TTIC 31230, Fundamentals of Deep Learning

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Latent Variable Models

Expectation Maximization (EM)

The Evidence Lower Bound (the ELBO)

Variational Autoencoders (VAEs)

Latent Variable Models

$$P_\Phi(y) = \sum_z P_\Phi(z) P_\Phi(y|z) = E_{z \sim P_\Phi(z)} P_\Phi(y|z)$$

Or

$$P_\Phi(y|x) = \sum_z P_\Phi(z|x) P_\Phi(y|z,x) = E_{z \sim P_\Phi(z|x)} P_\Phi(y|z,x)$$

Here z is a latent variable.

Latent Variable Models

$$P_\Phi(y) = \sum_z P_\Phi(z) P_\Phi(y|z) = E_{z \sim P_\Phi(z)} P_\Phi(y|z)$$

Here we often think of z as the causal source of y.

For example z might be a physical scene causing image y.

Or z might be the intended utterance causing speech signal y.

In these situations a latent variable model should more accurately represents the distribution on y.

Latent Variable Models

$$P_\Phi(y) = \sum_z P_\Phi(z) P_\Phi(y|z) = E_{z \sim P_\Phi(z)} P_\Phi(y|z)$$

$P_\Phi(z)$ is called the prior.

Given an observation of y (the evidence) $P_\Phi(z|y)$ is called the posterior.

Variational Bayesian inference involves approximating the posterior.

Colorization with Latent Segmentation

x $\hat{y}$ y

Larsson et al., 2016

Colorization is a natural self-supervised learning problem — we delete the color and then try to recover it from the grey-level image.

Can colorization be used to learn segmentation?

Segmentation is latent — not determined by the color label.

Colorization with Latent Segmentation

x $\hat{y}$ y

Larsson et al., 2016

x is a grey level image.

y is a color image drawn from $\text{Pop}(y|x)$.

$\hat{y}$ is an arbitrary color image.

$P_\Phi(\hat{y}|x)$ is the probability that model Φ assigns to the color image $\hat{y}$ given grey level image x.

Colorization with Latent Segmentation

Input | Our Method | Ground-truth

x $\hat{y}$ y

$$P_\Phi(\hat{y}|x) = \sum_z P_\Phi(z|x) P_\Phi(\hat{y}|z,x).$$

input x

$P_\Phi(z|x) = \ldots$ semantic segmentation

$P_\Phi(\hat{y}|z,x) = \ldots$ segment colorization

Assumptions

We assume models $P_\Phi(z)$ and $P_\Phi(y|z)$ are both samplable and computable.

In other words, we can sample from these distributions and for any given z and y we can compute $P_\Phi(z)$ and $P_\Phi(y|z)$.

These are nontrivial assumptions.

A loopy graphical model is neither (efficiently) samplable nor computable.

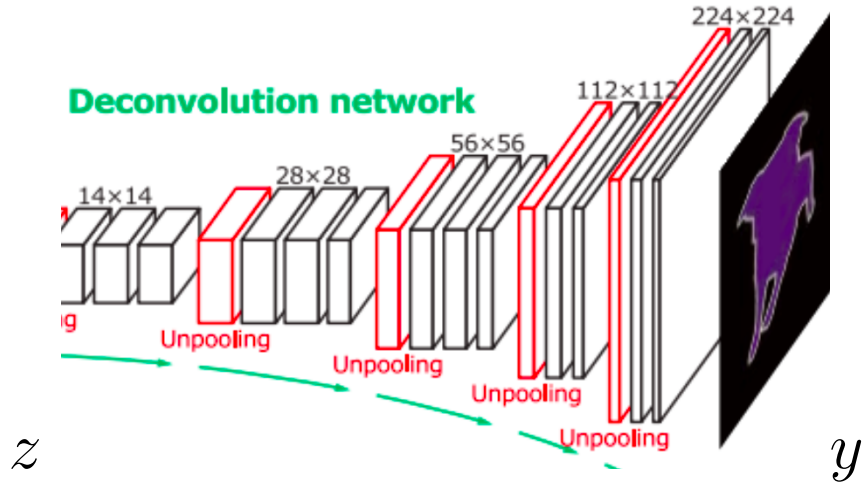
Cases Where the Assumptions Hold

In CTC we have that z is the sequence with blanks and y is the result of removing the blanks from z.

In a hidden markov model z is the sequence of hidden states and y is the sequence of emissions.

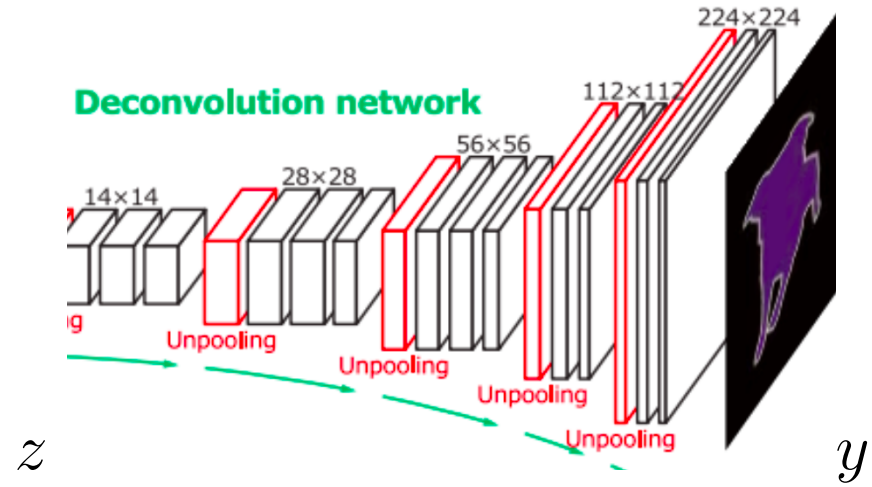
An autoregressive model, such as an autoregressive language model, is both samplable and computable.

Image Generators



We can generate an image y from noise z where $p_\Phi(z)$ and $p_\Phi(y|z)$ are both samplable and computable.

Image Generators



Typically $p_\Phi(z)$ is $\mathcal{N}(0, I)$ reshaped as $z[X, Y, J]$

We can generate an image y form noise z where $p_\Phi(z)$ and $p_\Phi(y|z)$ are both samplable and computable.

Assumptions

We assume models $P_\Phi(z)$ and $P_\Phi(y|z)$ are both samplable and computable.

When the assumptions hold we can sample from $P_\Phi(y)$ but we cannot typically compute $P_\Phi(y)$.

In particular, for an image generator we cannot compute $P_\Phi(y)$.

Hence it is not obvious how to optimize the fundamental equation.

$$\Phi^* = \operatorname*{argmin}_\Phi \; E_{y \sim \text{Pop}} \; - \ln P_\Phi(y)$$

Shifting the Difficulty

For any z we have

$$P_\Phi(y) = \frac{P_\Phi(y)P_\Phi(z|y)}{P_\Phi(z|y)}$$

$$= \frac{P_\Phi(z)P_\Phi(y|z)}{P_\Phi(z|y)}$$

The difficulty has now been shifted to estimating $P_\Phi(z|y)$ which remains intractable but is intuitively easier than estimating $P_\Phi(y)$.

The Evidence Lower Bound (The ELBO)

We introduce a samplable and computable model $Q_\Phi(z|y)$ to approximate $P_\Phi(z|y)$.

$$
\begin{aligned}
\ln P_\Phi(y) &= E_{z\sim Q_\Phi(z|y)} \ln \frac{P_\Phi(z)P_\Phi(y|z)}{P_\Phi(z|y)} \\
&= E_{z\sim Q_\Phi(z|y)} \left(\ln \frac{P_\Phi(z)P_\Phi(y|z)}{Q_\Phi(z|y)} + \ln \frac{Q_\Phi(z|y)}{P_\Phi(z|y)} \right) \\
&= \left(E_{z\sim Q_\Phi(z|y)} \ln \frac{P_\Phi(z)P_\Phi(y|z)}{Q_\Phi(z|y)} \right) + KL(Q_\Phi(z|y), P_\Phi(z|y)) \\
&\geq E_{z\sim Q_\Phi(z|y)} \ln \frac{P_\Phi(z)P_\Phi(y|z)}{Q_\Phi(z|y)} \quad \text{The ELBO}
\end{aligned}
$$

The Variational Autoencoder (VAE)

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y\sim \mathrm{Pop},\, z\sim Q_\Phi(z|y)} \quad \ln \frac{Q_\Phi(z|y)}{P_\Phi(z,y)}$$

VAE generalizes EM

VAE:

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y\sim\text{Train},\, z\sim Q_\Phi(z|y)} \quad \ln \frac{Q_\Phi(z|y)}{P_\Phi(z,y)}$$

EM: Alternately optimize Q then P.

$$\Phi^{t+1} = \underset{\Phi}{\operatorname{argmin}}\; E_{y\sim\text{Train}}\, E_{z\sim P_{\Phi^t}(z|y)} \; - \ln P_\Phi(z,y)$$

Update	Inference
(M Step)	(E Step)
Hold Q fixed	$Q^* = P_{\Phi^t}$

Hard VAEs

In hard EM we use $\text{argmax}_z \, P_{\Phi^t}(z|y)$ rather than $E_{z \sim P_{\Phi^t}(z|y)}$.

K-means is hard EM for mixtures of Gaussians (when all covariances matrices are fixed at I).

By analogy with hard EM we can formulate a notion of a hard VAE.

Hard VAEs

(Soft) VAE:

$$\begin{aligned}\Phi^* &= \operatorname*{argmin}_{\Phi} E_{y,\epsilon} \ \ln \frac{Q_\Phi(z|y)}{P_\Phi(z,y)} \\ &= \operatorname*{argmin}_{\Phi} \Big(E_{z\sim Q_\Phi(z|y)} \ - \ln P_\Phi(z,y) \Big) - H(Q_\Phi(z|y))\end{aligned}$$

Hard VAE:

$$\Phi^* = \operatorname*{argmin}_{\Phi} E_{z\sim Q_\Phi(z|y)} \ - \ln P_\Phi(z,y)$$

For a hard VAE we have that Q^* focuses on a single value. Even for a soft VAE Q can suffer from mode collapse.

The Reparameterization Trick

$$-\ln P_\Phi(y) \leq E_{z\sim Q_\Phi(z|y)} \ln \frac{Q_\Phi(z|y)}{P_\Phi(z)P_\Phi(y|z)}$$

$$= E_\epsilon \ln \frac{Q_\Phi(z|y)}{P_\Phi(z)P_\Phi(y|z)} \quad z := f_\Phi(y,\epsilon)$$

ϵ is parameter-independent noise.

This supports SGD: $\nabla_\Phi E_{y,\epsilon}[\ldots] = E_{y,\epsilon} \nabla_\Phi [\ldots]$

Posterior Collapse

Assume Universal Expressiveness for $P_\Phi(y|z)$.

This allows $P_\Phi(y|z) = \text{Pop}(y)$ independent of z.

We then get a completely optimized model with z taking a single (meaningless) determined value.

$$Q_\Phi(z|y) = P_\Phi(z|y) = 1$$

Colorization with Latent Segmentation

x $\hat{y}$ y

Larsson et al., 2016

Can colorization be used to learn latent segmentation?

We introduce a latent segmentation into the model.

In practice the latent segmentation is likely to "collapse" because the colorization can be done just as well without it.

Optimizing the VAE leaves $I(y, z)$ undetermined

Complete optimization gives $P_\Phi(y) = \text{Pop}(y)$. But this does not determine $Q_\Phi(z|y)$.

At complete optimization the value of the objective function is $H(y)$. But we have

$$H(y) = I(y, z) + H(y|z)$$

The VAE operates on the joint distribution on y and z determined by $\text{Pop}(y)$ and $Q_\Phi(z|y)$.

Posterior collapse is the case of $I(y, z) = 0$.

The β-VAE

β-VAE: Learning Basic Visual Concepts With A Constrained Variational Framework, Higgins et al., ICLR 2017.

The VAE:

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\ \ln \frac{Q_\Phi(z|y)}{P_\Phi(z)P_\Phi(y|z)}$$

The β-VAE:

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\quad \beta \ln \frac{Q_\Phi(z|y)}{P_\Phi(z)} - \ln P_\Phi(y|z)$$

The β-VAE

β-VAE: Learning Basic Visual Concepts With A Constrained Variational Framework, Higgins et al., ICLR 2017.

The β-VAE:

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon} \quad \beta \ln \frac{Q_\Phi(z|y)}{P_\Phi(z)} - \ln P_\Phi(y|z)$$

The paper claims that taking $\beta > 1$ can prevent posterior collapse. More Later.

Noisy-Channel RDAs vs. β-VAEs

Noisy-Channel RDA

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\ \ln \frac{p_\Phi(z|y)}{q_\Phi(z)} + \lambda \mathrm{Dist}(y, y_\Phi(z)) \quad z := f_\Phi(y, \epsilon)$$

β-VAE

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon} \quad \beta \ln \frac{q_\Phi(z|y)}{p_\Phi(z)} - \ln p_\Phi(y|z) \quad z := f_\Phi(y, \epsilon)$$

L_2 Distortion and Gaussian Image Noise

Using L_2 distortion and $p_\Phi(y|z) \propto \exp(-||y - y_\Phi(z)||/(2\sigma^2))$

Noisy-Channel RDA

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\ \ln \frac{p_\Phi(z|y)}{q_\Phi(z)} + \lambda||y - y_\Phi(z)||^2$$

β-VAE

$$\Phi^* = \underset{\Phi,\sigma}{\operatorname{argmin}}\, E_{y,\epsilon}\quad \beta \ln \frac{q_\Phi(z|y)}{p_\Phi(z)} + \left(\frac{1}{2\sigma^2}\right) ||y - y_\Phi(z)||^2 + \ln \sigma$$

Gaussian Image Noise

for $p_\Phi(y|z) \propto \exp(-||y - y_\Phi(z)||/(2\sigma^2))$ we have

β-VAE

$$\Phi^* = \underset{\Phi,\sigma}{\operatorname{argmin}} E_{y,\epsilon} \quad \beta \ln \frac{q_\Phi(z|y)}{p_\Phi(z)} + \left(\frac{1}{2\sigma^2}\right) ||y - y_\Phi(z)||^2 + \ln \sigma$$

where $\sigma^* = \sqrt{E_{y,\epsilon} \, ||y - y_\Phi(z)||^2}$

Partial Optimization

Noisy-Channel RDA

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\ \ln \frac{p_\Phi(z|y)}{q_\Phi(z)} + \lambda \mathrm{Dist}(y, y_\Phi(z))$$

$$q^*(z) = p_{\mathrm{pop}}(z) = E_{y \sim \mathrm{pop}}\, p_\Phi(z|y)$$

β-VAE

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\quad \beta \ln \frac{q_\Phi(z|y)}{p_\Phi(z)} - \ln p_\Phi(y|z)$$

$$p^*(z) = p_{\mathrm{pop}}(z) = E_{y \sim \mathrm{pop}}\, q_\Phi(z|y)$$

Inserting the Optima

Noisy-Channel RDA

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}} \quad I(y,z) + \lambda E_{y,\epsilon} \operatorname{Dist}(y, y_\Phi(z))$$

β-VAE

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}} \quad \beta I(y,z) - E_{y,\epsilon} \ln p_\Phi(y|z)$$

where the joint distribution on y and z is determined by $\operatorname{pop}(y)$ and the respective encoder distributions.

Semantics of the β-VAE seems unclear

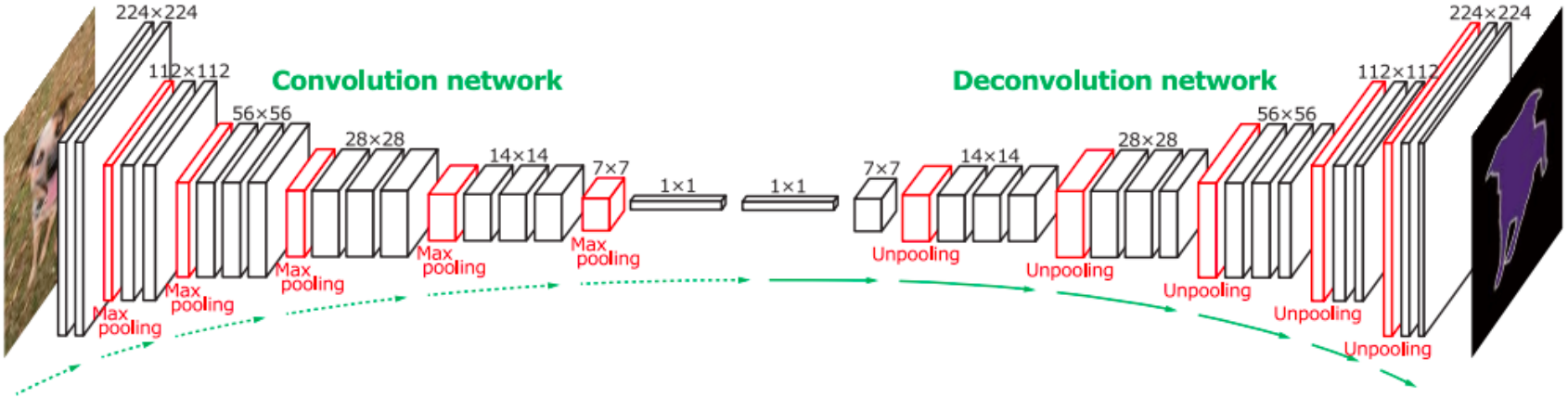
$$\begin{aligned}\Phi^* &= \operatorname*{argmin}_{\Phi} \quad \beta I(y,z) - E_{y,\epsilon}\ \ln p_\Phi(y|z) \\ &= \beta I(y,z) + H(y|z)\end{aligned}$$

We are minimizing the mutual information term. To encourage large mutual information we should take $\beta < 1$ not $\beta > 1$ as recommended.

A VAE for Images

Auto-Encoding Variational Bayes, Diederik P Kingma, Max Welling, 2013.

y $z_\Psi(y, \epsilon)$ $z\ p_\Phi(z)$ $\hat{y}_\Phi(z)$ $||y - \hat{y}||^2$



[Hyeonwoo Noh et al.]

Gaussian VAEs

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_{y,\epsilon}\ \ln \frac{p_\Phi(\tilde{z}|y)}{q_\Phi(\tilde{z})} + \lambda \mathrm{Dist}(y, y_\Phi(\tilde{z}))$$

$$\tilde{z}[i] = z_\Phi(y)[i] + \sigma_\Phi(y)\epsilon[i] \quad \epsilon[i] \sim \mathcal{N}(0,1)$$

$$p_\Phi(\tilde{z}[i]|y) = \mathcal{N}(z_\Phi(y)[i], \sigma_\Phi(y)[i])$$

$$q_\Phi(\tilde{z}[i]) = \mathcal{N}(\mu_q[i], \sigma_q[i]) \ \ \mathrm{WLOG} = \mathcal{N}(0,1)$$

$$p_\Phi(y[i]|z) = \mathcal{N}(y_\Phi(z)[i],\ \sigma_\Phi(z)[i])$$

Sampling

Sample $z \sim \mathcal{N}(0, I)$ and compute $y_\Phi(z)$

[Alec Radford]

Vector Quantized VAEs (VQ-VAE)

Neural Discrete Representation Learning, van den Ord et al., ArXiv 1711.00937, Neurips 2017.

Generating Diverse High-Fidelity Images with VQ-VAE-2, Razavi et al, arXiv 1906.00446

VQ-VAEs effectively perform k-means on vectors in the model so as to represent vectors by discrete cluster centers.

Vector Quantized VAEs (VQ-VAE)

For concreteness we will consider VQ-VAEs on images with a single layer of quantization.

We will use s (for signal) to denote images.

VQ-VAE Encoder-Decoder

We train a dictionary $C[K, I]$ where $C[k, I]$ is the center vector of cluster k.

$$
\begin{aligned}
L[X, Y, I] &= \mathrm{Enc}_\Phi(s) \\
k[x, y] &= \underset{k}{\mathrm{argmin}} \ ||L[x, y, I] - C[k, I]|| \\
\hat{L}[x, y, I] &= C[k[x, y], I] \\
\hat{s} &= \mathrm{Dec}_\Phi(\hat{L}[X, Y, I])
\end{aligned}
$$

VQ-VAE Training Loss

We will interpret the VQ-VAE as a noisy-channel RDA.

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_s\, I(s,k) + \lambda \mathrm{Dist}(s,\hat{s})$$

The mutual information $I(s,k)$ is limited by the entropy of $k[X,Y]$ which can be no larger than $\ln K^{XY} = XY \ln K$.

Maximizing $I(s,k)$ subject to this upper bound should reduce the distortion by providing the decoder with adequate information about the image.

VQ-VAE Training Loss

We preserve information about the image s by minimizing the distortion between $L[X, Y, I]$ and its reconstruction $\hat{L}[X, Y, I]$.

$$\Phi^* = \underset{\Phi}{\text{argmin}} \; E_s \sum_{x,y} ||L[x, y, I] - \hat{L}[x, y, I]||^2 + \lambda \text{Dist}(s, \hat{s})$$

This is a two-level rate-distortion auto-encoder where the rate is ultimately governed by the size K of the codebook $C[K, I]$.

VQ-VAE Training Loss

Unfortunately the latent variable $k[X, Y]$ is discrete and has no gradient. Hence some approximation must be used. They use:

$$L[x, y, I].\text{grad} = \hat{L}[x, y, I].\text{grad}$$

$$C[k, I].\text{grad} = \beta \sum_{x,y:k[x,y]=k} (C[k, I] - L[x, y, I])$$

VQ-VAE Training Loss

$$L[x, y, I].\text{grad} = \hat{L}[x, y, I].\text{grad}$$

$$C[k, I].\text{grad} = \beta \sum_{x,y:k[x,y]=k} (C[k, I] - L[x, y, I])$$

The first equation is the "straight through" gradient. This makes sense for low distortion between $L[X, Y, I]$ and $\hat{L}[X, Y, I]$.

If the second gradient is zero then $C[k, I]$ is the mean of the vectors assigned to k. Then $C[K, I]$ is a minimizer of the distortion between $L(X, Y, I)$ and $\hat{L}(X, Y, I)$.

Training Phase II

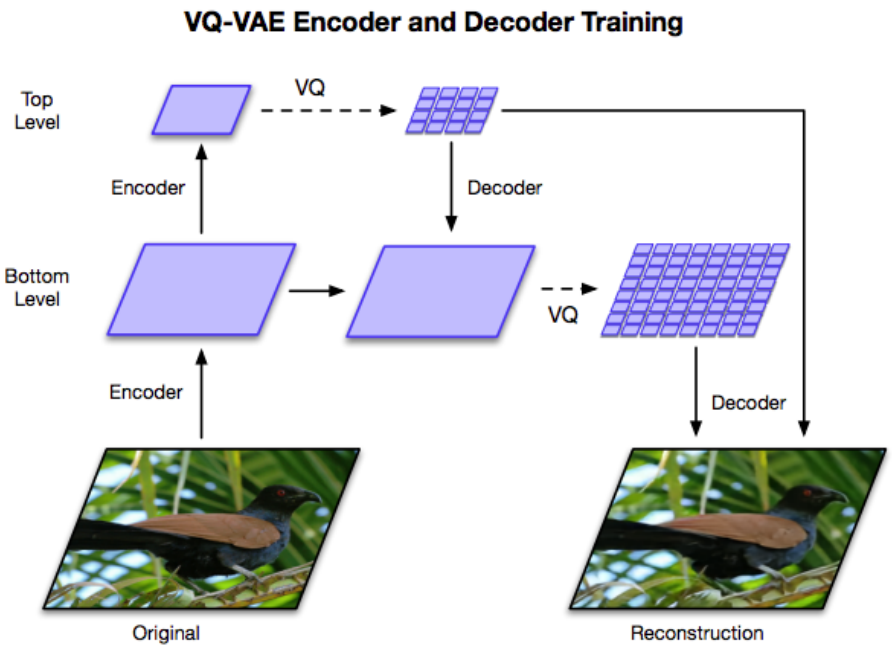
Once the model is trained we can sample images s and compute the "symbolic image" $k[X, Y]$.

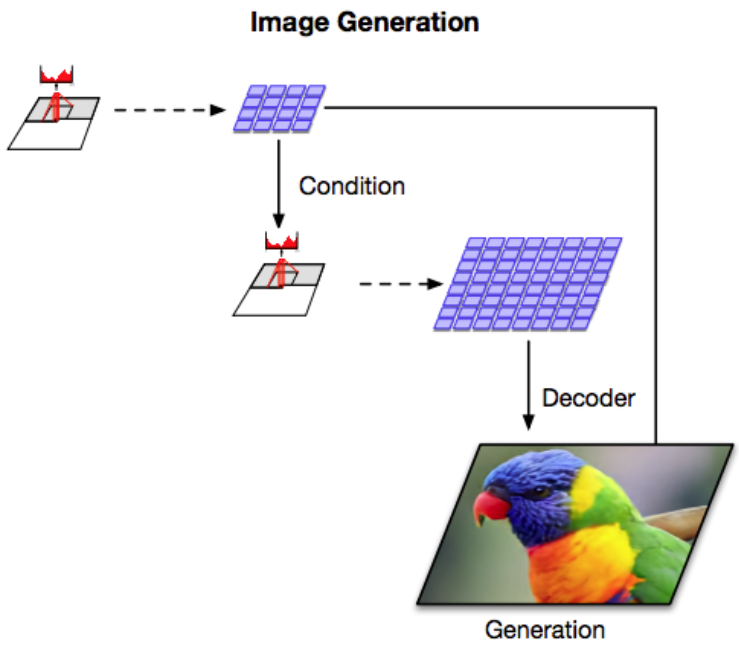
Given samples of symbolic images $k[X, Y]$ we can learn an auto-regressive model of these symbolic images using a pixal-CNN.

This yields a prior probability distribution $P_\Phi(k[X, Y])$ which provides a tighter upper bound on the rate.

We can then measure compression and distortion for test images. This is something GANs cannot do.

Multi-Layer Vector Quantized VAEs





VAEs in 2019

VQ-VAE-2, Razavi et al. June, 2019

VAEs in 2019

Figure 1: Class-conditional 256x256 image samples from a two-level model trained on ImageNet.

VQ-VAE-2, Razavi et al. June, 2019

Quantitative Evaluation

The VQ-VAE2 paper reports a classification accuracy score (CAS) for class-conditional image generation.

We generate image-class pairs from the generative model trained on the ImageNet training data.

We then train an image classifier from the generated pairs and measure its accuracy on the ImageNet test set.

	Top-1 Accuracy	Top-5 Accuracy
BigGAN deep	42.65	65.92
VQ-VAE	54.83	77.59
VQ-VAE after reconstructing	58.74	80.98
Real data	73.09	91.47

Direct Rate-Distortion Evaluation.

Rate-distortion metrics for image compression to discrete representations support unambiguous rate-distortion evaluation.

Rate-distortion metrics also allow one to explore the rate-distortion trade-off.

	Train NLL	Validation NLL	Train MSE	Validation MSE
Top prior	3.40	3.41	-	-
Bottom prior	3.45	3.45	-	-
VQ Decoder	-	-	0.0047	0.0050

Table 1: Train and validation negative log-likelihood (NLL) for top and bottom prior measured by encoding train and validation set resp., as well as Mean Squared Error for train and validation set. The small difference in both NLL and MSE suggests that neither the prior network nor the VQ-VAE overfit.

Vector Quantization (Emergent Symbols)

Vector quantization represents a distribution (or density) on vectors with a discrete set of embedded symbols.

Vector quantization optimizes a rate-distortion tradeoff for vector compression.

The VQ-VAE uses vector quantization to construct a discrete representation of images and hence a measurable image compression rate-distortion trade-off.

Symbols: A Better Learning Bias

Do the objects of reality fall into categories?

If so, shouldn't a learning architecture be designed to categorize?

Whole image symbols would yield emergent whole image classification.

Symbols: Improved Interpretability

Vector quantization shifts interpretation from linear threshold units to the emergent symbols.

This seems related to the use of t-SNE as a tool in interpretation.

Symbols: Unifying Vision and Language

Modern language models use word vectors.

Word vectors are embedded symbols.

Vector quantization also results in models based on embedded symbols.

Symbols: Addressing the "Forgetting" Problem

When we learn to ski we do not forget how to ride a bicycle.

However, when a model is trained on a first task, retraining on a second tasks degrades performance on the first (the model "forgets").

But embedded symbols can be task specific.

The embedding of a task-specific symbol will not change when training on a different task.

Symbols: Improved Transfer Learning.

Embedded symbols can be domain specific.

Separating domain-general parameters from domain-specific parameters may improve transfer between domains.

Final Thought: Attention and Latent Variables

In machine translation attention is used to handle a latent alignment between the input sentence and the gold label translation.

In general, attention can be viewed as defining a probability distribution over a latent choice.

The precise relationship between attention and latent variables is unclear.

END