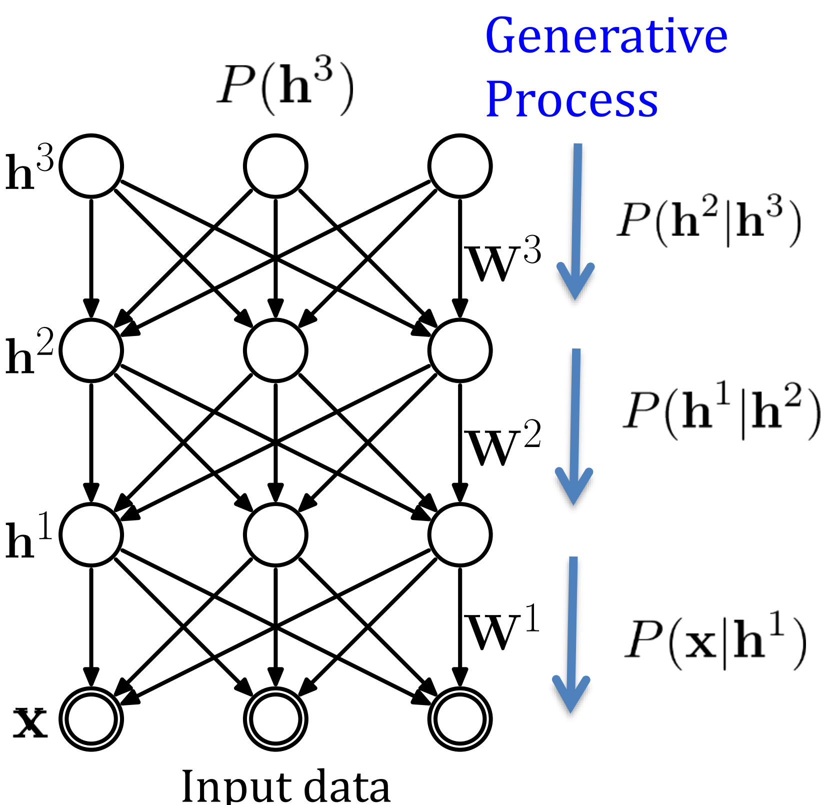


Variational autoencoders

"*Decoder/generator*": directed Bayesian network with Gaussian layers

$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{\mathbf{h}^1,\ldots,\mathbf{h}^L} p(\mathbf{h}^L|\boldsymbol{\theta})p(\mathbf{h}^{L-1}|\mathbf{h}^L,\boldsymbol{\theta})\cdots p(\mathbf{x}|\mathbf{h}^1,\boldsymbol{\theta})$$

Each term may denote a complicated nonlinear relationship



Typically, directed layers are parametrized as:

$$p(\boldsymbol{h}^{L-1}|\boldsymbol{h}^L,\boldsymbol{\theta}) = \mathcal{N}(\mu_{\boldsymbol{\theta}}(\boldsymbol{h}^L),\Sigma_\theta(\boldsymbol{h}^L))$$

Gaussians, means/covariances functions (e.g. one-layer neural net) of previous layer and model parameters θ.

Easy to sample!

Where does an "encoder" come in?

"*Decoder/generator*": directed Bayesian network with Gaussian layers

$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{\mathbf{h}^1,\ldots,\mathbf{h}^L} p(\mathbf{h}^L|\boldsymbol{\theta})p(\mathbf{h}^{L-1}|\mathbf{h}^L,\boldsymbol{\theta})\cdots p(\mathbf{x}|\mathbf{h}^1,\boldsymbol{\theta})$$

Recall *learning via variational inference*:

ELBO:
$$\log\ p(x) = \max_{q(h^L|x)} H\big(q(h^L|x)\big) + \mathbb{E}_{q(h^L|x)}[\log p(x,h^L)]$$

Max-likelihood can be written as:

$$\max_{\theta\in\Theta} \max_{\{q(h^L|x)\}} \sum_{i=1}^{n} H(q(h^L|x)) + \mathbb{E}_{q(h^L|x)}[\log p(x,h^L)]$$

"*Encoder:*" a directed Bayesian network approximating $q(h^L|x)$

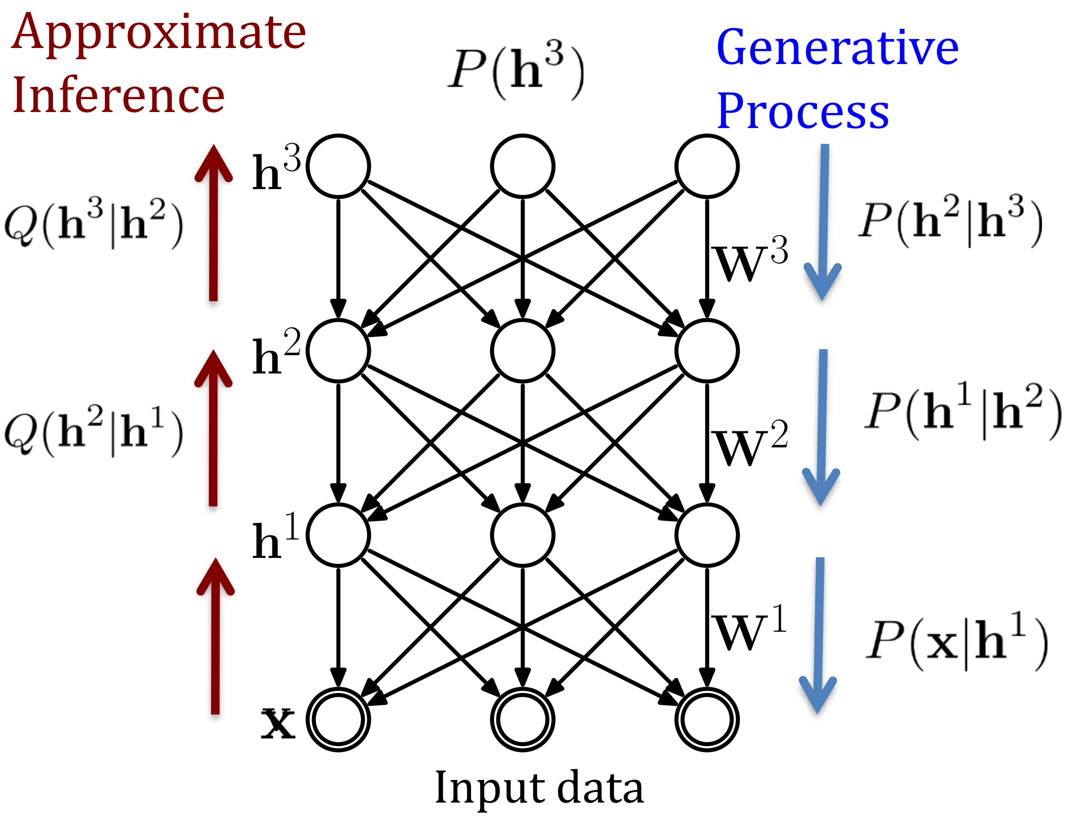
It will be a directed Bayesian network in the "reverse" direction.

Encoder: A "recognition network"

The encoder is defined in terms of an analogous factorization:

$$q(\boldsymbol{h}|\boldsymbol{x},\boldsymbol{\theta}) = q(\boldsymbol{h}^1|\boldsymbol{x},\boldsymbol{\theta})q(\boldsymbol{h}^2|\boldsymbol{h}^1,\boldsymbol{\theta}) \ldots q(\boldsymbol{h}^L|\boldsymbol{h}^{L-1},\boldsymbol{\theta})$$

Each term may denote a complicated nonlinear relationship



Typically, directed layers are parametrized as:

$$q(\boldsymbol{h}^l|\boldsymbol{h}^{l-1},\boldsymbol{\theta}) = \mathcal{N}(\mu_{\boldsymbol{\theta}}(\boldsymbol{h}^{l-1}),\Sigma_{\boldsymbol{\theta}}(\boldsymbol{h}^{l-1}))$$

Means/covariances fns (e.g. one-layer neural net) of previous layer and parameters $\boldsymbol{\theta}$.

Why is this called an "encoder"?

Max-likelihood can be written as:

$$\max_{\theta\in\Theta} \max_{\{q(h^L|x)\}} \sum_{i=1}^{n} H(q(h^L|x)) + \mathbb{E}_{q(h^L|x)}[\log p(x,h^L)]$$

Let's rewrite the ELBO a bit:

$$H\big(q(h^L|x)\big) + \mathbb{E}_{q(h^L|x)}[\log p(x,h^L)] = \mathbb{E}_{q(h^L|x)}[\log p(x,h^L) - \log q(h^L|x)]$$

$$= \mathbb{E}_{q(h^L|x)}[\log p(h^L) + \log p(x|h^L) - \log q(h^L|x)]$$

$$= \mathbb{E}_{q(h^L|x)} \log p(x|h^L) - \mathbb{E}_{q(h^L|x)} \log \frac{q\big(h^L|x\big)}{p(h^L)}$$

$$= \underbrace{\mathbb{E}_{q(h^L|x)} \log p(x|h^L)} - \underbrace{KL\big(q(h^L|x)\big|\big|p(h^L)\big)}$$

"Reconstruction" error
Use q as a "probabilistic" encoder,
Use p as a "probabilistic" decoder,

$$x \to h^L \to x$$

"Regularization
towards prior"

How to train?

Max-likelihood can be written as:

$$\max_{\theta \in \Theta} \max_{\{q_\theta(h^L|x)\}} \sum_x \mathbb{E}_{q_\theta(h^L|x)} \log \frac{p_\theta(x, h^L)}{q_\theta(h^L|x)}$$

As usual: we need to be able to take gradients in θ

Denote $f(\theta, h^L) := \log \frac{p_\theta(x,h^L)}{q_\theta(h^L|x)}$. We have:

$$\nabla_\theta \mathbb{E}_{q_\theta(h^L|x)} f(\theta, h^L) = \int \nabla_\theta f(\theta, h^L) q_\theta(h^L|x) dh^L + \int f(\theta, h^L) \nabla_\theta q_\theta(h^L|x) dh^L$$

$$= \mathbb{E}_{q_\theta(h^L|x)} \nabla_\theta f(\theta, h^L) + \int f(\theta, h^L) \nabla_\theta q_\theta(h^L|x) dh^L$$

The first term is easy to estimate, e.g. by drawing samples from $q_\theta(h^L|x)$

But what do we do with the second term??

How to train?

Max-likelihood can be written as:

$$\max_{\theta \in \Theta} \max_{\{q_\theta(h^L|x)\}} \sum_x \mathbb{E}_{q_\theta(h^L|x)} \log \frac{p_\theta(x, h^L)}{q_\theta(h^L|x)}$$

As usual: we need to be able to take gradients in θ

***Try 1**:* $\int f(\theta, h^L) \nabla_\theta q_\theta(h^L|x) dh^L$

$$= \int f(\theta, h^L) \frac{q_\theta(h^L|x)}{q_\theta(h^L|x)} \nabla_\theta q_\theta(h^L|x) dh^L$$

$$= \int f(\theta, h^L)\, q_\theta(h^L|x)\, \nabla_\theta \log\, q_\theta(h^L|x) dh^L$$

$$= \mathbb{E}_{q_\theta(h^L|x)} f(\theta, h^L)\, \nabla_\theta \log\, q_\theta(h^L|x)$$

Expectation, so can be estimated by samples, but typically high variance.

How to train?

Max-likelihood can be written as:

$$\max_{\theta \in \Theta} \max_{\{q_\theta(h^L|x)\}} \sum_x \mathbb{E}_{q_\theta(h^L|x)} \log \frac{p_\theta(x, h^L)}{q_\theta(h^L|x)}$$

As usual: we need to be able to take gradients in θ

Try 2: if we could instead reduce the problem to calculating an expectation of the type $\nabla_\theta \mathbb{E}_{q(h^L|x)} f(\theta, h^L)$ (i.e. the expectation is with respect to a variable that doesn't depend on the parameters we are taking derivatives wrt), the problematic term from prior slide would vanish!

Reparametrization trick

Max-likelihood can be written as:

$$\max_{\theta\in\Theta} \max_{\{q_\theta(h^L|x)\}} \sum_x \mathbb{E}_{q_\theta(h^L|x)} \log \frac{p_\theta(x,h^L)}{q_\theta(h^L|x)}$$

As usual: we need to be able to take gradients in θ

Try 2: write the expectation $\mathbb{E}_{q_\theta(h^L|x)} \log \frac{p_\theta(x,h^L)}{q_\theta(h^L|x)}$ as an expectation over a distribution not dependent on θ.

Kingma-Welling '13: reparametrization trick!

Main idea: a sample from $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ can be generated as follows

Sample $\mathbf{x} \sim \mathcal{N}(0, \mathrm{I})$.

Output $\boldsymbol{y} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{x}$.

Reparametrization trick

Max-likelihood can be written as:

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As usual: we need to be able to take gradients in θ

Recall that $q(\boldsymbol{h}|\boldsymbol{x},\boldsymbol{\theta}) = q(\boldsymbol{h}^1|\boldsymbol{x},\boldsymbol{\theta})q(\boldsymbol{h}^2|\boldsymbol{h}^1,\boldsymbol{\theta}) \dots q(\boldsymbol{h}^L|\boldsymbol{h}^{L-1},\boldsymbol{\theta})$

where $q(\boldsymbol{h}^l|\boldsymbol{h}^{l-1},\boldsymbol{\theta}) = \mathcal{N}(\mu_{\boldsymbol{\theta}}(\boldsymbol{h}^{l-1}), \Sigma_{\boldsymbol{\theta}}(\boldsymbol{h}^{l-1}))$

To produce a sample from $q(\boldsymbol{h}|\boldsymbol{x},\boldsymbol{\theta})$, sample iid standard Gaussians $\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \dots, \boldsymbol{\epsilon}_L$. Set

$$\mathbf{h}^\ell\left(\boldsymbol{\epsilon}^\ell, \mathbf{h}^{\ell-1}, \boldsymbol{\theta}\right) = \boldsymbol{\Sigma}(\mathbf{h}^{\ell-1}, \boldsymbol{\theta})^{1/2}\boldsymbol{\epsilon}^\ell + \boldsymbol{\mu}(\mathbf{h}^{\ell-1}, \boldsymbol{\theta})$$

Using the reparametrization trick

Max-likelihood can be written as:

$$\max_{\theta\in\Theta} \max_{\{q_\theta(h)\}} \sum_x \mathbb{E}_{q_\theta(h|x)} \log \frac{p_\theta(x,h)}{q_\theta(h|x)}$$

We can hence write the gradient wrt to θ :

$$\nabla_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{h}\sim q(\mathbf{h}|\mathbf{x},\boldsymbol{\theta})} \left[\log \frac{p(\mathbf{x},\mathbf{h}|\boldsymbol{\theta})}{q(\mathbf{h}|\mathbf{x},\boldsymbol{\theta})} \right]$$

$$= \nabla_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{\epsilon}^1,\ldots,\boldsymbol{\epsilon}^L\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})} \left[\log \frac{p(\mathbf{x},\mathbf{h}(\boldsymbol{\epsilon},\mathbf{x},\boldsymbol{\theta})|\boldsymbol{\theta})}{q(\mathbf{h}(\boldsymbol{\epsilon},\mathbf{x},\boldsymbol{\theta})|\mathbf{x},\boldsymbol{\theta})} \right]$$

$$= \mathbb{E}_{\boldsymbol{\epsilon}^1,\ldots,\boldsymbol{\epsilon}^L\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})} \left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\mathbf{x},\mathbf{h}(\boldsymbol{\epsilon},\mathbf{x},\boldsymbol{\theta})|\boldsymbol{\theta})}{q(\mathbf{h}(\boldsymbol{\epsilon},\mathbf{x},\boldsymbol{\theta})|\mathbf{x},\boldsymbol{\theta})} \right]$$

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We can approximate the expectation by an empirical average as before.

For **fixed** $\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \ldots, \boldsymbol{\epsilon}_L$: log p and log q are easy to take gradients of via backpropagating.

It's common to have **diagonal covariance mxs** for training efficiency.

Part II: Evaluating representations

Desiderata for representations

What do we want out a representation?

Many possible answers here. First, a few uncontroversial desiderata:

Interpretability: if the derived features are semantically meaningful, and interpretable by a human, they can be easily evaluated.
(e.g. noisy-OR: "features" are diseases a patient has)

Sparsity of a representation is an important subcase: "explanatory" features for sample can be examined if there are a small number of them.

Downstream usability: the features are "useful" for downstream tasks. Some examples:

Improving label efficiency: if, for a task, a linear (or otherwise "simple") classifier can be trained on features and it works well, smaller # of labeled samples are needed.

Desiderata for representations

Obvious issue: interpretability and "usefulness" are not easily mathematically expressed. We need some "proxies" that induce such properties.

This is a lot more contraversial – here we survey some general desiderata, proposed as early as *Bengio-Courville-Vincent '14:*

Hierarchy/compositionality: video/images/text/ are expected to have hierarchical structure – depth helps induce such structure.

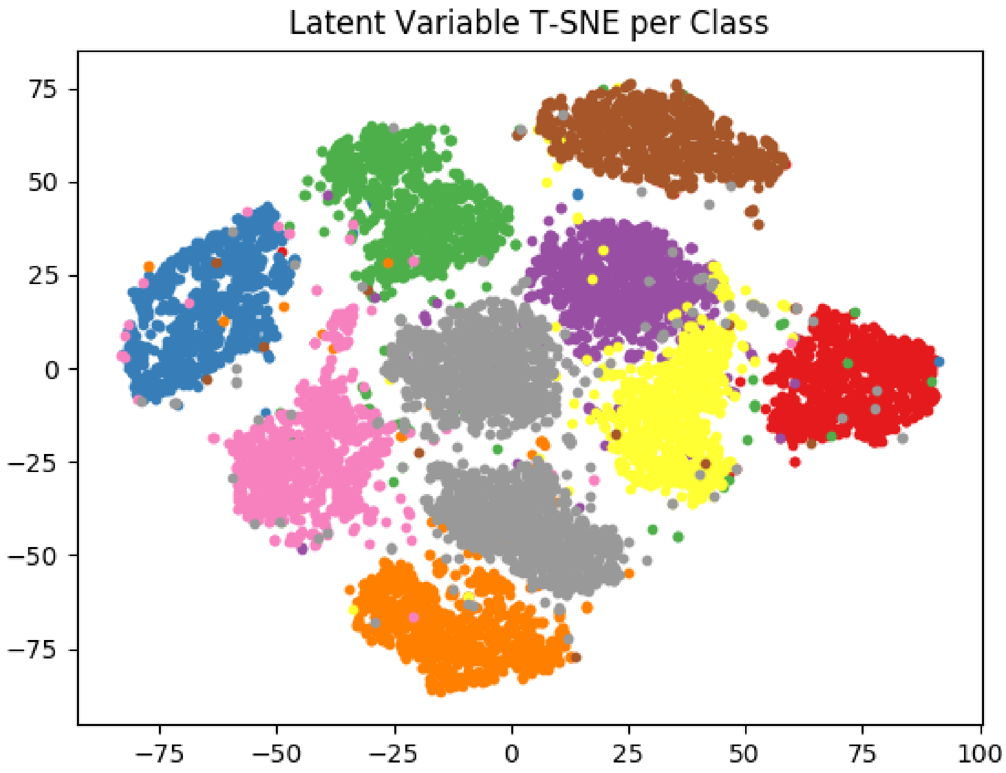
Semantic clusterability: features of the same "semantic class" (e.g. images in the same category) are clustered.

Linear interpolation: in representation space, linear interpolations produce meaningful data points (i.e. "latent space is convex"). Sometimes called *manifold flattening*.

Disentangling: features capture "independent factors of variation" of data. (*Bengio-Courville-Vincent '14).* Has been very popular in modern unsupervised learning, though many potential issues with it.

Semantic clustering

Semantic clusterability: features of the same "semantic class" (e.g. images in the same category) are clustered together.



The intuition:

If semantic classes are linearly (or other simple function) separable, and labels on downstream tasks depend linearly on semantic classes – can afford to learn a simple classifier !!

t-SNE projection of VAE-learned features of the 10 MNIST classes.
Image from https://pyro.ai/examples/vae.html

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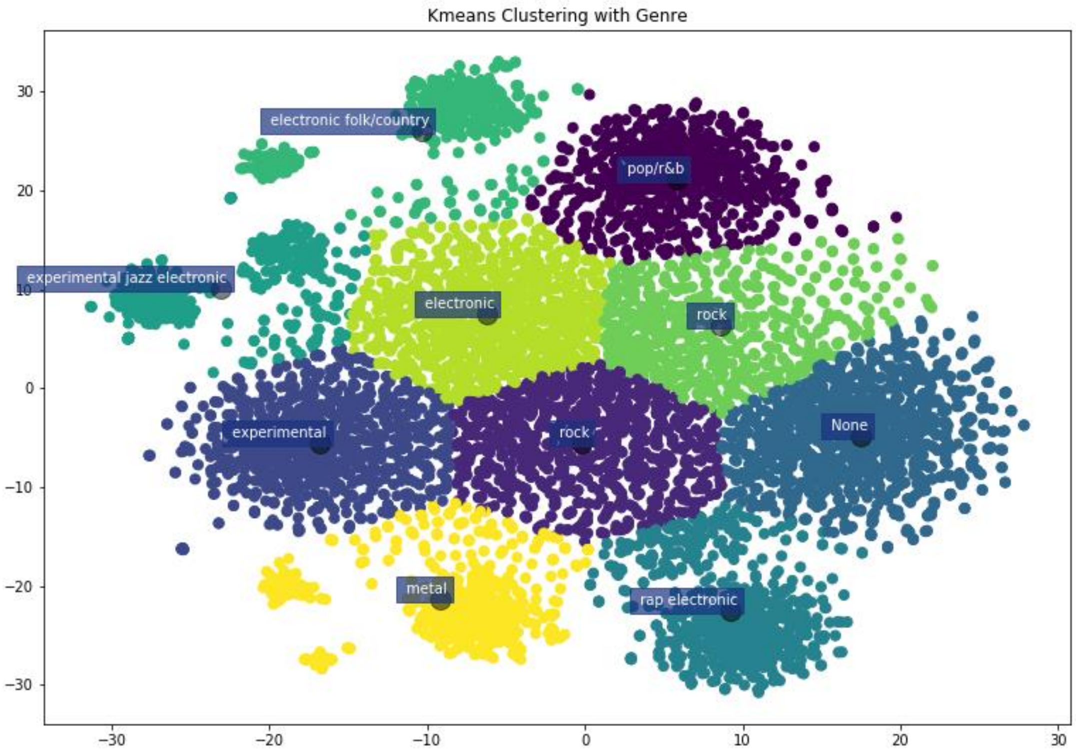
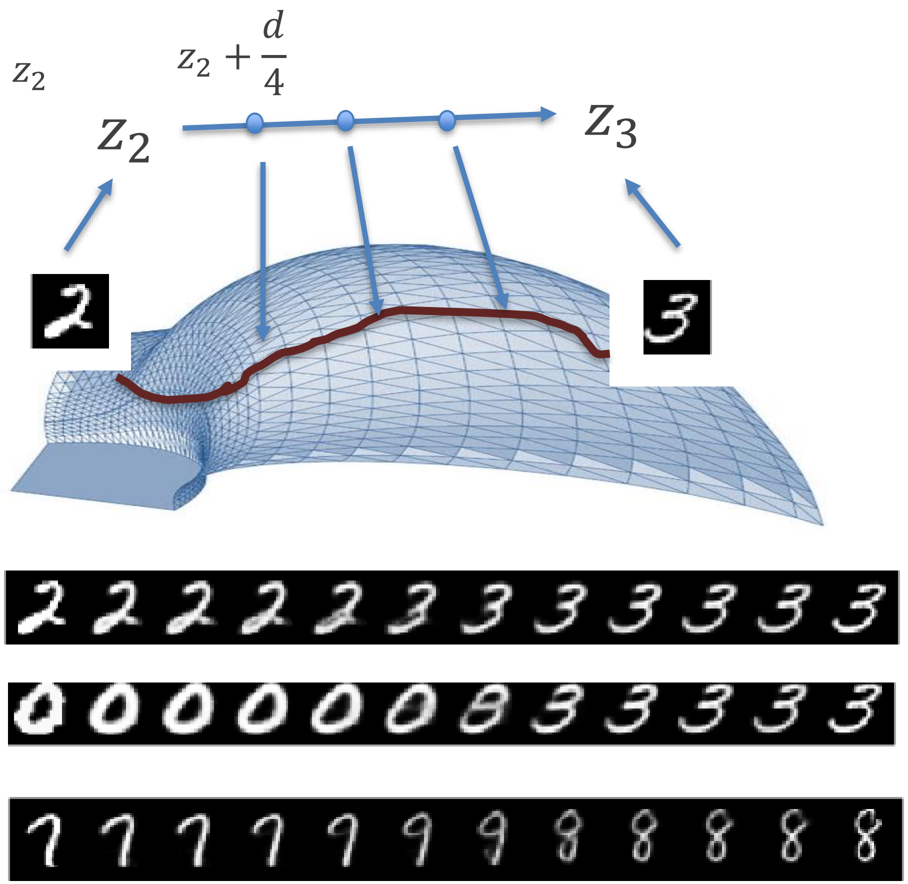


t-SNE projection of word embeddings for artists (clustered by genre). Image from https://medium.com/free-code-camp/learn-tensorflow-the-word2vec-model-and-the-tsne-algorithm-using-rock-bands-97c99b5dcb3a

Linear interpolation

Linear interpolation: in representation space, linear interpolations produce meaningful data points. (i.e. “latent space is convex”)

$d = z_3 - z_2$



Interpolations for a VAE trained on MNIST.

The intuition:

The data manifold is complicated/curved.

The latent variable manifold is a convex set – moving in straight lines keeps us on it.

Linear interpolation

Linear interpolation: in representation space, linear interpolations produce meaningful data points. (i.e. "latent space is convex")

Interpolations for a BigGAN, image from
https://thegradient.pub/bigganex-a-dive-into-the-latent-space-of-biggan/

Disentangled representations

Disentangling: features capture "independent factors of variation" of data. (*Bengio-Courville-Vincent '14).* Has been very popular in modern unsupervised learning, though many potential issues with it.

For concreteness, let's assume that we have a latent variable model for data with latent variables $\boldsymbol{z}$, observables $\boldsymbol{x}$, and joint distribution $p_{\boldsymbol{\theta}}(\boldsymbol{z}, \boldsymbol{x})$

There are (at least) two ways to formalize this (literature is not always clear on which one is aimed for!):

Prior disentangling: $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ is a product distribution, i.e. $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \Pi_i p_{\boldsymbol{\theta}}(\boldsymbol{z_i})$

Classical example: ICA (independent component analysis)

Posterior disentangling: fit a variational posterior $q_{\boldsymbol{\theta}}$ s.t. $q_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ is (on average over **x**) a product distribution

In other words, $\int_x q_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})\, p(\boldsymbol{x}) d\boldsymbol{x}$ – usually called the *aggregate posterior* – is close to a product "distribution".

Disentangled representations

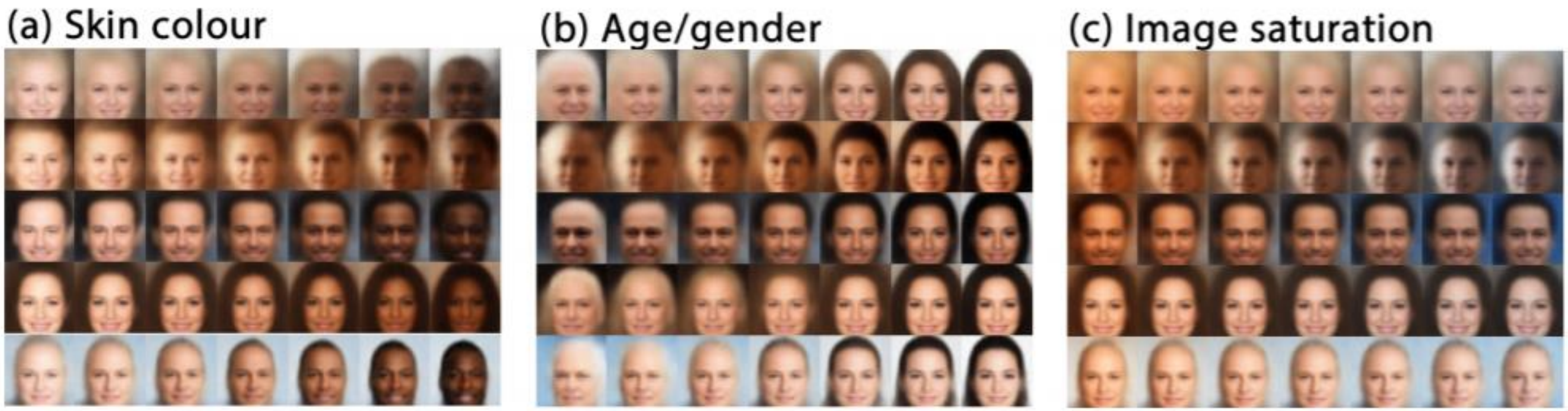


Figure 4: **Latent factors learnt by β-VAE on celebA:** traversal of individual latents demonstrates that β-VAE discovered in an unsupervised manner factors that encode skin colour, transition from an elderly male to younger female, and image saturation.

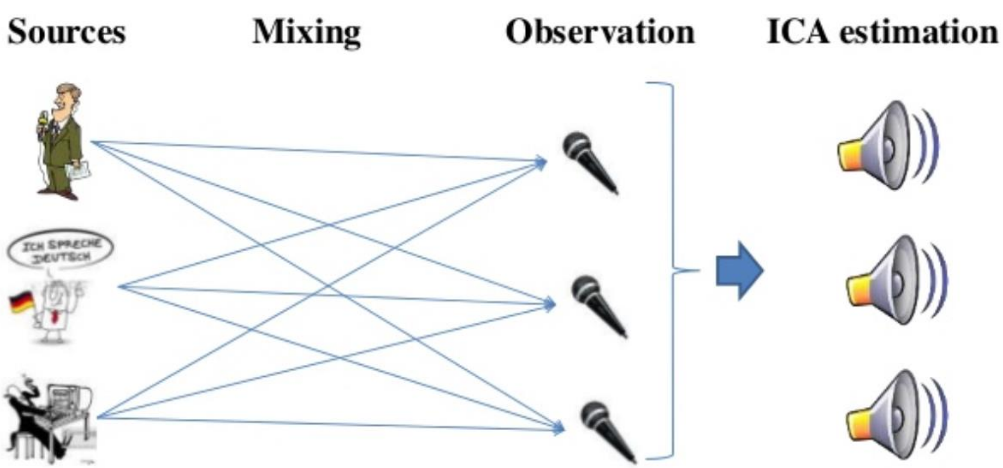
Posterior disentangling in β −VAE. To produce plots, infer latent variable for an image, then change a single latent variable gradually.
Image from Higgins et al. '17.

Prior disentangling

Prior disentangling: $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ is a product distribution, i.e. $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \Pi_i p_{\boldsymbol{\theta}}(\boldsymbol{z_i})$

Classical example: ICA (independent component analysis), also called the "cocktail party problem".

Assume data is generated as $x = Az,\ z \in \mathbb{R}^d, A \in \mathbb{R}^{d \times d}$



If z has an independent, *non-Gaussian* prior, model is identifiable and efficiently learnable.

Other examples: noisy-OR networks (diseases are independent), general Bayesian nets, viewing top variables as z's

Posterior disentanglement in VAEs

Recall the "regularization" view of the VAEs objective:

$$\underbrace{\sum_x \mathbb{E}_{q(h^L|x)} \log p(x|h^L)}_{\text{"Reconstruction" error}} - \underbrace{KL\left(q(h^L|x) \| p(h^L)\right)}_{\text{"Regularization towards prior"}}$$

Consider a prior which is a product distribution (e.g. standard Gaussian):

The KL term implicitly penalizes distributions for which

$$\sum_x KL\left(q(h^L|x) \| p(h^L)\right) \approx \mathbb{E}_{x \sim p^*} KL\left(q(h^L|x) \| p(h^L)\right)$$

is large – i.e. the aggregated posterior is far from a product distribution.

Posterior disentanglement in VAEs

Recall the "regularization" view of the VAEs objective:

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The KL term implicitly penalizes distributions for which

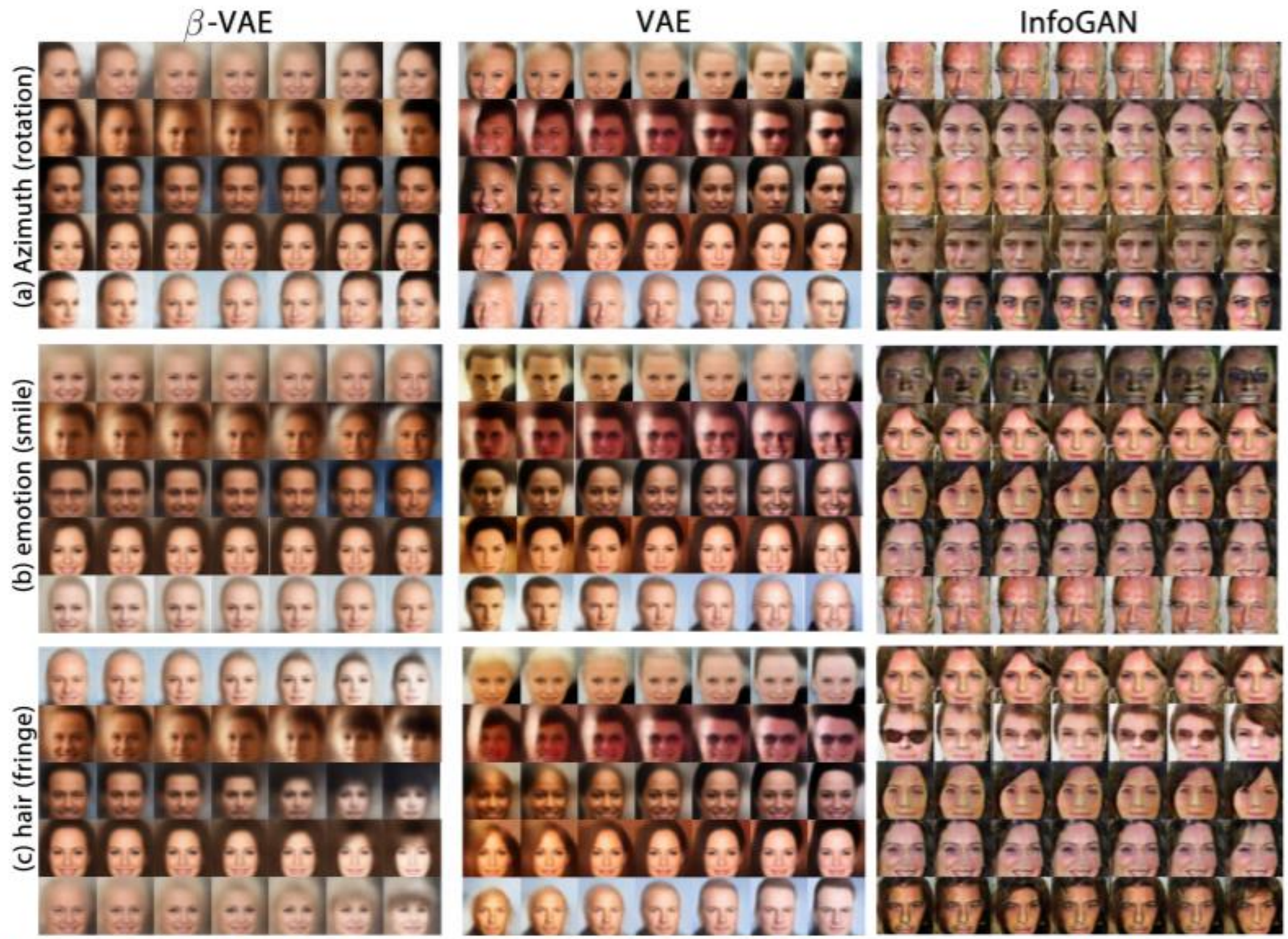
$$\sum_x KL(q(h^L|x)||p(h^L)) \approx \mathbb{E}_{x\sim p^*} KL(q(h^L|x)||p(h^L))$$

The idea of *Higgins et al '17*: introduce a "weighting" factor to put more weight on reconstruction or disentanglement:

β −VAE objective: $\sum_x \mathbb{E}_{q(h^L|x)} \log p(x|h^L) - \beta\, KL(q(h^L|x)||p(h^L))$

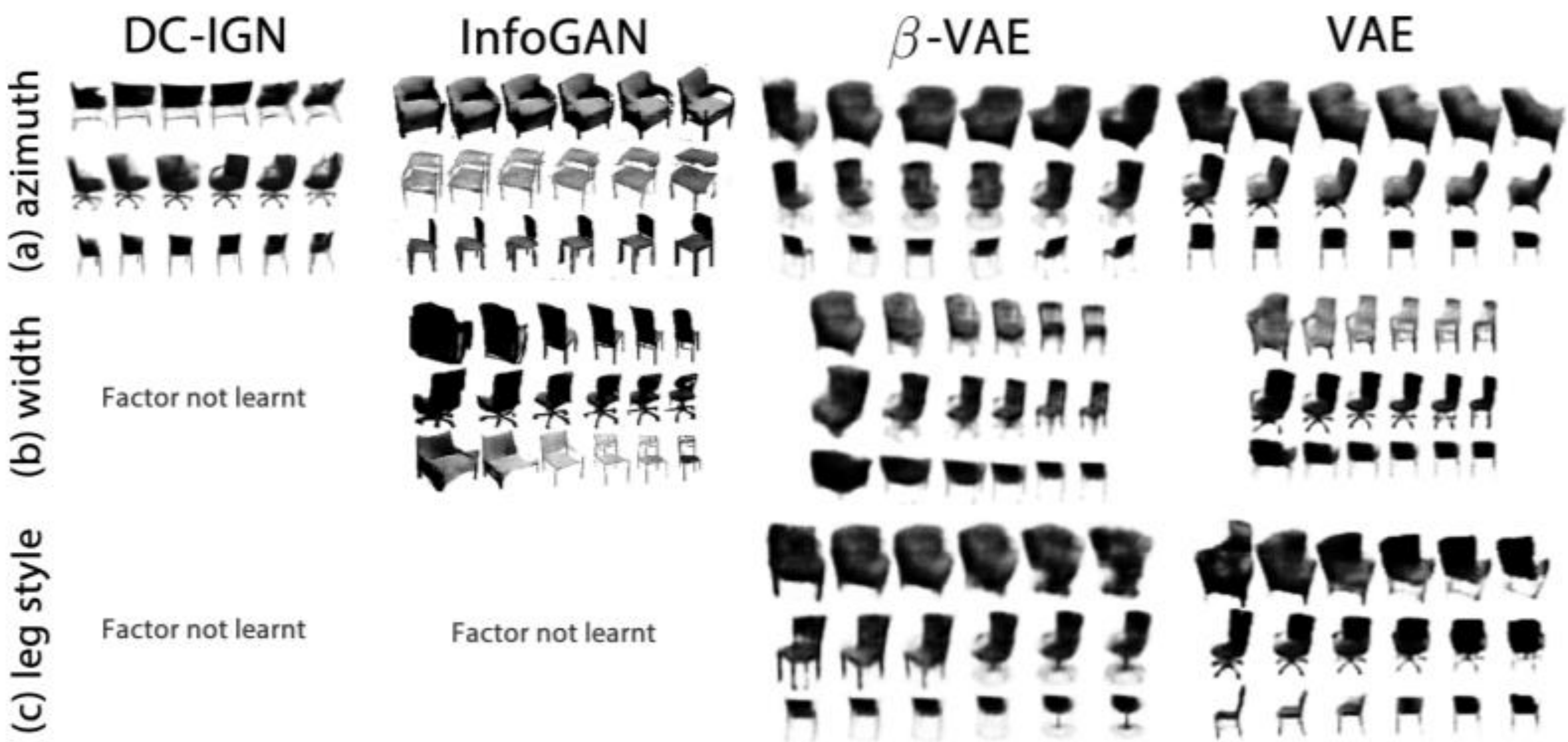
β large: more weight on disentanglement

Posterior disentanglement in VAEs



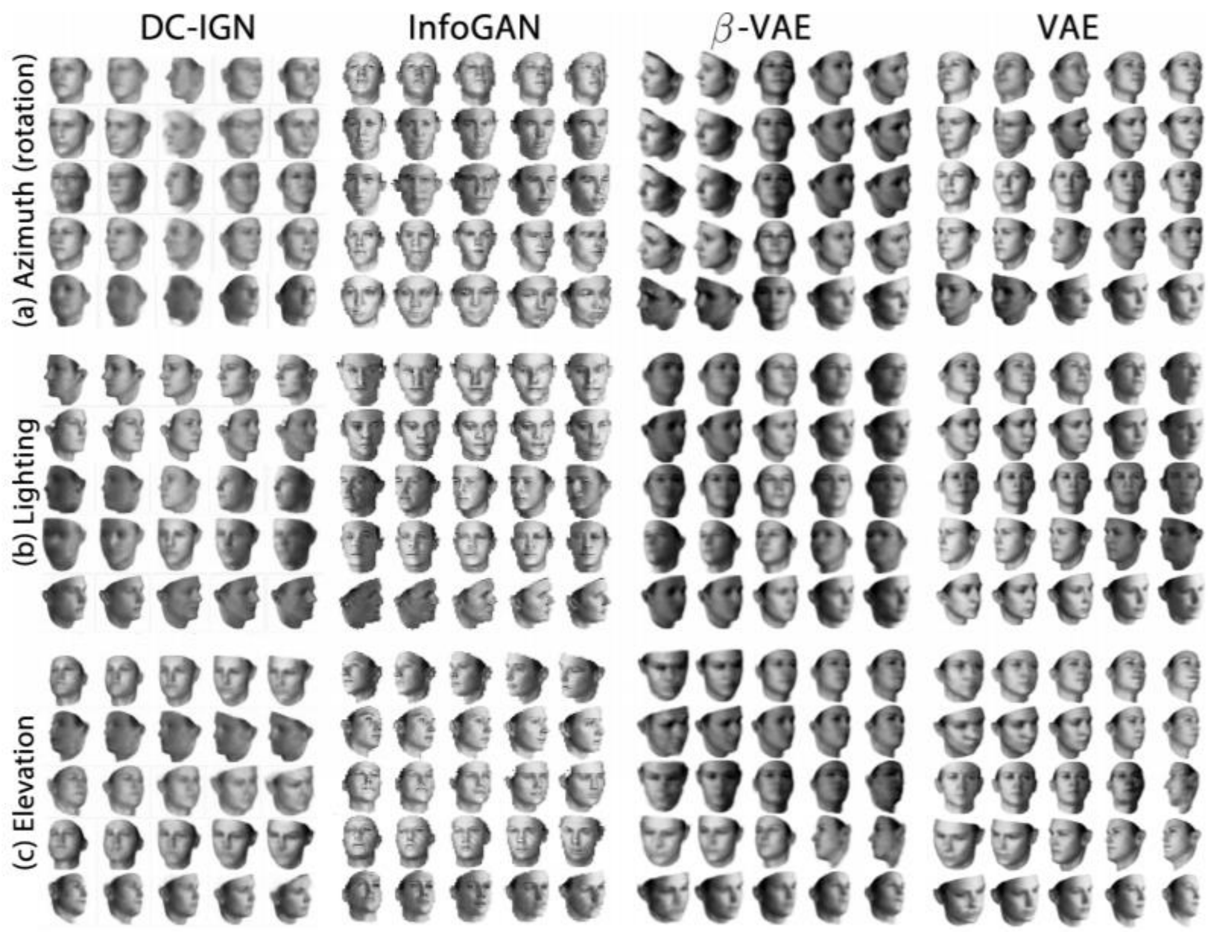
Comparing disentangling of different types of generative models.
Image from Higgins et al. '17.

Posterior disentanglement in VAEs



Comparing disentangling of different types of generative models. Image from Higgins et al. '17.

Posterior disentanglement in VAEs



Comparing disentangling of different types of generative models. Image from Higgins et al. '17.

Measuring disentanglement

Locatello et al '19, "Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations" (Best paper award at ICML '19): A large-scale study of disentanglement measures, as well as gen. models.

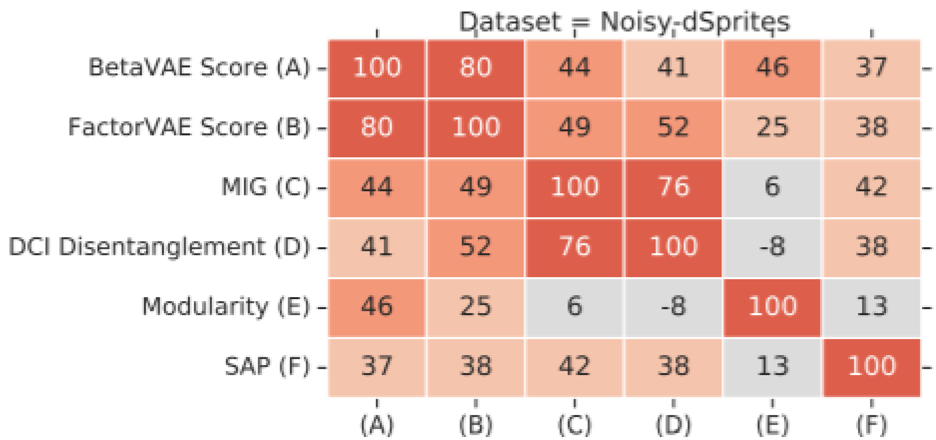


Figure 2. Rank correlation of different metrics on Noisy-dSprites. Overall, we observe that all metrics except Modularity seem mildly correlated with the pairs BetaVAE and FactorVAE, and MIG and DCI Disentanglement strongly correlated with each other.

Usefulness of disentanglement?

Locatello et al '19, "Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations" (Best paper award at ICML '19): A large-scale study of disentanglement measures, as well as gen. models.

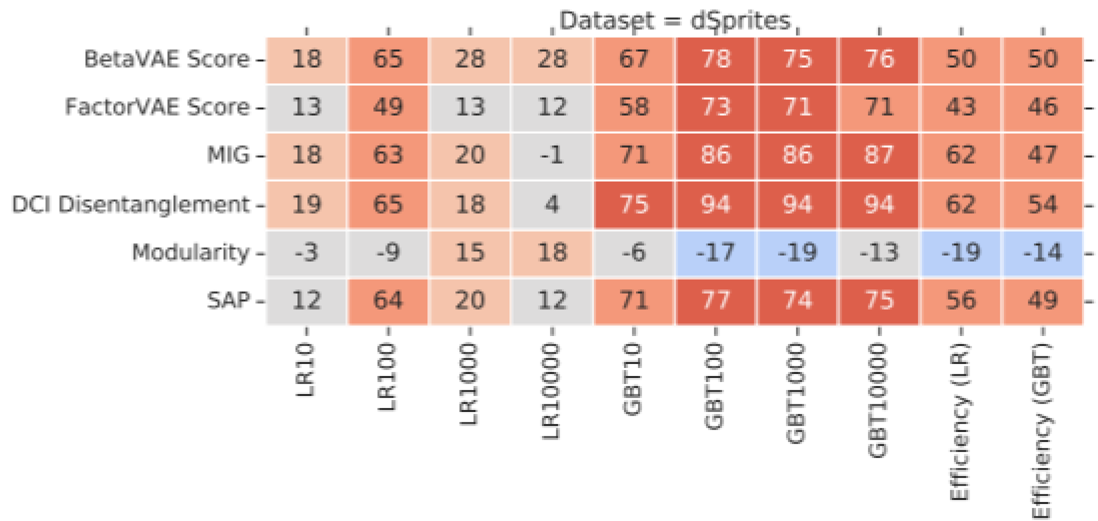


Figure 5. Rank correlations between disentanglement metrics and downstream performance (accuracy and efficiency) on dSprites.

Downstream classification task: predict **true** ground-truth factors (w/ multiclass logistic regression)
Carefull to extrapolate too much – task/setup is a little contrived.

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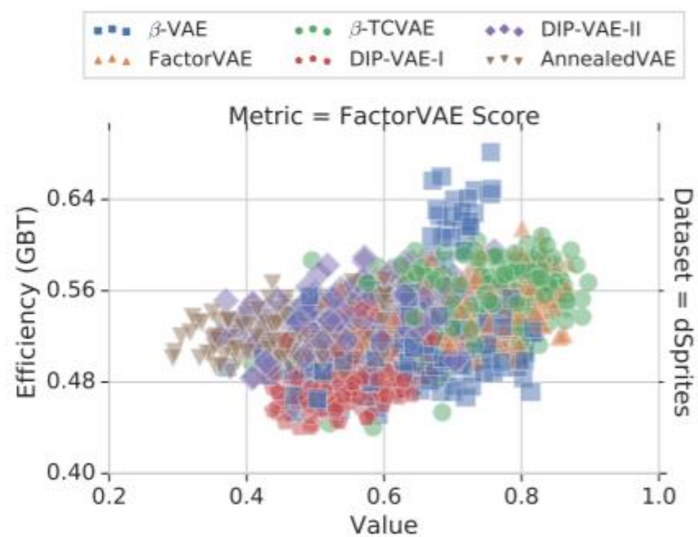

Figure 6. Statistical efficiency of the FactorVAE Score for learning a GBT downstream task on dSprites.

Statistical efficiency measure: average accuracy based on 100 samples divided by the average accuracy based on 10 000 samples

Issue of ill-posedness?

Locatello et al '19, "Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations" (Best paper award at ICML '19):

A model can be re-parametrized, s.t. the distribution over the data and latents is unchanged, but it can be arbitrarily more "entangled".

Thus, some kind of inductive bias both on model class and data seems necessary.

As a simple example: consider $\boldsymbol{z} \sim \mathcal{N}(0, \boldsymbol{I})$, let $\boldsymbol{z}' = \boldsymbol{U}\boldsymbol{z}$, for any non-identity orthogonal matrix U.

Then, under any "intuitive" understanding of entangling, $\boldsymbol{z}'$ seems entangled with $\boldsymbol{z}$ – small changes of coordinates of z cause global changes in $\boldsymbol{z}'$.