DATA SCIENCE

Variational autoencoders.

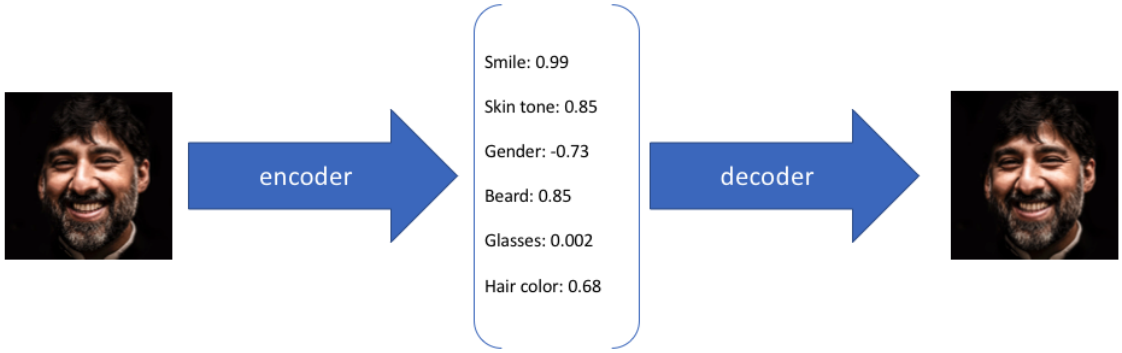
JEREMY JORDAN
19 MAR 2018 • 8 MIN READ

In my introductory post on autoencoders, I discussed various models (undercomplete, sparse, denoising, contractive) which take data as input and discover some latent state representation of that data. More specifically, our input data is converted into an *encoding vector* where each dimension represents some learned attribute about the data. The most important detail to grasp here is that our encoder network is outputting a *single value* for each encoding dimension. The decoder network then subsequently takes these values and attempts to recreate the original input.

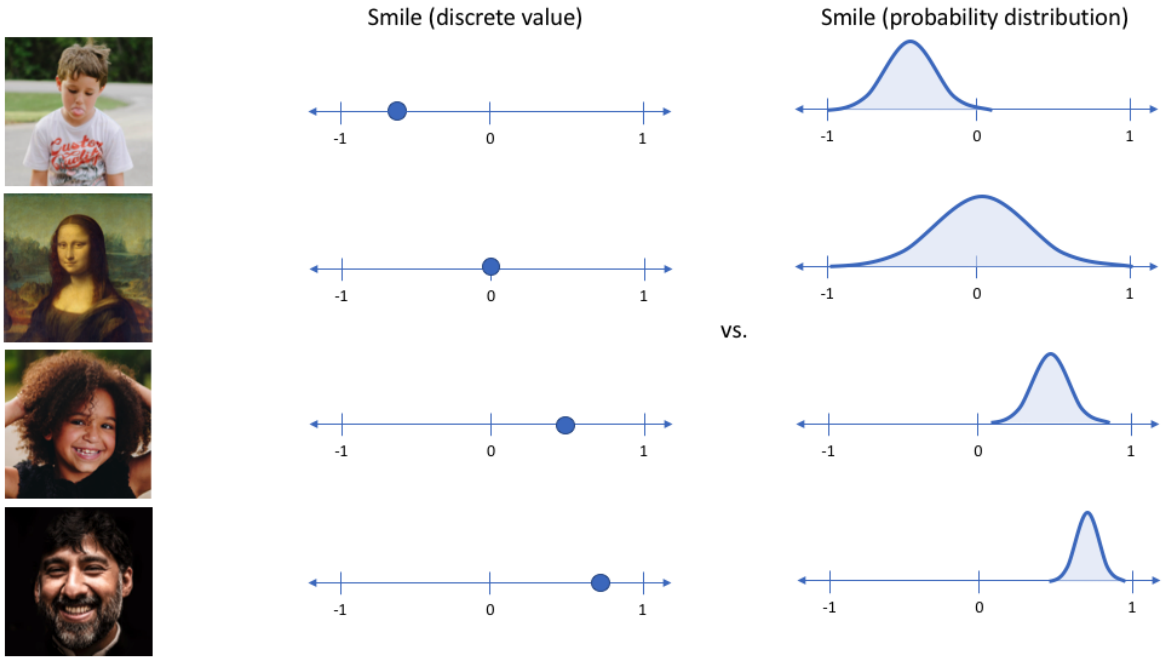
A variational autoencoder (VAE) provides a *probabilistic* manner for describing an observation in latent space. Thus, rather than building an encoder which outputs a single value to describe each latent state attribute, we'll formulate our encoder to describe a probability distribution for each latent attribute.

Intuition

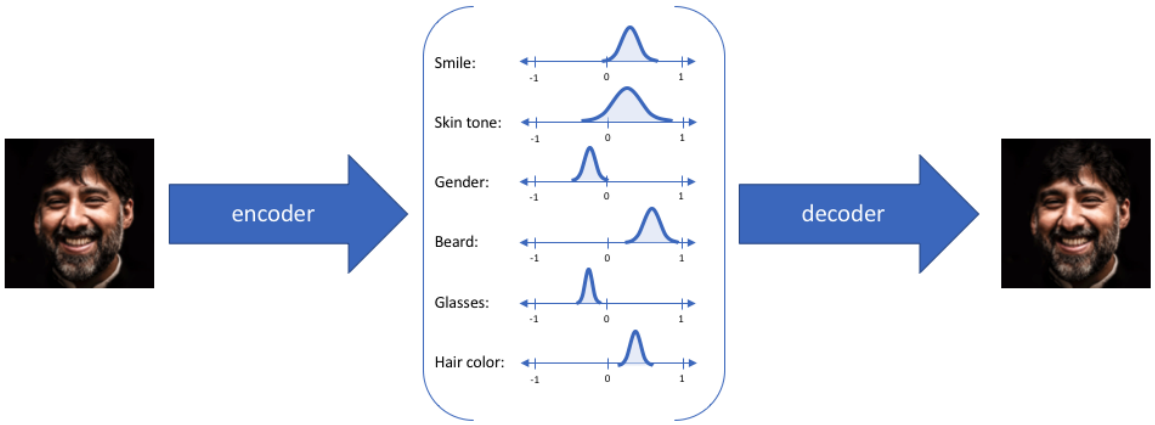
To provide an example, let's suppose we've trained an autoencoder model on a large dataset of faces with a encoding dimension of 6. An ideal autoencoder will learn descriptive attributes of faces such as skin color, whether or not the person is wearing glasses, etc. in an attempt to describe an observation in some compressed representation.



In the example above, we've described the input image in terms of its latent attributes using a single value to describe each attribute. However, we may prefer to represent each latent attribute as a range of possible values. For instance, what *single value* would you assign for the smile attribute if you feed in a photo of the Mona Lisa? Using a variational autoencoder, we can describe latent attributes in probabilistic terms.

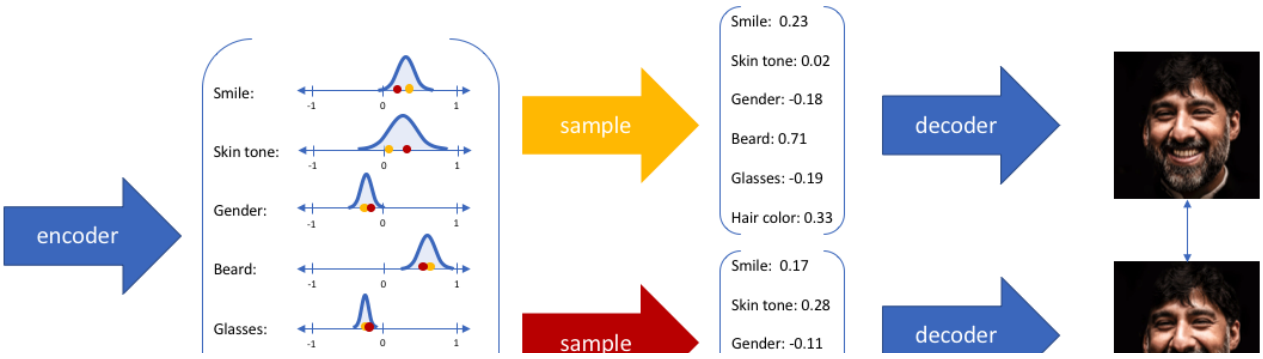


With this approach, we'll now represent *each latent attribute* for a given input as a probability distribution. When decoding from the latent state, we'll randomly



*Note: For variational autoencoders, the encoder model is sometimes referred to as the **recognition model** whereas the decoder model is sometimes referred to as the **generative model**.*

By constructing our encoder model to output a range of possible values (a statistical distribution) from which we'll randomly sample to feed into our decoder model, we're essentially enforcing a continuous, smooth latent space representation. For any sampling of the latent distributions, we're expecting our decoder model to be able to accurately reconstruct the input. Thus, values which are nearby to one another in latent space should correspond with very similar reconstructions.



Statisical motivation

Suppose that there exists some hidden variable z which generates an observation x.

We can only see x, but we would like to infer the characteristics of z. In other words, we'd like to compute $p(z|x)$.

$$p(z|x) = \frac{p(x|z)\,p(z)}{p(x)}$$

Unfortunately, computing $p(x)$ is quite difficult.

$$p(x) = \int p(x|z)\,p(z)\,dz$$

varitational inference to estimate this value.

Let's approximate $p(z|x)$ by another distribution $q(z|x)$ which we'll define such that it has a tractable distribution. If we can define the parameters of $q(z|x)$ such that it is very similar to $p(z|x)$, we can use it to perform approximate inference of the intractable distribution.

Recall that the KL divergence is a measure of difference between two probability distributions. Thus, if we wanted to ensure that $q(z|x)$ was similar to $p(z|x)$, we could minimize the KL divergence between the two distributions.

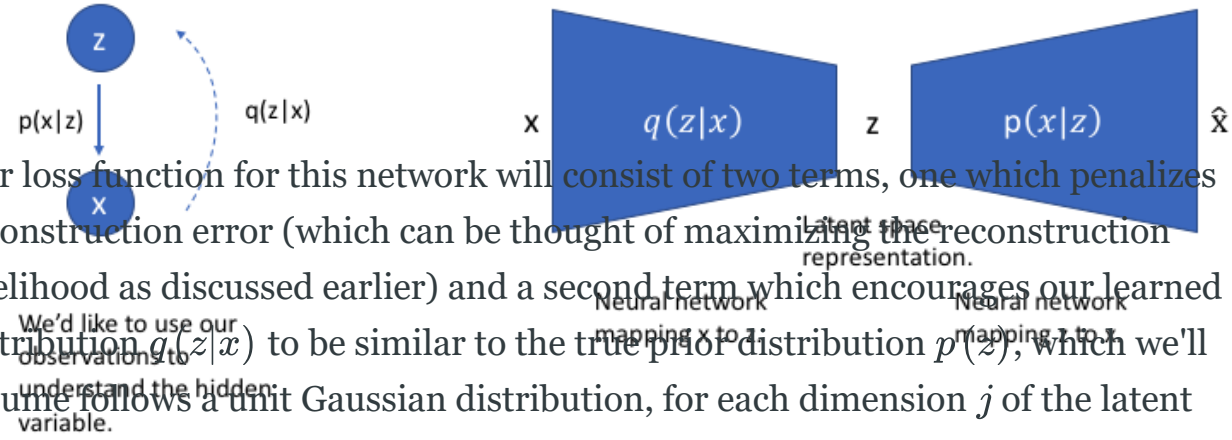
$$\min KL\left(q(z|x)\,||p(z|x)\right)$$

Dr. Ali Ghodsi goes through a full derivation here, but the result gives us that we can minimize the above expression by maximizing the following:

$$E_{q(z|x)}\log p(x|z) - KL\left(q(z|x)\,||p(z)\right)$$

The first term represents the reconstruction likelihood and the second term ensures that our learned distribution q is similar to the true prior distribution p.

To revisit our graphical model, we can use q to infer the possible hidden variables (ie. latent state) which was used to generate an observation. We can further construct this model into a neural network architecture where the encoder model learns a mapping from x to z and the decoder model learns a mapping from z back to x.



Our loss function for this network will consist of two terms, one which penalizes reconstruction error (which can be thought of maximizing the reconstruction likelihood as discussed earlier) and a second term which encourages our learned distribution $q(z|x)$ to be similar to the true prior distribution $p(z)$, which we'll assume follows a unit Gaussian distribution, for each dimension j of the latent space.

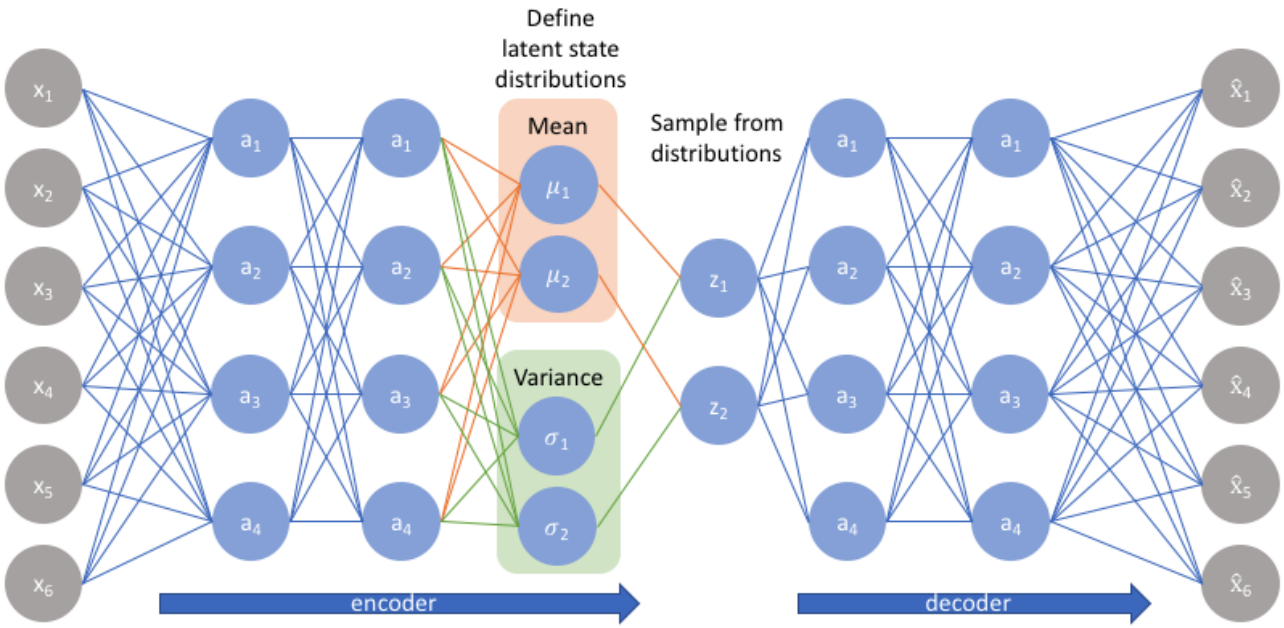
$$\mathcal{L}(x, \hat{x}) + \sum_j KL(q_j(z|x)||p(z))$$

Implementation

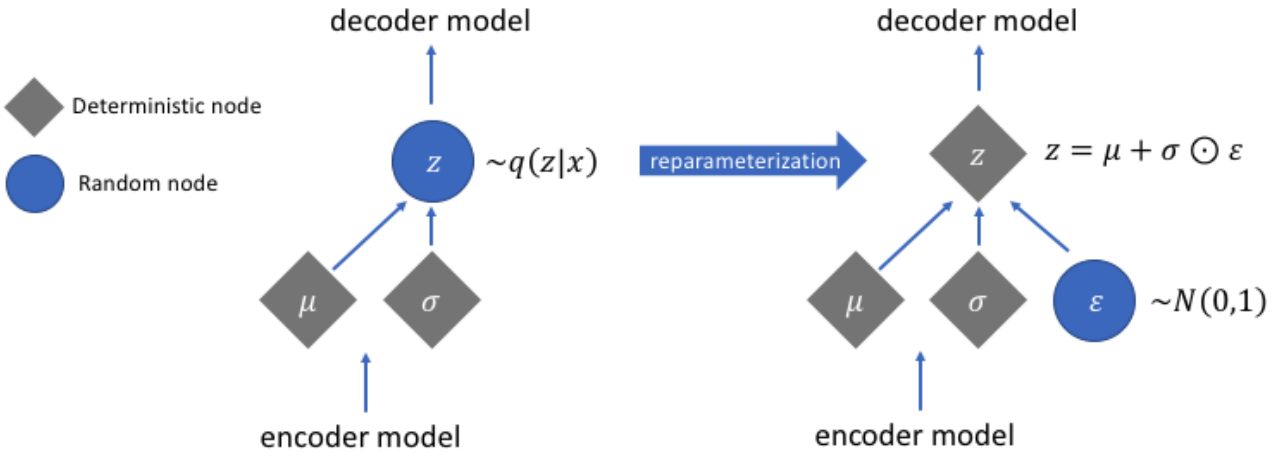
In the previous section, I established the statistical motivation for a variational autoencoder structure. In this section, I'll provide the practical implementation details for building such a model yourself.

Rather than directly outputting values for the latent state as we would in a standard autoencoder, the encoder model of a VAE will output parameters describing a distribution for each dimension in the latent space. Since we're assuming that our prior follows a normal distribution, we'll output *two* vectors describing the mean and variance of the latent state distributions. If we were to build a true multivariate Gaussian model, we'd need to define a covariance matrix describing how each of the dimensions are correlated. However, we'll make a simplifying assumption that our covariance matrix only has nonzero values on the diagonal, allowing us to describe this information in a simple vector.

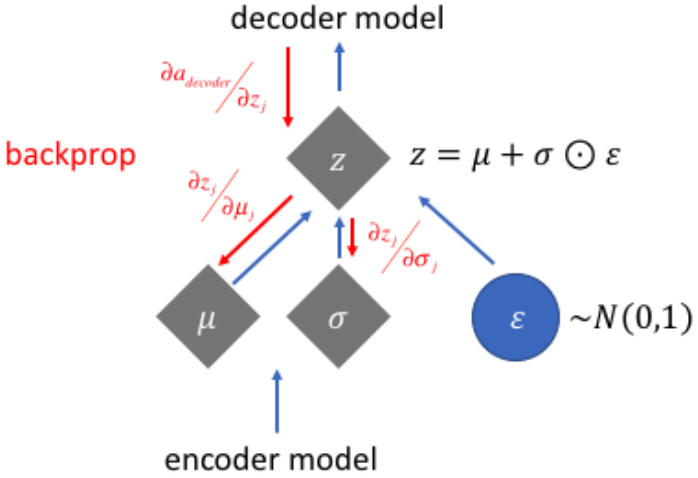
Our decoder model will then generate a latent vector by sampling from these



However, this sampling process requires some extra attention. When training the model, we need to be able to calculate the relationship of each parameter in the network with respect to the final output loss using a technique known as backpropagation. However, we simply cannot do this for a *random sampling* process. Fortunately, we can leverage a clever idea known as the "reparameterization trick" which suggests that we randomly sample ε from a unit Gaussian, and then shift the randomly sampled ε by the latent distribution's mean μ and scale it by the latent distribution's variance σ.



distribution while still maintaining the ability to randomly sample from that distribution.



Note: In order to deal with the fact that the network may learn negative values for σ, we'll typically have the network learn $\log \sigma$ and exponentiate this value to get the latent distribution's variance.

Visualization of latent space

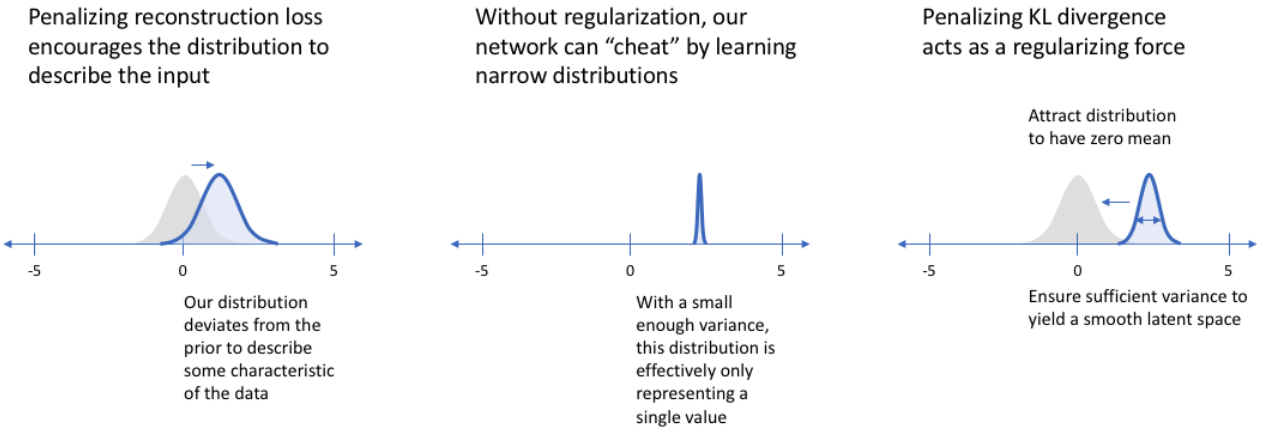
To understand the implications of a variational autoencoder model and how it differs from standard autoencoder architectures, it's useful to examine the latent space. This blog post introduces a great discussion on the topic, which I'll summarize in this section.

The main benefit of a variational autoencoder is that we're capable of learning *smooth* latent state representations of the input data. For standard autoencoders, we simply need to learn an encoding which allows us to reproduce the input. As you can see in the left-most figure, focusing only on reconstruction loss *does* allow us to separate out the classes (in this case, MNIST digits) which should allow our decoder model the ability to reproduce the original handwritten digit, but there's an uneven distribution of data within the latent space. In other words, there are areas in latent space which don't represent *any* of our observed data.

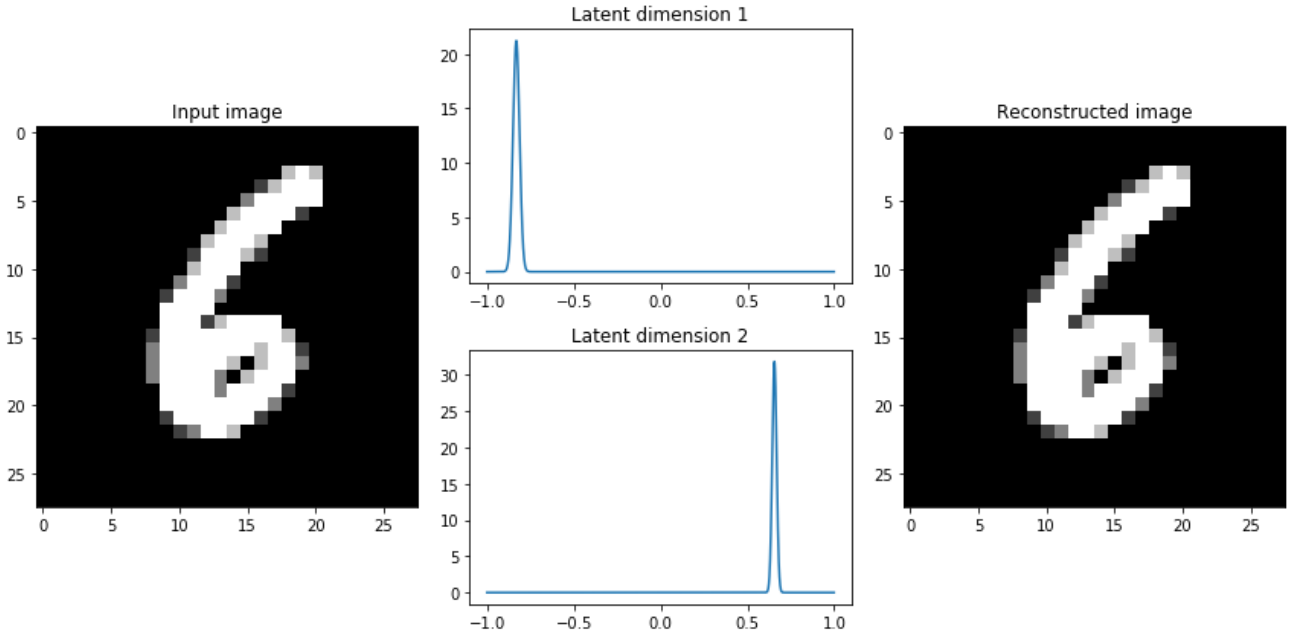
Image credit (modified)

On the flip side, if we only focus only on ensuring that the latent distribution is similar to the prior distribution (through our KL divergence loss term), we end up describing *every* observation using the same unit Gaussian, which we subsequently sample from to describe the latent dimensions visualized. This effectively treats every observation as having the same characteristics; in other words, we've failed to describe the original data.

However, when the two terms are optimized simultaneously, we're encouraged to describe the latent state for an observation with distributions close to the prior but deviating when necessary to describe salient features of the input.



When I'm constructing a variational autoencoder, I like to inspect the latent



If we observe that the latent distributions appear to be very tight, we may decide to give higher weight to the KL divergence term with a parameter $\beta > 1$, encouraging the network to learn broader distributions. This simple insight has led to the growth of a new class of models - disentangled variational autoencoders. As it turns out, by placing a larger emphasis on the KL divergence term we're also implicitly enforcing that the learned latent dimensions are uncorrelated (through our simplifying assumption of a diagonal covariance matrix).

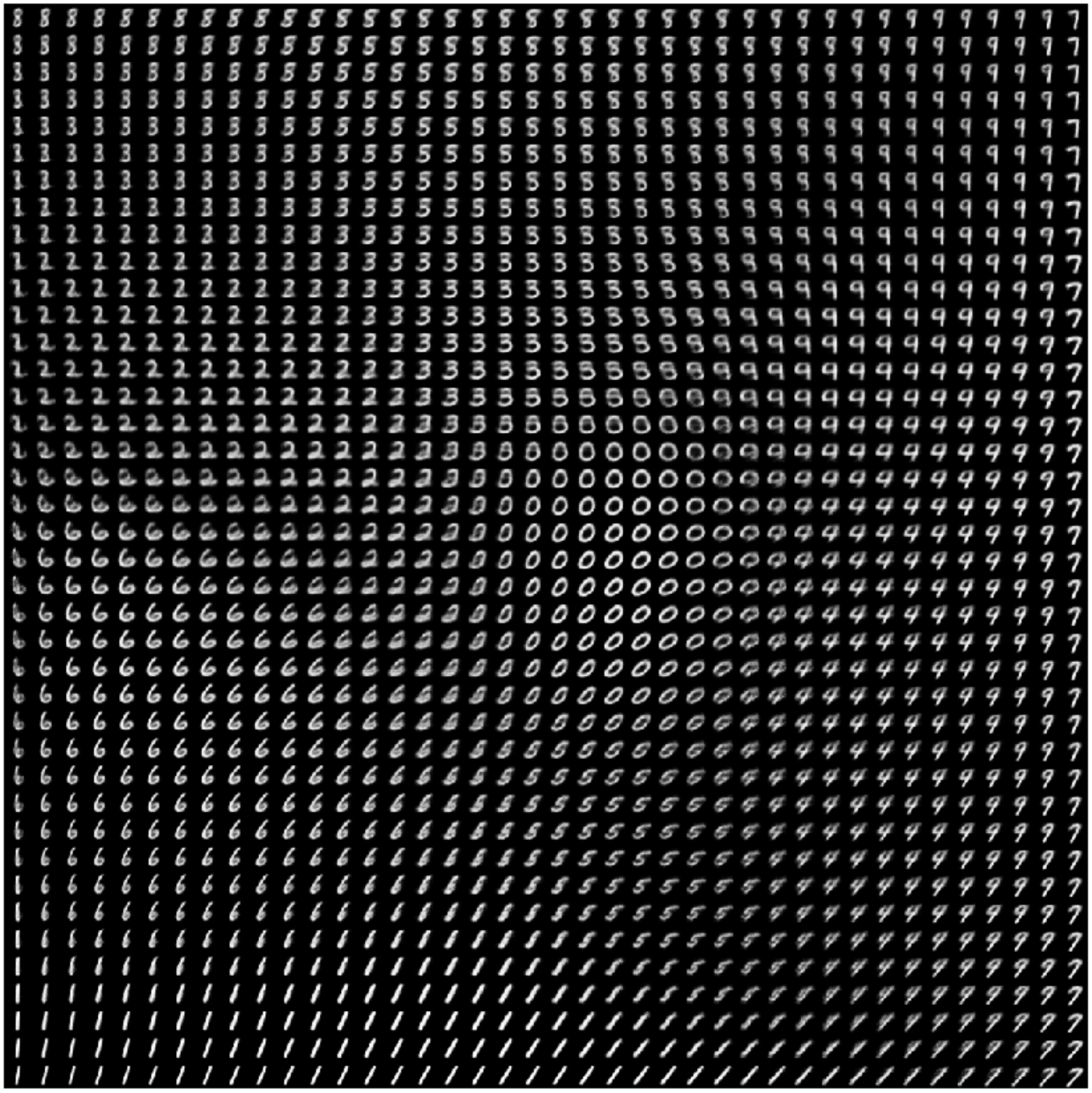
$$\mathcal{L}\left(x, \hat{x}\right) + \beta \sum_{j} KL\left(q_j\left(z|x\right)||N\left(0,1\right)\right)$$

Variational autoencoders as a generative model

By sampling from the latent space, we can use the decoder network to form a generative model capable of creating new data similar to what was observed during training. Specifically, we'll sample from the prior distribution $p\left(z\right)$ which we assumed follows a unit Gaussian distribution.

The figure below visualizes the data generated by the decoder network of a

the output of our decoder network.



As you can see, the distinct digits each exist in different regions of the latent space and smoothly transform from one digit to another. This smooth transformation can be quite useful when you'd like to interpolate between two observations, such as this recent example where Google built a model for interpolating between two music samples.

Further reading

Lectures

- Ali Ghodsi: Deep Learning, Variational Autoencoder (Oct 12 2017)
- UC Berkley Deep Learning Decall Fall 2017 Day 6: Autoencoders and Representation Learning
- Stanford CS231n: Lecture on Variational Autoencoders

Blogs/videos

- Building Variational Auto-Encoders in TensorFlow (with great code examples)
- Building Autoencoders in Keras
- Variational Autoencoders - Arxiv Insights
- Intuitively Understanding Variational Autoencoders
- Density Estimation: A Neurotically In-Depth Look At Variational Autoencoders
- Pyro: Variational Autoencoders
- Under the Hood of the Variational Autoencoder

- Kullback-Leibler Divergence Explained
- Neural Discrete Representation Learning

Papers/books

- Deep learning book (Chapter 20.10.3): Variational Autoencoders
- Variational Inference: A Review for Statisticians
- A tutorial on variational Bayesian inference
- Auto-Encoding Variational Bayes
- Tutorial on Variational Autoencoders

Papers on my reading list

- Neural Discrete Representation Learning
- Early Visual Concept Learning with Unsupervised Deep Learning
- Multimodal Unsupervised Image-to-Image Translation
  - Video from paper

Lester • 3 years ago

Great post! Never understood why KL and reconstruction loss were used. The other thing I wonder about is why MSE is not as the reconstruction loss but rather I usually see binary cross-entropy applied to the pixels?

1 • Reply • Share ›

Jeremy Jordan Mod Lester • 3 years ago

That's a really good question! I believe it has to do with the nature (ie. distribution) of your data - Dr. Ghodsi alludes to this in his lecture.

2 • Reply • Share ›

is how is mean and variance vector representation different. if we interchange mean and variance variables, will it still be the same?

Naveen Vishnu Kinnal ↪ Rajesh T • 8 days ago

It would not be the same. Since during learning and backpropogation, the mean and variance are updated by different factors, such that the losses are minimized.

• Reply • Share ›

Asifa Junaid • 2 months ago

wonderful post, article is written in simple way. I understand the concepts very well.Thanks a lot

• Reply • Share ›

Pietro Fusco • 2 months ago • edited

This is an amazing post. I would kindly ask you if you can suggest or refer a post about Normalizing Flows. Thanks in advance.

• Reply • Share ›

parekh vivek • 3 months ago

How to learn distribution numerical data? For examples, input parameters of housing price prediction dataset.

• Reply • Share ›

MM • 5 months ago

Your blog was the first result on Google when I searched "Variational Autoencoder". Such wonderful explanations!

• Reply • Share ›

Omer • 7 months ago

Hi, great post!
1 question if I may... You have written "When I'm constructing a variational autoencoder, I like to inspect the latent dimensions for a few samples from the data to see the characteristics of the distribution."
You mean taking a single specific sample x_i from the data and observing the histogram of the z_i's the encoder produces? I can simply look at the std or I'm mistaken?
Or maybe you have meant lookong on the full histogram of the z_i's obtained from all the data x_1,x_2,...x_N ? What do you get by that? Isn't it simply Q(z_i | X) ?

• Reply • Share ›

Wesley Neill • 8 months ago

I'm super stoked that you turned me on to Dr. Ghodsi's Lectures. I

Weierstraß • a year ago

Anandamoy Bandyopadhyay • 2 years ago

The best article on the net about VAEs that I've come across. Thanks a lot for this!
The KL term essentially tries to attract each of the latent feature means to zero and variance as close as to 1 as possible, right?
However, for data with large variability does this restriction not adversely affect the geneartive performance of the model? Does it make sense to use *N(0, s)* instead of *N(0, 1)* where *s* is a data-dependent hyperparameter?
Also, can any differentiable image-image comparison measure be used in place of the reconstruction loss?

Would be much obliged if you could find the time to leave a reply!

• Reply • Share ›

Manjiro Kawakami • 2 years ago

Other 1 is here.
Please advise me about KL(q(z|x)||N(01)). Does P(z) represent classes of normal distributions with the coefficients with Maximum Likelihood? For example, the pictures of mountains, lakes, clouds, to be z1 and z2 and z3 being, say, 0.3, 0.5, and 0.2? Or, is this z simply the one to correspond to x, one by one in the reduced dimension space, with several Gaussian peaks to be confined in N(0,1)? I got lost. Please help.

• Reply • Share ›

Manjiro Kawakami • 2 years ago

2 questions more, thank you for many help. 1 is here.
Re-parametrization. With reconstruction loss, I thought it is basically, supervised training with backpropagation like CNN to Make X and X-bar identical. Why εnecessary? For each X, correspondent Z will be selected and Z will be distributed anyway. Where am I mistaken?

• Reply • Share ›

Manjiro Kawakami • 2 years ago

Thank you very much for your articles!
How you could put "SMILE" label in features for unsupervised learning?
I meaning is, you already labeling to training material with "SMILE" before VAE training, or labeling after VAE traning as put "SMILE"

Jeremy Jordan Mod ↷ Manjiro Kawakami • 2 years ago

Yeah good question, I put human-interpretable concepts for the dimensions in latent space so that people could understand

are uncorrelated and represent distinct concepts. When you train generative models, one thing you can do is search for a vector in the latent space which does represent a concept, and modify the values along this vector to adjust an explicit concept.

• Reply • Share ›

Manjiro Kawakami Jeremy Jordan • 2 years ago

Thank you again. Questions. Can I understand that we can input X into Encoder randomly without categorizing smile, glass, color-of-skin, etc, in advance, right?

I naturally presume such features like “smile” cannot be coincidentally eigenvalue (in case of PCA). Do you mean that we can tame the feature to be independent (diagonal) by tampering somehow?

• Reply • Share ›

Manjiro Kawakami Jeremy Jordan • 2 years ago

Thank you very much for your prompt reply, exciting.
I have a interesting what is the "human-interpretable concepts" in actual program but I trying to understand your advice detail first. Again, thank you very much for your articles and reply !

• Reply • Share ›

issy • 2 years ago

hi jeremy, if we take a random encoding and do nearest neighbor search, do we end up with similar neighbors? i don't see many similars though.

• Reply • Share ›

Jeremy Jordan Mod issy • 2 years ago

what do you mean by random encoding? a randomly selected image (and its encoding) from your dataset or a randomly generated vector? can you provide more details surrounding the problem you're working on?

• Reply • Share ›

issy Jeremy Jordan • 2 years ago • edited

my goal is to get similar images clustered. So, when i do a nearest neighbor search, i could find all the visually

that there are lot of neighbors which belong to different classes as the clusters in latent representation are close

interpolate.
Training the model and throwing away the decoder and using the encoder seems like just doing the PCA and knn.

• Reply • Share ›

Jeremy Jordan Mod ➚ issy
• 2 years ago • edited

if you have a good VAE model then the encoding space should capture a visual similarity metric. for example, notice how model trained on MNIST data has a smooth latent space with similar numbers (eg. 1 and 7) occurring nearby. your hypothesis makes sense, have you tried adjusting the hyperparameter to balance between reconstruction loss and KL divergence?

it also sounds like this paper https://arxiv.org/abs/1907.... would be a good approach to explore for your problem.

• Reply • Share ›

issy ➚ Jeremy Jordan • 2 years ago

Thanks, will look into it. i do not want the visual similar metric in the generated. i just want to find out the visually similar in my dataset. I will not be using image generation at all.

• Reply • Share ›

Mithi Sevilla • 2 years ago • edited

Hi Jeremy! Thanks for writing this well-explained article about VAEs . I included it in this little project of mine called Deep Blueberry Book, a very focused collection of must-see deep-learning videos and articles.

If you know a cool link that you think should be included in this tiny

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A simple solution for monitoring ML systems.
2 Jan 2021 – 10 min read

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Common architectures in convolutional neural networks.

In this post, I'll discuss commonly used architectures for convolutional networks. As you'll see, almost all CNN architectures follow the same general design principles of successively applying convolutional layers to the input, periodically downsampling the spatial dimensions while increasing the number of feature maps.

JEREMY JORDAN
19 APR 2018 • 9 MIN READ

DATA SCIENCE

Introduction to autoencoders.

Autoencoders are an unsupervised learning technique in which we leverage neural networks for the task of representation learning. Specifically, we'll design a neural network architecture such that we impose a bottleneck in the network which forces a compressed knowledge representation of the original input.

JEREMY JORDAN
19 MAR 2018 • 10 MIN READ