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May 14th, 2020

Unsupervised Learning: Introduction to Generative Models

Olivier Dubrule and Navjot Kukreja

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Objectives of the Day

- Recall what unsupervised learning is, with PCA as simplest linear case
- Autoencoders and latent vectors for image parametrization
- Introduce transposed convolution
- Variational Autoencoders for coding and generating random images
- Generative Adversarial Networks for generating random images

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Introduction to Generative Models

1. PCA and Autoencoders
2. Transposed Convolution
3. Variational Autoencoders
4. Generative Adversarial Networks

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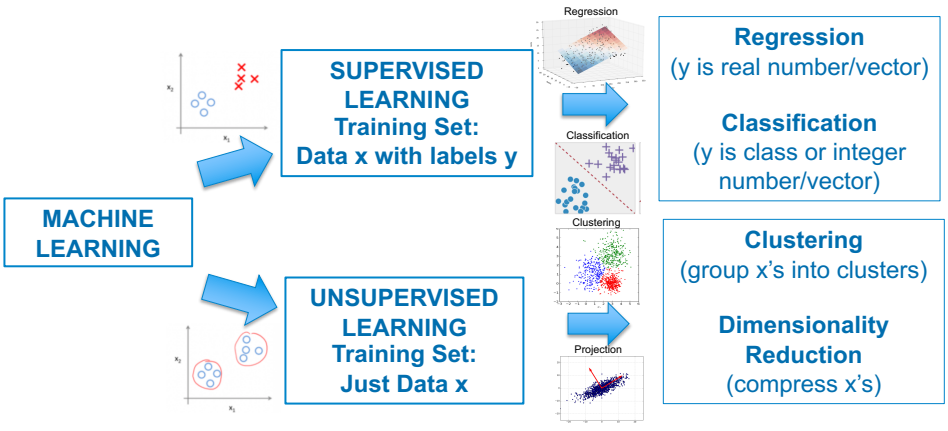
Supervised vs Unsupervised Learning



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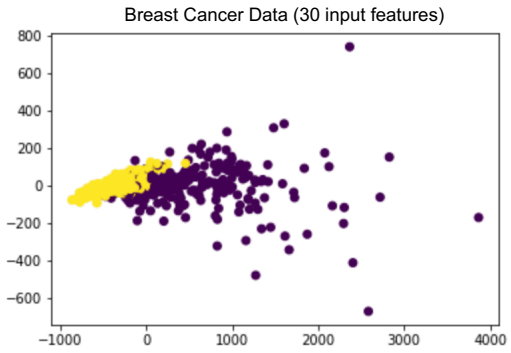
PCA Dimensionality Reduction



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The PCA Method is Linear Dimensionality Reduction

If the first p eigenvectors are denoted as $(\varphi_k)_{k=1,..,p}$, each data vector $x^{(i)}$ of dimension n can be approximated by a linear combination of the eigenvectors:

$$x^{(i)} \approx \sum_{k=1}^{p} z_k^{(i)} \varphi_k$$

So, instead of being defined by its n original features, each $x^{(i)}$ is now defined by its p coordinates $z_k^{(i)}$ in the basis $(\varphi_k)_{k=1,..,p}$, where $p \ll n$: this is Dimensionality Reduction.

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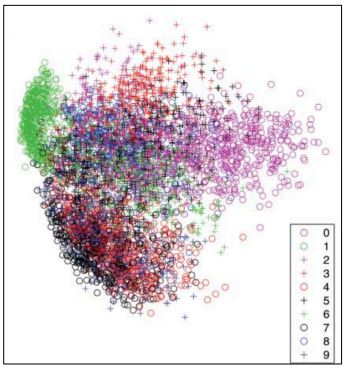
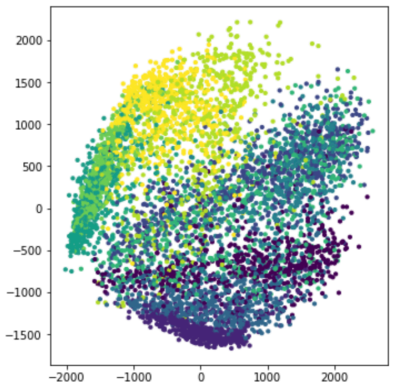
PCA Dimensionality Reduction on Images

MNIST (784 input features)



Fashion MNIST (784 input features)



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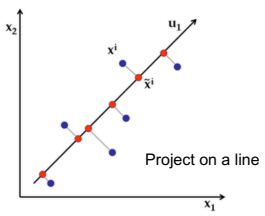
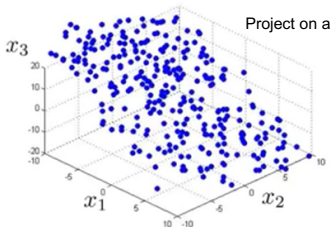
Dimensionality Reduction with Latent Vectors

Idea:

PCA projects only on a linear manifold, we wish to generalize to non-linear manifolds.





Potential applications

Simple parametrization of images, classification or regression based on the feature vectors $z^{(i)}$ rather than the raw data $x^{(i)}$, visualization, data compression, inversion….

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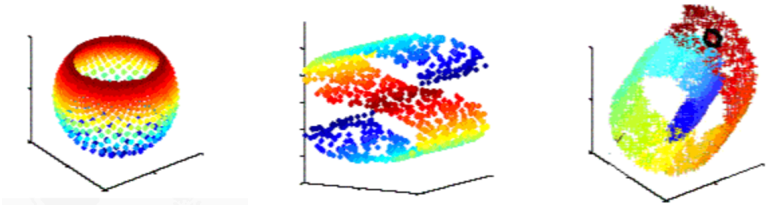
Why do we Need a Non-Linear Approach ?



Examples of data that cannot be separated by projecting on a linear manifold.

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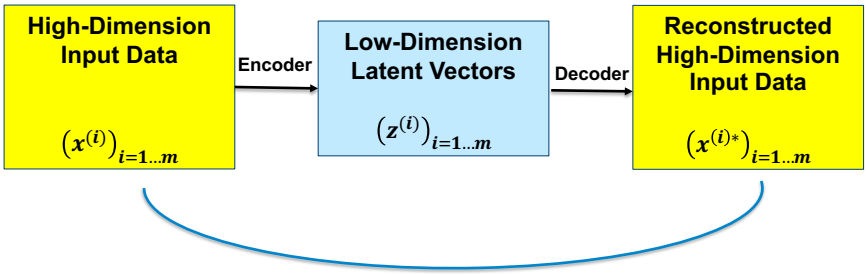
Autoencoders: the Basic Idea



Minimize the reconstruction loss
$\sum_{i=1}^{m} \|x^{(i)} - x^{(i)*}\|^2$ ***if real numbers***
(or cross-entropy if classes)

Note that we use Supervised Learning to address an Unsupervised Learning problem!

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Autoencoders Historical Example on MNIST (~12,000 citations)

Reducing the Dimensionality of Data with Neural Networks

G. E. Hinton* and R. R. Salakhutdinov

High-dimensional data can be converted to low-dimensional codes by training a multilayer neural network with a small central layer to reconstruct high-dimensional input vectors. Gradient descent can be used for fine-tuning the weights in such "autoencoder" networks, but this works well only if the initial weights are close to a good solution. We describe an effective way of initializing the weights that allows deep autoencoder networks to learn low-dimensional codes that work much better than principal components analysis as a tool to reduce the dimensionality of data.

Dimensionality reduction facilitates the classification, visualization, communication, and storage of high-dimensional data. A simple and widely used method is principal components analysis (PCA), which finds the directions of greatest variance in the data set and represents each data point by its coordinates along each of these directions. We describe a nonlinear generalization of PCA that uses an adaptive, multilayer "encoder" network

2006 VOL 313 SCIENCE www.sciencemag.org

From Hinton and Salakhutdinov, Science, Science, July 2006
https://www.youtube.com/watch?v=_Ex1Ur85AVs

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Autoencoder Historical Example on MNIST

Structure of Hinton and Salakhutdinov's autoencoders (loss function is cross-entropy)

Each MNIST image represented now in p=30 dimensions instead of originally in 28x28=784 dimensions.

From Hinton and Salakhutdinov, Science, Science, July 2006
https://www.youtube.com/watch?v=_Ex1Ur85AVs

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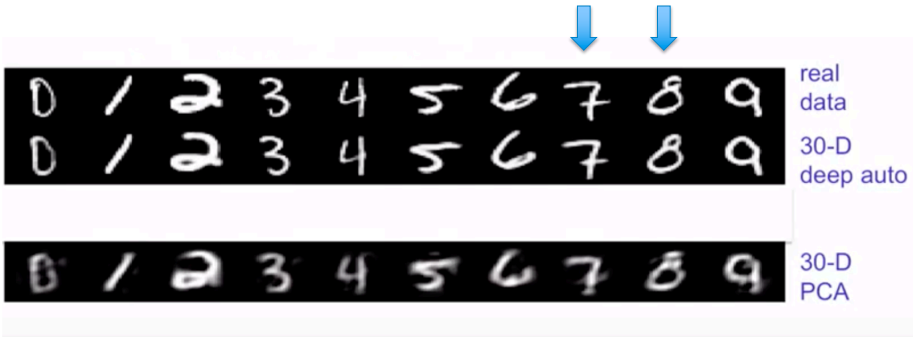
Autoencoder Historical Example on MNIST



The reconstructed numbers (second line) look better than the originals, because the autoencoder model does not have enough capacity to represent the subtle variations/noise in the data.

From Hinton and Salakhutdinov, Science, Science, July 2006
https://www.youtube.com/watch?v=_Ex1Ur85AVs

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Autoencoder Historical Example on MNIST

Now using a 2-dimensional instead of 30-dimensional code

Each MNIST number represented now in p=2 dimensions instead of originally in 28x28=784 dimensions!

From Hinton and Salakhutdinov, Science, Science, July 2006
https://www.youtube.com/watch?v=_Ex1Ur85AVs

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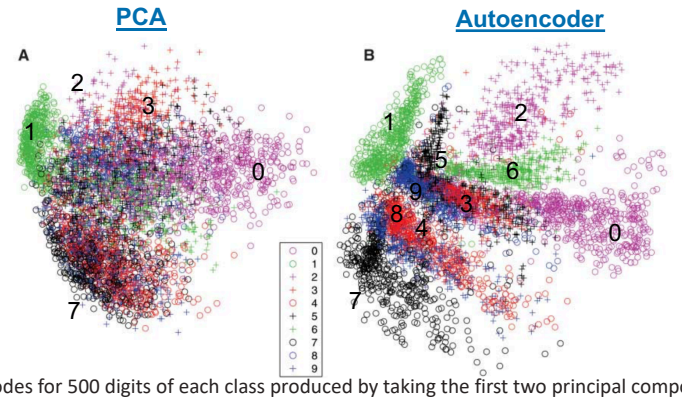
Autoencoder Historical Example on MNIST

Now representing 28x28 MNIST images by just two coordinates



(A) The 2-D codes for 500 digits of each class produced by taking the first two principal components of all 60,000 training images. (B) The two-dimensional codes found by a 784- 1000-500-250-2 autoencoder.

From Hinton and Salakhutdinov, Science, Science, July 2006

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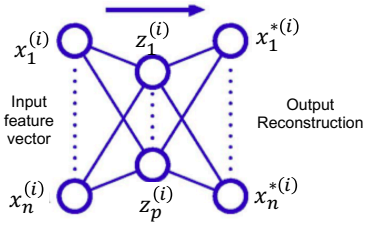
Question

What result will the autoencoder produce if there is just one hidden layer and no non-linear activation function in the encoder and decoder networks?



$z = Wx$

$x^* = W'z$

Minimize:

$$\sum_{i=1}^{m} \|x_i - x_i^*\|^2$$

PCA!

https://www.cs.toronto.edu/~urtasun/courses/CSC411/14_pca.pdf

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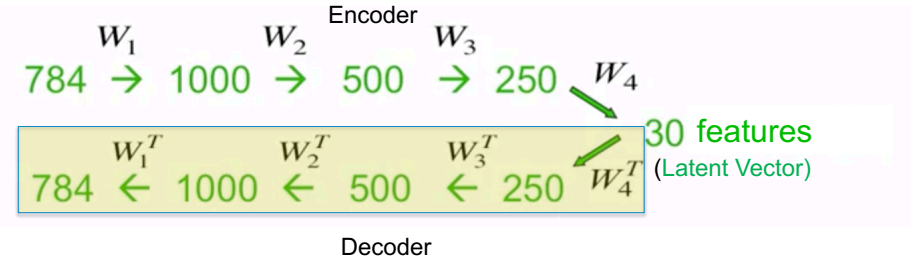
Transposed Convolution Filters



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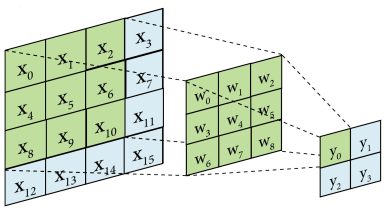
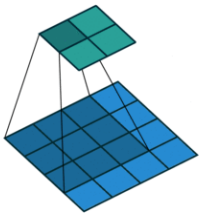
Encoder: Convolution Reduces Dimensionality

Simple 2-D Convolution Example (stride 1, no-padding)





$$y_0 = w_0x_0+w_1x_1+w_2x_2+w_3x_4+w_4x_5+w_5x_6+w_6x_8+w_7x_9+w_8x_{10} + \boldsymbol{b}$$

Can we write the Convolution Operation in Matrix Form?

https://github.com/vdumoulin/conv_arithmetic
https://towardsdatascience.com/up-sampling-with-transposed-convolution-9ae4f2df52d0

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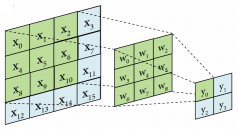

Encoder: Writing Convolution as a Matrix Operation

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} w_0 & w_1 & w_2 & 0 & w_3 & w_4 & w_5 & 0 & w_6 & w_7 & w_8 & 0 & 0 & 0 & 0 & 0 \\ 0 & w_0 & w_1 & w_2 & 0 & w_3 & w_4 & w_5 & 0 & w_6 & w_7 & w_8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_0 & w_1 & w_2 & 0 & w_3 & w_4 & w_5 & 0 & w_6 & w_7 & w_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & w_0 & w_1 & w_2 & 0 & w_3 & w_4 & w_5 & 0 & w_6 & w_7 & w_8 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \\ x_{14} \\ x_{15} \end{pmatrix}$$

Convolution can be written in matrix form $\boldsymbol{y} = \boldsymbol{W}\boldsymbol{x}$ with x reshaped as a 16x1 vector, y reshaped as a 4x1 vector, and a 4x16 matrix W.

https://github.com/vdumoulin/conv_arithmetic
https://towardsdatascience.com/up-sampling-with-transposed-convolution-9ae4f2df52d0

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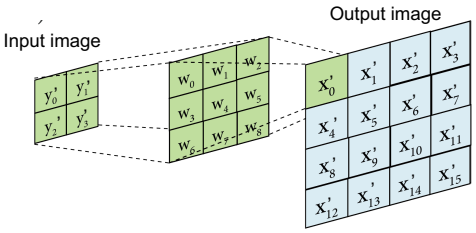
Decoder: Transposed Convolution to Increase Dimensionality



y' reshaped into 4x1 vector, x' reshaped into 16x1 vector and W^T 16x4 transposed of W

$$x' = W^T y'$$

$$\begin{pmatrix} x'_0 \\ x'_1 \\ x'_2 \\ x'_3 \\ x'_4 \\ x'_5 \\ x'_6 \\ x'_7 \\ x'_8 \\ x'_9 \\ x'_{10} \\ x'_{11} \\ x'_{12} \\ x'_{13} \\ x'_{14} \\ x'_{15} \end{pmatrix} = \begin{pmatrix} w_0 & 0 & 0 & 0 \\ w_1 & w_0 & 0 & 0 \\ w_2 & w_1 & 0 & 0 \\ 0 & w_2 & 0 & 0 \\ w_3 & 0 & w_0 & 0 \\ w_4 & w_3 & w_1 & w_0 \\ w_5 & w_4 & w_2 & w_1 \\ 0 & w_5 & 0 & w_2 \\ w_6 & 0 & w_3 & 0 \\ w_7 & w_6 & w_4 & w_3 \\ w_8 & w_7 & w_5 & w_4 \\ 0 & w_8 & 0 & w_5 \\ 0 & 0 & w_6 & 0 \\ 0 & 0 & w_7 & w_6 \\ 0 & 0 & w_8 & w_7 \\ 0 & 0 & 0 & w_8 \end{pmatrix} \times \begin{pmatrix} y'_0 \\ y'_1 \\ y'_2 \\ y'_3 \end{pmatrix}$$

https://github.com/vdumoulin/conv_arithmetic

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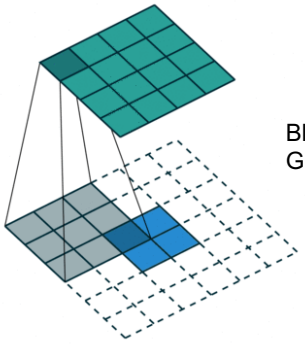
Transposed Convolution can also be Calculated by Convolution

Apply padding = 2 to array

$$\begin{matrix} y'_0 & y'_1 \\ y'_2 & y'_3 \end{matrix}$$

And convolve by filter W with stride 1.



Blue : input image
Green: output image

See afternoon exercise

https://github.com/vdumoulin/conv_arithmetic

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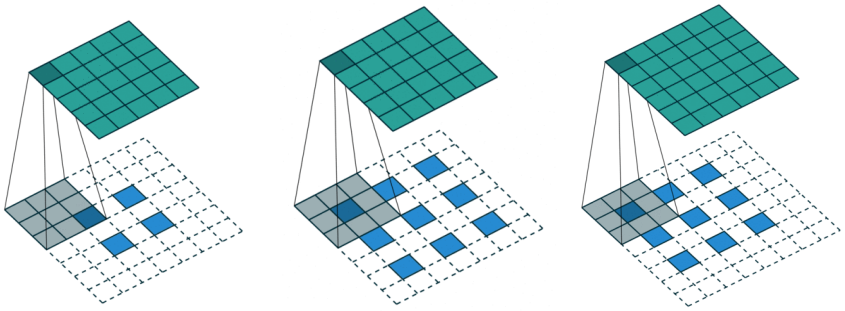
Transposed Convolution can also be Calculated by Convolution



Blue : input image
Green: output image

Issue of checker board artefacts: https://distill.pub/2016/deconv-checkerboard/

https://github.com/vdumoulin/conv_arithmetic

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Approach to calculate Transposed Convolution Operator

1. Identify the associated Direct Convolution
2. Calculate the Matrix associated with the Direct Convolution
3. Obtain Transposed Convolution from Transposed Matrix
4. Identify the Direct Convolution mimicking the Transposed one

https://arxiv.org/pdf/1603.07285.pdf

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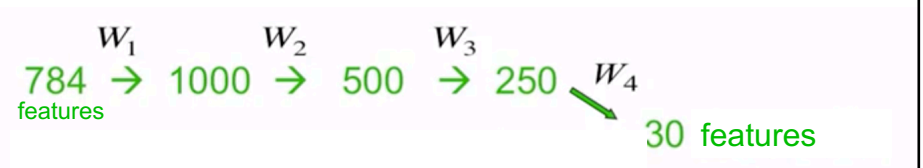
Which Use for Autoencoders?



Once the autoencoder has been trained, throw away the calibrated Decoder and use the Encoder for Dimensionality Reduction!

Every Image of MNIST Dataset now represented by only 30 features instead of by 784 pixel values.

Possible Application: a Supervised Learning exercise on the MNIST Dataset can use the 30 features as input features, instead of the 784 pixel values. Helps avoid overfitting the $x^{(i)}$ when not many input images are labelled.

From Hinton and Salakhutdinov, Science, Science, July 2006

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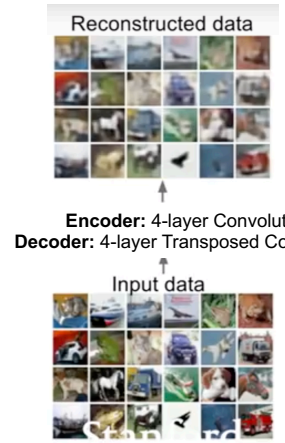
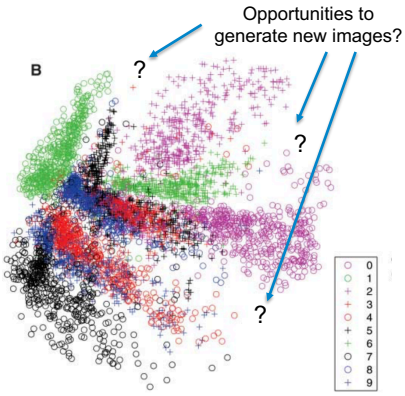
Autoencoders only Encode and Decode Existing Images





… we have not used the decoder yet. Why not make it generate more random images than just the existing ones?

https://www.youtube.com/watch?v=5WoItGTWV54 From Hinton and Salakhutdinov, Science, Science, July 2006

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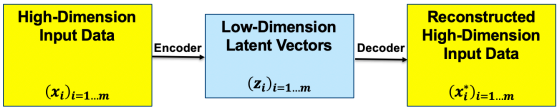
Variational Autoencoders (VAEs)



Variational autoencoders will be used to generate new images, that is images that are "variations" or belong to the same general pdf as images from the training set .

Make z and x random, instead of keeping them deterministic.

By sampling z, we will generate images that are not in the Training Set!

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How Variational Autoencoders Work (1)

The Encoding Step

Input Image x

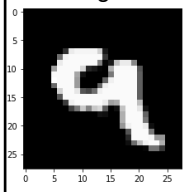


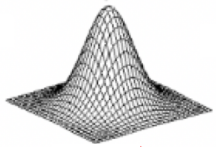
Image is of dimension n

Neural Network

$\mu(x)$

$\sigma^2(x)$

$\mu(x)$ and $\sigma^2(x)$ of dimension p



pdf of Latent Vector z

$\mathrm{N}(z; \mu(x), \sigma^2(x) I_{p\times p}))$

z is of dimension p

z

Value of z sampled by Monte-Carlo

z is of dimension p

We choose $p \ll n$!

https://www.kaggle.com/rvislaywade/visualizing-mnist-using-a-variational-autoencoder#

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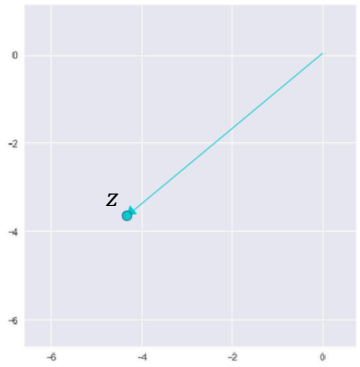
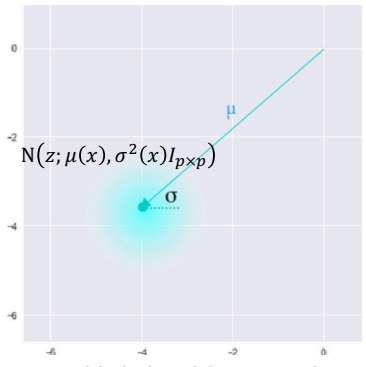
Encoding: From Deterministic to Probabilistic Latent Vector

Case where Latent Space Dimension = 2



Basic Autoencoder

(Deterministic encoding coordinates z In latent space)



Variational Autoencoder

$\mu(x)$ and $\sigma(x)$ now define a pdf:

z is stochastic

https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

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How Variational Autoencoders Work (2)

The Decoding Step

Latent Vector z

z

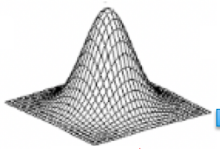
z is of dimension p

Neural Network

$\mu(z)$

$\sigma^2(z)$

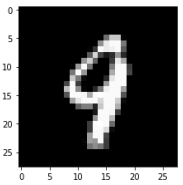
$\mu(z)$ and $\sigma^2(z)$ of dimension n



pdf of Generated Image x

$\mathrm{N}(x; \mu(z), \sigma^2(z) I_{n \times n}))$

x is of dimension n



Value of x sampled by Monte-Carlo

https://www.kaggle.com/rvislaywade/visualizing-mnist-using-a-variational-autoencoder#

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Some Important Definitions

The encoder network is also called the ***recognition*** or ***inferenc***e network.

The decoder network is also called the ***generative*** network.

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How Variational Autoencoders Work (3)

Call $q_\phi(z/x)$ the multivariate normal diagonal pdf $\mathrm{N}(z; \mu(x), \sigma^2(x) I_{p\times p})$ of dimension p

$q_\phi(z/x)$ is the pdf of the latent vectors z associated with a given image x

$\mu(x)$ and $\sigma(x)$, which have the dimension p of z, are calculated from x using a neural network. The parameters of this neural network are the $\phi's$ of $q_\phi(z/x)$.

Call $p_\theta(x/z)$ the multivariate normal diagonal pdf $\mathrm{N}(x; \mu(z), \sigma^2(z) I_{n\times n})$ of dimension n

$p_\theta(z/x)$ is the pdf of the images x associated with a given latent vector z

$\mu(z)$ and $\sigma(z)$, which have the dimension n of x, are calculated from z using a neural network. The parameters of this neural network are the $\theta's$ of $p_\theta(x/z)$.

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The Variational Autoencoder Model (in case of images)

Training Set Images $\left(\boldsymbol{x^{(i)}}\right)_{i=1,\ldots,m}$

Going back-and-forth between images $\boldsymbol{x^{(i)}}$ *and Latent vectors* $\boldsymbol{z^{(i)}}$:

How to calculate the parameters of the Neural Networks calculating $\mu(x)$ *and* $\sigma(x)$ *from* x *and* $\mu(z)$ *and* $\sigma(z)$ *from z?*

By maximizing the likelihood of the Training Set images $\left(\boldsymbol{x^{(i)}}\right)_{i=1,\ldots,m}$***!***

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How Variational Autoencoders Work (4) (Kingma & Welling, 2014)

For one single data point $x^{(i)}$ the exact log-likelihood $\log p(x^{(i)})$ cannot be calculated, only a lower bound can

$$\log p(x^{(i)}) \geq E_{z\sim q_\phi(z/x^{(i)})}(\log p_\theta(x^{(i)}/z)) - \mathrm{KL}(q_\phi(z/x^{(i)})||q(z))$$

The right-hand side is called the Evidence Lower Bound (ELBO).
The ELBO is negative, as the sum of two negative terms.

The first term of the ELBO is a **reconstruction likelihood**, quantifying the quality of the match to the data point $x^{(i)}$, or of the « round trip » between the training image $x^{(i)}$ and its associated latent vector pdf $q_\phi(z/x^{(i)})$. The second one is a **KL Divergence** that aims to « spread » the range of latent vectors associated to the image $x^{(i)}$ by making their pdf close to a multivariate standardized Gaussian $q(z)$.

For a mini-batch of m images $(x^{(i)})_{i=1,\ldots,m}$, the ELBO is summed over the data.

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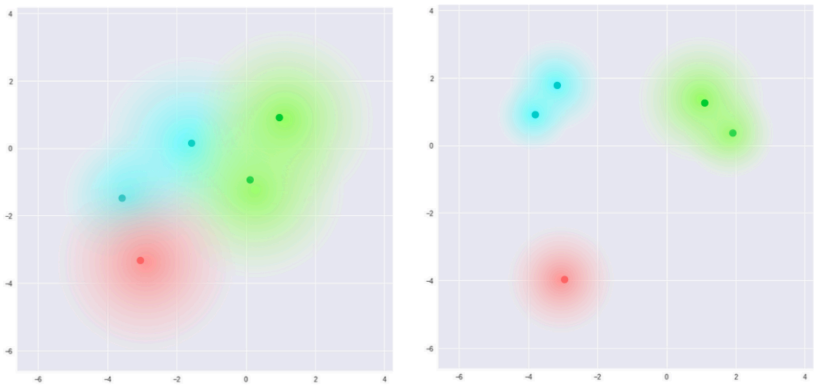
If Only First Term of Objective Function is Used…



We want a continuous latent space……..……But the Likelihood Term tends to create clusters

https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

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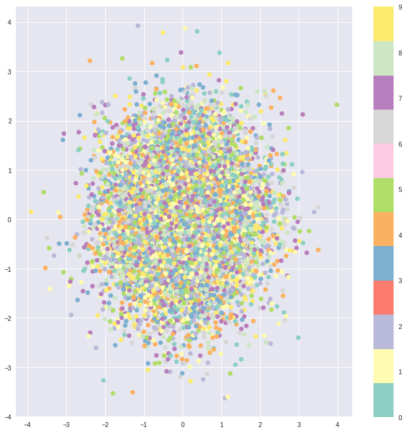
If Only Second Term of Objective Function is Used



Now the space is nicely continuous but there is no more difference between coded digits!

https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

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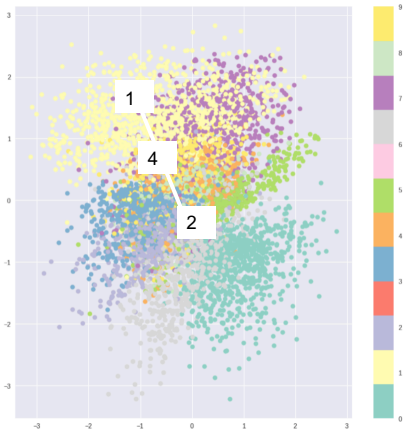
If Both Terms of Objective Function are Used



Digits are nicely separated but in a continuous space!

https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

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This slide can be skipped

How Variational Autoencoders Work (5) (Kingma & Welling, 2014)

Calculating $-\mathbf{KL}(\boldsymbol{q_\phi}(\boldsymbol{z}/\boldsymbol{x}^{(i)})\|\boldsymbol{q}(\boldsymbol{z}))$

This is the KL divergence between two Gaussian distributions, each of dimension p:

$q_\phi(z/x^{(i)})$ is $\mathrm{N}(z;\mu(x^{(i)}),\sigma^2(x^{(i)})I_{p\times p})$ or $\mathrm{N}\left(z;\mu^{(i)},{\sigma^{(i)}}^2\right)$

$q(z)$ is $\mathrm{N}(z;0_p,I_{p\times p})$

Using the formula giving the KL divergence of two multivariate Gaussians (see next slide) we get

$$-KL(q_\phi(z/x^{(i)})\|q(z))=\frac{1}{2}\sum_{j=1}^{p}\left[1+\log\left(\left(\sigma_j^{(i)}\right)^2\right)-\left(\mu_j^{(i)}\right)^2-\left(\sigma_j^{(i)}\right)^2\right]$$

Where p is the dimension of the latent vector

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This slide can be skipped

Recall: KL divergence of 2 Multivariate Gaussians

Suppose the two distributions are: $N(\mu_1,\Sigma_1)$ and $N(\mu_2,\Sigma_2)$, each of dimension p.

The KL divergence between the two distributions is:

$$KL=\frac{1}{2}\left[\log\frac{det\Sigma_2}{det\Sigma_1}-p+tr\left(\boldsymbol{\Sigma_2}^{-1}\boldsymbol{\Sigma_1}\right)+(\mu_2-\mu_1)^T\boldsymbol{\Sigma_2}^{-1}(\mu_2-\mu_1)\right]$$

In our case the first distribution is that of the conditional Gaussian of mean $\mu=\begin{pmatrix}\mu_1\\ \vdots\\ \mu_p\end{pmatrix}$ and diagonal variance-covariance $\Sigma=\begin{pmatrix}\sigma_1^2 & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \sigma_p^2\end{pmatrix}$ and the second one is the standardized multivariate normal: $\mu_2=0$ and $\Sigma_2=I_{p\times p}$. Thus, in our case:

$$KL=\frac{1}{2}\left[\log\frac{1}{\prod_{i=1}^{p}\sigma_i^2}-p+\sum_{i=1}^{p}\sigma_i^2+\sum_{i=1}^{p}\mu_i^2\right]=\frac{1}{2}\left[-\sum_{i=1}^{p}\left(1+\log(\sigma_i^2)\right)+\sum_{i=1}^{p}\left(\sigma_i^2+\mu_i^2\right)\right]$$

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This slide can be skipped

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How Variational Autoencoders Work (6) (Kingma & Welling, 2014)

Calculating $E_{z\sim q_\phi(z/x^{(i)})}(log\, p_\theta(x^{(i)}/z))$ for one data point $x^{(i)}$

This expression looks complex but simply quantifies the likelihood associated with the « round trip » between the image x_i and the pdf of associated latent vectors z. This is an expectation (because z does not take just one value as with autoencoders, but many possible values), which can be calculated by Monte Carlo sampling and averaging over a large set of L simulated values of z.

$$E_{z\sim q_\phi(z/x^{(i)})}\left(\log p_\theta(x^{(i)}/z)\right) = \frac{1}{L}\sum_{l=1}^{L}\log p_\theta(x^{(i)}/z^{(i,l)})$$

Since $z^{(i,l)}$ must be a sample from the multivariate diagonal normal pdf $q_\phi(z/x^{(i)})$ of mean $\mu^{(i)} = \mu(x_i)$ and variance $\sigma_i^2 = \sigma^2(x_i)$, we write:

$$z^{(i,l)} = \mu^{(i)} + \sigma^{(i)} \odot \varepsilon^{(l)} \text{ where } \varepsilon^{(l)} \text{ is } \mathrm{N}(\varepsilon; 0, I_{p\times p})$$

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Likelihood for Decoder $p_\theta(x/z)$ Multivariate Diagonal Gaussian

$$f(x) = (2\pi)^{-\frac{n}{2}}[\Sigma]^{-\frac{1}{2}}\exp\left[-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right]$$

If $\Sigma = \sigma^2 I_n$, this simplifies into: $f(x) = (2\pi)^{-\frac{n}{2}}\frac{1}{\prod_{j=1}^{j=n}\sigma_j}\exp\left[-\frac{1}{2}\sum_{i=1}^{n}\left(\frac{x_j-\mu_j}{\sigma_j}\right)^2\right]$

$$\log p_\theta(x^{(i)}/z^{i,l}) = -\frac{n}{2}\log(2\pi) - \sum_{j=1}^{n}\log\left(\sigma_j(z^{i,l})\right) - \frac{1}{2}\sum_{j=1}^{n}\left(\frac{x_j^{(i)}-\mu_j(z^{i,l})}{\sigma_j(z^{i,l})}\right)^2$$

https://stats.stackexchange.com/questions/351549/maximum-likelihood-estimators-multivariate-gaussian

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Likelihood for Decoder $p_\theta(x/z)$ Multivariate Bernouilli

$$\log p_\theta\left(x^{(i)}/z^{i,l}\right) = -\frac{1}{n}\sum_{j=1}^{n}\left[x_j^{(i)}\log\left(p_{j,l}^{i}\right) + \left(1 - x_j^{(i)}\right)\log\left(1 - p_{j,l}^{i}\right)\right]$$

Where $p_{j,l}^{i}$ is the j^{th} coordinate of the n – dimensional probability vector p_l^i associated (via neural network with final sigmoid activation) with $z^{i,l}$.

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Summarizing how we calculate a VAE

We have defined the ELBO as the right-hand side of :

$$log\, p\left(x^{(i)}\right) \geq \boldsymbol{E}_{z\sim q_\phi\left(z/x^{(i)}\right)}\left(\boldsymbol{log}\, \boldsymbol{p_\theta}\left(\boldsymbol{x^{(i)}}/\boldsymbol{z}\right)\right) - \mathbf{KL}\left(\boldsymbol{q_\phi}\left(\boldsymbol{z}/\boldsymbol{x^{(i)}}\right)\|\boldsymbol{q}(\boldsymbol{z})\right)$$

$\boldsymbol{E}_{\boldsymbol{z\sim q_\phi}\left(\boldsymbol{z}/\boldsymbol{x^{(i)}}\right)}\left(\boldsymbol{log}\, \boldsymbol{p_\theta}\left(\boldsymbol{x^{(i)}}/\boldsymbol{z}\right)\right)$ *is a function of the vectors* $\mu(x_i), \sigma^2(x_i)$ *and* $\mu(z), \sigma^2(z)$ *for known samples of* z,

$-\boldsymbol{KL}\left(\boldsymbol{q_\phi}\left(\boldsymbol{z}/\boldsymbol{x^{(i)}}\right)\|\boldsymbol{q}(\boldsymbol{z})\right)$ *is a function of the vectors* $\mu(x_i), \sigma^2(x_i)$

The ELBO, sum of these two terms, is thus a function of the parameter vectors θ *and* ϕ *of the neural networks respectively calculating* $\mu(x), \sigma^2(x)$ as a function of x and $\mu(z), \sigma^2(z)$ as a function of z. θ *and* ϕ *are obtained by maximizing the ELBO .*

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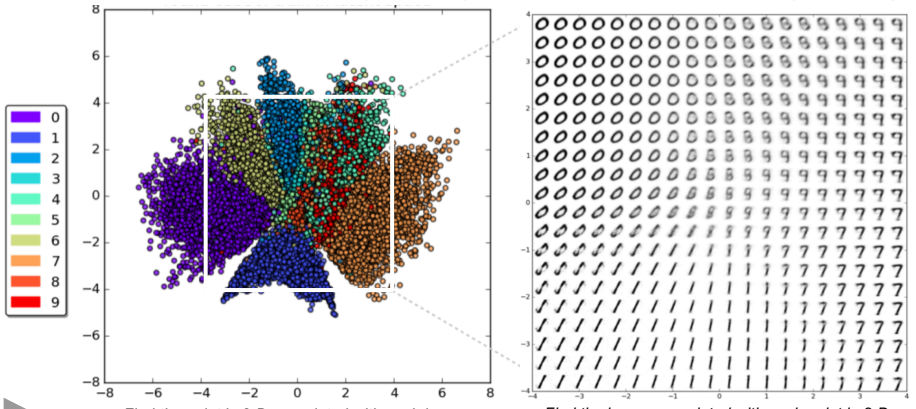
MNIST: Each Point of $N(z; 0_2, I_{2\times 2})$ now associated to an Image!

An Inference Network (Encoder) *A Generation Network (Decoder)*



Find the point in 2-D associated with each image *Find the image associated with each point in 2-D*

Can the two axes be interpreted?

https://blog.fastforwardlabs.com/2016/08/12/introducing-variational-autoencoders-in-prose-and.html

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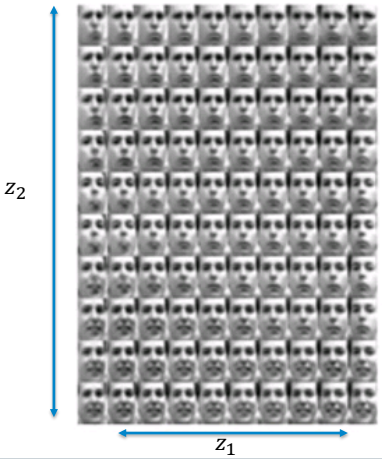
Case of 2-D Latent Vector: Interpreting the 2 Coordinates



z_1: Head Pose

z_2: Degree of Smile

Kingma and Welling, 2014

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VAEs: Decoder for Generating Samples

Sample image x from $N(x; \mu(x/z), \Sigma^2(x/z))$

Calculate $\mu(x/z)$ and $\Sigma^2(x/z)$ thanks to neural network

Sample latent vector z from $N(z; 0_p, I_{p\times p})$

Generative Network

https://www.youtube.com/watch?v=5WoItGTWV54

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Why Generative Models?

Generate Synthetic Images, Music, Text….

Training Data

Samples from $p_{data}(x)$

Samples from Model

Samples from $p_{model}(x)$

Goal: learn $p_{model}(x)$ from $p_{data}(x)$ in order to generate more samples "looking like" the data

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Introduction to Generative Models

1. PCA and Autoencoders
2. Transposed Convolution
3. Variational Autoencoders
4. Generative Adversarial Networks

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Do you know any of these people?

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Do you know any of these people?

https://thispersondoesnotexist.com/

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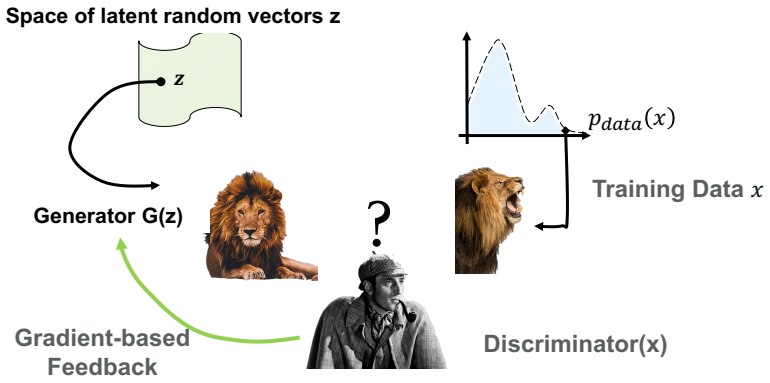
Generative Adversarial Networks – Toy Example



(Goodfellow et. al. 2014)

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Compare two pdfs: Generative Adversarial Networks

If $x = G(z)$ is a sample from $p_{model}(x)$, a Discriminator function $D(x)$ is applied to x and calculates a number between 0 and 1. The closest $D(x)$ is to 1, the higher the probability that the Discriminator will accept x as a sample of $p_{data}(x)$.

Both $D(x)$ and $G(z)$ are neural networks.

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Generative Adversarial Networks

- **Two Neural Networks are required:**
  - **Generator (or Decoder) – creates sample images x**

    $x = G_\theta(z)$ **with pdf of vector z:** $\mathrm{N}(z; 0_p, I_{p\times p})$
  - **Discriminator – evaluates images, to help decide whether "fake" or "real"**

    $D_\omega(x) \in [0,1]$

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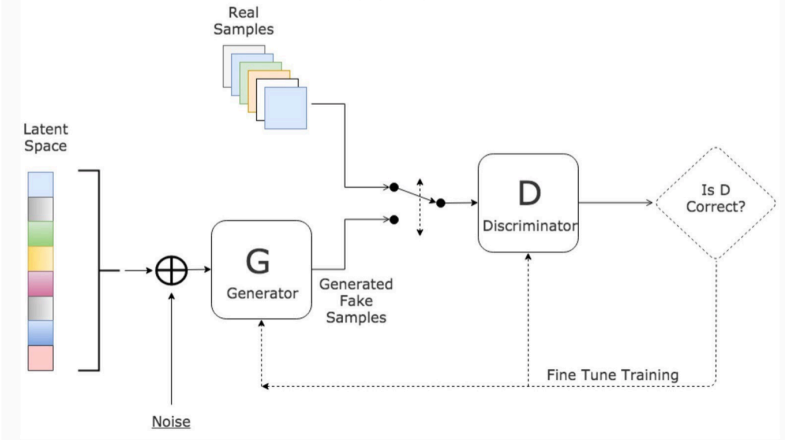
The GAN Training Workflow



https://www.kdnuggets.com/2017/01/generative-adversarial-networks-hot-topic-machine-learning.html

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Generative Adversarial Networks – Objective

- For Generator minimize (with D_ω fixed):

$$E_{x\sim p_z}\left[\log\left(1 - D_\omega\left(G_\theta(z)\right)\right)\right]$$

- For Discriminator maximize (with G_θ fixed):

$$E_{x\sim p_{data}}[\log D_\omega(x)] + E_{x\sim p_z}\left[\log\left(1 - D_\omega\left(G_\theta(z)\right)\right)\right]$$

Binary Cross-Entropy!

Other Objective functions or formulations possible e.g. Wasserstein GANs

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GAN Training Example - MNIST

Training Images

Training Iterations

https://www.youtube.com/watch?v=R7HTX79JlBg&feature=youtu.be

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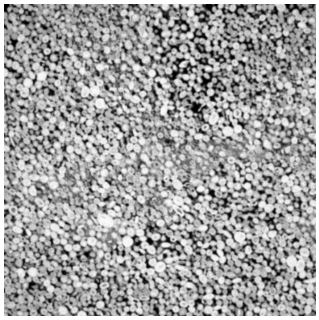
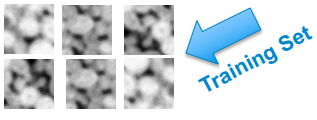
Ketton Limestone Dataset and Preprocessing

- Oolitic Limestone
- Intergranular pores
- Intragranular Micro-Porosity
- Ellipsoidal grains
- 99% Calcite
- Image Size:
  - 900^3 voxels @ 26.7 μm

Extract Non-Overlapping Training Images (64^3 $voxels$)





Mosser et al, 2017

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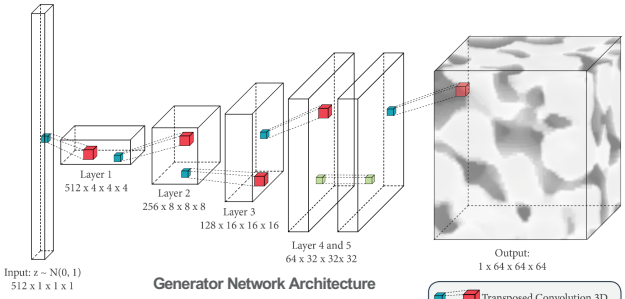
Network Architecture - 3D Convolutional Network

Represent $G(z)$ and $D(x)$ as deep neural networks:



Generator Network Architecture

Discriminator: Binary Classification Network -> Real / Fake

Mosser et al, 2017

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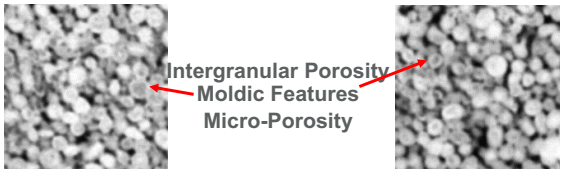
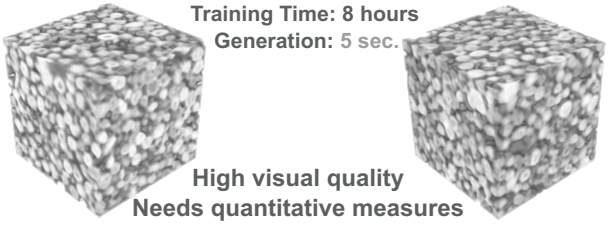
Reconstruction Quality

Ketton Training Image

GAN Generated Sample



Intergranular Porosity
Moldic Features
Micro-Porosity



Training Time: 8 hours
Generation: 5 sec.

High visual quality
Needs quantitative measures

Mosser et al, 2017

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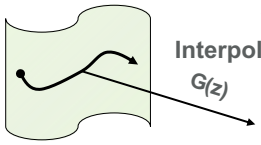
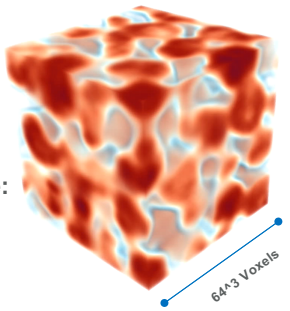
Latent Space Interpolation

Latent space **z**

$$z^* = \beta\, z_{start} + (1-\beta)\, z_{end}, \beta \in [0,1]$$



Interpolation path visualization



Interpolation in latent space:

Shows that generator has learned a meaningful representation in a lower dimensional space!

Mosser et al, 2017

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Latent Space Interpolation for fake celebrities

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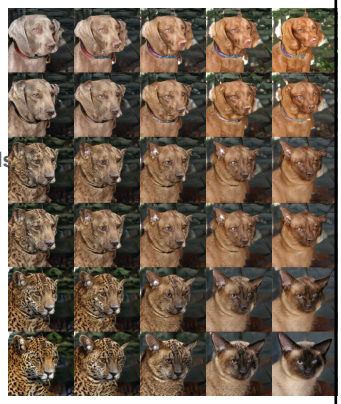
Conditioning of Generative Models

(Cat, Dog, Leopard, Dachshund)



Generative model can incorporate additional information:
$G(z, class)$ -> $G(z, class = \{Cat, Dog, Bird\})$

Train generative model on images with associated class labels

Generative model input: Latent Vector + Class

Possible to perform smooth inter-class interpolation

This model -> Trained on Imagenet (1000 classes)

(Miyato and Koyama 2018)

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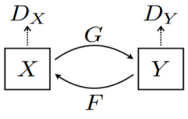
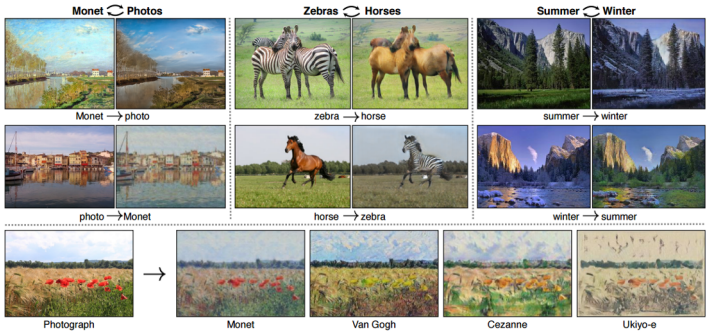
Domain Transfer with CycleGANs (Zhu et al, 2017)





Find functions G(X) and F(Y) to map between two unpaired domains

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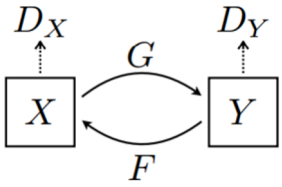
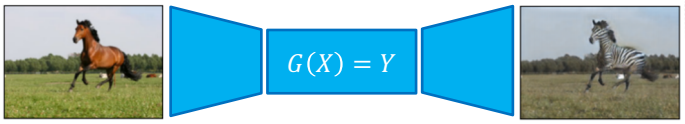
CycleGAN – Detailed Analysis (1)

CycleGAN consists of 4 Convolutional Neural Networks:
- 2 Transformer Networks: $G(X) = Y \; and \; F(Y) = X$
- 2 Discriminators: $D(X) \; and \; D(Y)$



Transformer Networks:

- Perform A -> B mapping, where A and B are images
  e.g.: (Horse -> Zebra), (Winter -> Summer), (Blurred -> Detailed)



X ~ Horse → Y ~ Zebra

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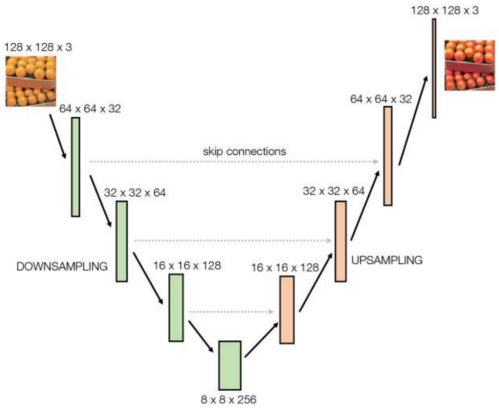
CycleGAN – Detailed Analysis (2)



Example of U-Net Generator for CycleGan (Foster, 2019)

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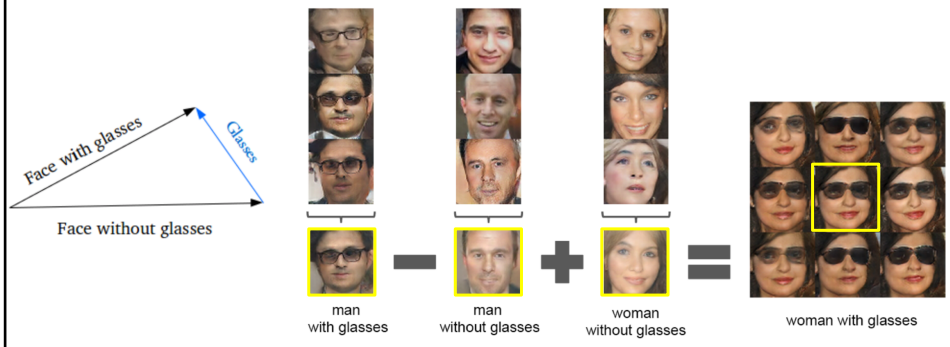
Arithmetic Operations on Latent Vectors



(Radford et al, 2016)

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Comparison VAE's and GANs

VAE

- Generative + Inference Model
- Encoder + Decoder
- For data point x, provides:
  - Reconstruction x^*
  - Latent Vector z
- Trained by maximizing ELBO

GAN

- Generative Model Only
- Generator - Discriminator
- Can only sample new data
- For data point x, does not directly provide z or x^*
- Adversarial Training

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Conclusion

- Autoencoders a Generalization of PCAs to non-Linear Manifolds
- Variational Autoencoders give a Probabilistic Spin to Autoencoders
- Variational Autoencoders produce both an Inference and a Generative Network
- Generative Adversarial Networks are a simpler Generative method, but which does not produce Inference.