Variational Autoencoders with Application to Unsupervised Representation Learning

Guo-Jun Qi, Liheng Zhang, Chang Wen Chen, Qi Tian; The IEEE International Conference on Computer Vision (ICCV), 2019

Yash Patel
Visual Recognition Group, Czech Technical University in Prague
Presentation Outline


2. Transformation Equivariant Representations.

Variational Autoencoders - Objective

Unknown GT distribution

$P_{\text{GT}}$

Objective is to learn

$P \approx P_{\text{GT}}$

Collection of Samples $\mathbf{x}$
Variational Autoencoders - Applications

- Image Compression
- Predicting future from static images
- Graphic designing
- etc...


An Uncertain Future: Forecasting from Static Images using Variational Autoencoders, Walker et al. ECCV 2016
Latent Variable Models

- Say, that we have a vector $\mathbf{z}$ in a high-dimensional space $\mathbb{Z}$
- We can easily sample $\mathbf{z}$ according to a probability distribution function (PDF) $\mathbf{P}(\mathbf{z})$
- Say that we have a family of deterministic functions $\mathbf{f}(\mathbf{z}; \mathbf{\Theta})$
- $\mathbf{\Theta}$ are the parameters of the function $\mathbf{f}$ in some space $\mathbf{\Theta}$

$$f: \mathbb{Z} \times \mathbf{\Theta} \rightarrow \mathcal{X}$$

Objective: optimize $\mathbf{\Theta}$ such that sampling $\mathbf{z}$ via $\mathbf{P}(\mathbf{z})$ will result in real looking images.
Latent Variable Models

- Say, that we have a vector \( \mathbf{z} \) in a high-dimensional space \( \mathcal{Z} \)
- We can easily sample \( \mathbf{z} \) according to a probability distribution function (PDF) \( \mathbf{P}(\mathbf{z}) \)
- Say that we have a family of deterministic functions \( \mathbf{f}(\mathbf{z}; \Theta) \)
- \( \Theta \) are the parameters of the function \( \mathbf{f} \) in some space \( \Theta \)

\[
\mathbf{f} : \mathcal{Z} \times \Theta \to \mathcal{X}
\]

Objective: optimize \( \Theta \) such that sampling \( \mathbf{z} \) via \( \mathbf{P}(\mathbf{z}) \) will result in real looking images.

\[
\mathbf{P}(\mathbf{X}) = \int \mathbf{P}(\mathbf{X}|\mathbf{z}; \Theta)\mathbf{P}(\mathbf{z}) \, d\mathbf{z}
\]

\[
\mathbf{P}(\mathbf{X}|\mathbf{z}; \Theta) = \mathcal{N}(\mathbf{X} \mid \mathbf{f}(\mathbf{z}; \Theta), \sigma(\mathbf{z}; \Theta)^2\mathbf{I})
\]
Variational Autoencoders - Challenges

Objective: $P(X) = \int P(X|z; \Theta)P(z) \, dz$

Two main problems:

a. How to define the latent variables $z$ (that is decide what information they represent).

b. How to deal with the integral over $z$. 
Latent Variable Models - Graphical Model
a. How to define the latent variables $\mathbf{z}$

Objective: $P(X) = \int P(X|z; \Theta) P(z) \, dz$

VAEs solve this by assuming that $\mathbf{z}$ is drawn from a normal distribution with zero mean and identity covariance:

$$P(\mathbf{z}) = N(\mathbf{z} \mid 0, I)$$

How is this possible? How can a simple distribution $P(\mathbf{z}) = N(\mathbf{z} \mid 0, I)$ can lead to the generation of complex data samples?
a. How to define the latent variables $\mathbf{z}$

How can a simple distribution $\mathbf{P}(\mathbf{z}) = \mathcal{N}(\mathbf{z} \mid 0, \mathbf{I})$ lead to the generation of complex data samples?

Remember $\mathbf{P}(\mathbf{X} \mid \mathbf{z}; \Theta) = \mathcal{N}(\mathbf{X} \mid \mathbf{f}(\mathbf{z}; \Theta), \sigma(\mathbf{z}; \Theta)^2 \mathbf{I})$?

If $\mathbf{f}(\mathbf{z}; \Theta)$ is a powerful function approximator, generating data samples is possible!

**NEURAL NETWORK DECODER**

$$\mathbf{f}(\mathbf{z}) = \mathbf{z}/10 + \mathbf{z}/||\mathbf{z}||$$
a. How to define the latent variables $\mathbf{z}$

Objective: $P(X) = \int P(X|\mathbf{z}; \Theta)P(\mathbf{z}) \, d\mathbf{z}$

Not all $\mathbf{z}$ will lead to the generation of meaningful samples. During training VAEs sample $\mathbf{z}$ efficiently by using another function $Q(\mathbf{z} | X)$.

Let us compute $E_{\mathbf{z} \sim Q} P(X|\mathbf{z}; \Theta)$ relatively easily.

NEURAL NETWORK ENCODER
Relating $E_{z \sim Q} P(X|z; \Theta)$ and $P(X)$

The two distributions are compared using Kullback-Leibler divergence (KL divergence)

$$KL[Q(z | X) \ || \ P(z|X)] = E_{z \sim Q}[\log Q(z | X) - \log P(z|X)]$$

From Bayes rule: $\log P(z|X) = \log P(X|z) + \log P(z) - \log P(X)$

Substituting

$$KL[Q(z | X) \ || \ P(z|X)] = E_{z \sim Q}[\log Q(z | X) - \log P(X|z) - \log P(z)] + \log P(X)$$

Rearranging

$$\log P(X) - KL[Q(z | X) \ || \ P(z|X)] = E_{z \sim Q}[\log P(X|z)] - KL[Q(z | X) \ || \ P(z)]$$

Does not depend on $z$
Understanding the Objective

\[
\log P(X) - KL[Q(z \mid X) \parallel P(z \mid X)] = E_{z \sim Q}[\log P(X \mid z)] - KL[Q(z \mid X) \parallel P(z)]
\]

What we want to maximize

Ensures that the encoder outputs \( z \) that can compute \( X \)

Objective for the decoder

Objective for the encoder

Can be optimized using SGD!
Understanding the Objective

Assumption: High capacity

\[ \log P(X) - KL[Q(z | X) \parallel P(z|X)] = E_{z \sim Q}[\log P(X|z)] - KL[Q(z | X) \parallel P(z)] \]

Can’t be computed analytically (not tractable)
Understanding the Objective

\[ \log P(X) - KL[Q(z \mid X) \parallel P(z \mid X)] = E_{z \sim Q} [\log P(X \mid z)] - KL[Q(z \mid X) \parallel P(z)] \]

Nearly zero! Thus we can use \( Q(z \mid X) \) to compute \( P(z \mid X) \)
Optimizing the Objective

$$R.H.S = E_{z \sim Q}[\log P(X|z)] - KL[Q(z | X) || P(z)]$$

$$Q(z | X) = N(z|\mu(X;\phi), \Sigma(X;\phi))$$

Parameterized deterministic functions

$$\Sigma(X;\phi)$$ is constrained to be a diagonal matrix to compute the KL divergence efficiently

$$KL[Q(z | X) || P(z)] = KL[N(z|\mu(X;\phi), \Sigma(X;\phi)) || N(z | 0, I)]$$

$$= 0.5(tr(\Sigma(X;\phi)) + \mu(X;\phi)^T \mu(X;\phi) - \log(\text{det}(\Sigma(X;\phi))))$$

Number of dimensions
Back-propagation - Reparameterization Trick

\[ \mathbb{KL}[\mathcal{N}(\mu(X), \Sigma(X)) || \mathcal{N}(0, I)] \]

Sample \( z \) from \( \mathcal{N}(\mu(X), \Sigma(X)) \)

\[ ||X - f(z)||^2 \]

\( f(z) \)

Decoder \((P)\)

\( \mu(X) \quad \Sigma(X) \)

Encoder \((Q)\)

\( X \)
Back-propagation - Reparameterization Trick
Note: The notations for equations and the figures of the AVT (ICCV’19) paper have been adjusted to align with the VAE tutorial.
Training data: \((x, y) \sim X\)

Model output: \(\hat{y} = f(\text{aug}(x))\)

Objective fnc: \(\min[\Sigma \text{loss}(\hat{y}, y)]\)

Can TERs be a criteria for learning unsupervised representations?
Unsupervised Representation Learning

Doersch et al. 2015

Agrawal et al. 2015

Wang et al. 2015

Owens et al. 2016

Gidaris et al. 2018

Use of non-visual signals, intrinsically correlated to the image, as a form to supervise visual feature learning.
Transformation Equivariant Representations

Parameterized Transformation: $t \sim p(t)$
Image: $x \sim p(x)$
Transformed Image: $t(x)$

Model with parameters $\varphi$

$Q(z | t(x); \varphi)$
Representation of the transformed image

$Q(\tilde{z} | x; \varphi)$
Representation of the original image

Objective: Use transformation equivariant property as a supervisory signal for learning unsupervised representations $Q(x; \varphi)$. 
AET: Auto-Encoders for Predicting Transformations

Objective fnc: \( \min \left[ E_{t \sim p(t), x \sim p(x)} \text{loss}(\hat{t}, t) \right] \)

L2 between projective transformation metrics
AVT: Auto-encoding Variational Transformations

\[ Q(z \mid x; \varphi), Q_x(x; \varphi) \]

Sample \( z \) from \( N(z \mid Q_\mu(x; \varphi), Q_x(x; \varphi)) \)

\[ Q(z \mid x; \varphi), Q_x(x; \varphi) \]

Sample \( \tilde{z} \) from \( Q_\mu(t(x); \varphi), Q_x(t(x); \varphi) \)

Sample \( t \) from \( N(t \mid f_\mu(z, \tilde{z}; \Theta), f_x(z, \tilde{z}; \Theta)) \)

\[ f(t \mid z, \tilde{z}; \Theta) \]
AVT: Optimization

\[ I(t; \tilde{z}|z) = H(t|z) - H(t; z) \]

mutual information conditional entropies (from the definition of mutual information)

\[ I(t; \tilde{z}|z) = H(t|z) + E_{z, \tilde{z} \sim Q(\varphi), t \sim p(t)} \left[ \log Q(t|\tilde{z}, z; \varphi) \right] \]

from the definition of conditional entropy

\[ I(t; \tilde{z}|z) = H(t|z) + E_{z, \tilde{z} \sim Q(\varphi), t \sim p(t)} \left[ \log f(t | z, \tilde{z}; \Theta) \right] + E_{z, \tilde{z} \sim Q(\varphi), t \sim p(t)} \text{KL}[Q(t|\tilde{z}, z; \varphi) \| f(t | z, \tilde{z}; \Theta)] \]

Always non-negative

\[ I(t; \tilde{z}|z) \geq H(t|z) + E_{z, \tilde{z} \sim Q(\varphi), t \sim p(t)} \left[ \log f(t | z, \tilde{z}; \Theta) \right] \]
AVT: Optimization

\[ I(t;\hat{z}|z) \geq H(t|z) + \mathbb{E}_{z,\hat{z} \sim Q(\varphi), t \sim p(t)}[\log f(t | z, \hat{z}; \Theta)] \]

Does not depend on model parameters

Objective: \[ \max_{\varphi, \Theta} E_{z,\hat{z} \sim Q(\varphi), t \sim p(t)}[\log f(t | z, \hat{z}; \Theta)] \]

\[ \max_{\theta, \varphi} \frac{1}{n} \sum_{i=1}^{n} \mathcal{N}(t_i | f_{\mu}(z_i, \hat{z}; \theta), f_{\sigma}(z_i, \hat{z}; \theta)) \]
AVT: Results on CIFAR-10 dataset

Table 2: Error rates of different classifiers trained on top of the learned representations on CIFAR 10, where $n$-FC denotes a classifier with $n$ fully connected layers and conv denotes the third NIN block as a convolutional classifier. Two AET variants are chosen for a fair direct comparison since they are based on the same architecture as the AVT and have outperformed the other unsupervised representations before [37].

<table>
<thead>
<tr>
<th></th>
<th>1 FC</th>
<th>2 FC</th>
<th>3 FC</th>
<th>conv</th>
</tr>
</thead>
<tbody>
<tr>
<td>AET-affine [37]</td>
<td>17.16</td>
<td>9.77</td>
<td>10.16</td>
<td>8.05</td>
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<tr>
<td>AET-project [37]</td>
<td>16.65</td>
<td>9.41</td>
<td>9.92</td>
<td>7.82</td>
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<tr>
<td>(Ours) AVT</td>
<td><strong>16.19</strong></td>
<td><strong>8.96</strong></td>
<td><strong>9.55</strong></td>
<td><strong>7.75</strong></td>
</tr>
</tbody>
</table>

Deterministic models

Probabilistic models used projective transformations for training
AVT: Results on ImageNet dataset

TABLE 6: Top-1 accuracy with linear layers on ImageNet. AlexNet is used as backbone to train the unsupervised models under comparison. A 1,000-way linear classifier is trained upon various convolutional layers of feature maps that are spatially resized to have about 9,000 elements. Fully supervised and random models are also reported to show the upper and the lower bounds of unsupervised model performances. Only a single crop is used and no dropout or local response normalization is used during testing, except the models denoted with * where ten crops are applied to compare results.

<table>
<thead>
<tr>
<th>Method</th>
<th>Conv1</th>
<th>Conv2</th>
<th>Conv3</th>
<th>Conv4</th>
<th>Conv5</th>
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<tbody>
<tr>
<td>ImageNet labels (Upper Bound)</td>
<td>19.3</td>
<td>36.3</td>
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<td>24.5</td>
<td>23.2</td>
<td>20.6</td>
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<tr>
<td>Context [21]</td>
<td></td>
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</tr>
<tr>
<td>Context Encoders [39]</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Colorization [26]</td>
<td>12.5</td>
<td>24.5</td>
<td>30.4</td>
<td>31.5</td>
<td>30.3</td>
</tr>
<tr>
<td>Jigsaw Puzzles [20]</td>
<td>18.2</td>
<td>28.8</td>
<td>34.0</td>
<td>33.9</td>
<td>27.1</td>
</tr>
<tr>
<td>BIGAN [13]</td>
<td>17.7</td>
<td>24.5</td>
<td>31.0</td>
<td>29.9</td>
<td>28.0</td>
</tr>
<tr>
<td>Split-Brain [40]</td>
<td>17.7</td>
<td>29.3</td>
<td>35.4</td>
<td>35.2</td>
<td>32.8</td>
</tr>
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<td>Counting [40]</td>
<td>18.0</td>
<td>30.6</td>
<td>34.3</td>
<td>32.5</td>
<td>25.7</td>
</tr>
<tr>
<td>RotNet [23]</td>
<td>18.8</td>
<td>31.7</td>
<td>38.7</td>
<td>38.2</td>
<td>36.5</td>
</tr>
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<tr>
<td>AVT-project</td>
<td>19.5</td>
<td>33.6</td>
<td>41.3</td>
<td>40.3</td>
<td>39.1</td>
</tr>
<tr>
<td>DeepCluster* [37]</td>
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<td>41.0</td>
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</tr>
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<td>AET-project*</td>
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<td>44.0</td>
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<td>42.4</td>
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<td>44.3</td>
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</table>
AVT: Results on Places dataset

TABLE 7: Top-1 accuracy on the Places dataset. A 205-way logistic regression classifier is trained on top of various layers of feature maps that are spatially resized to have about 9,000 elements. All unsupervised features are pre-trained on the ImageNet dataset, and then frozen when training the logistic regression classifiers with Places labels. We also compare with fully-supervised networks trained with Places Labels and ImageNet labels, as well as with random models. The highest accuracy values are in bold and the second highest accuracy values are underlined.

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Thank you!

@yash0307

patelyas@fel.cvut.cz

Homepage: https://yash0307.github.io