Introduction to Deep Learning

Autoencoders

Andres Mendez-Vazquez

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Outline

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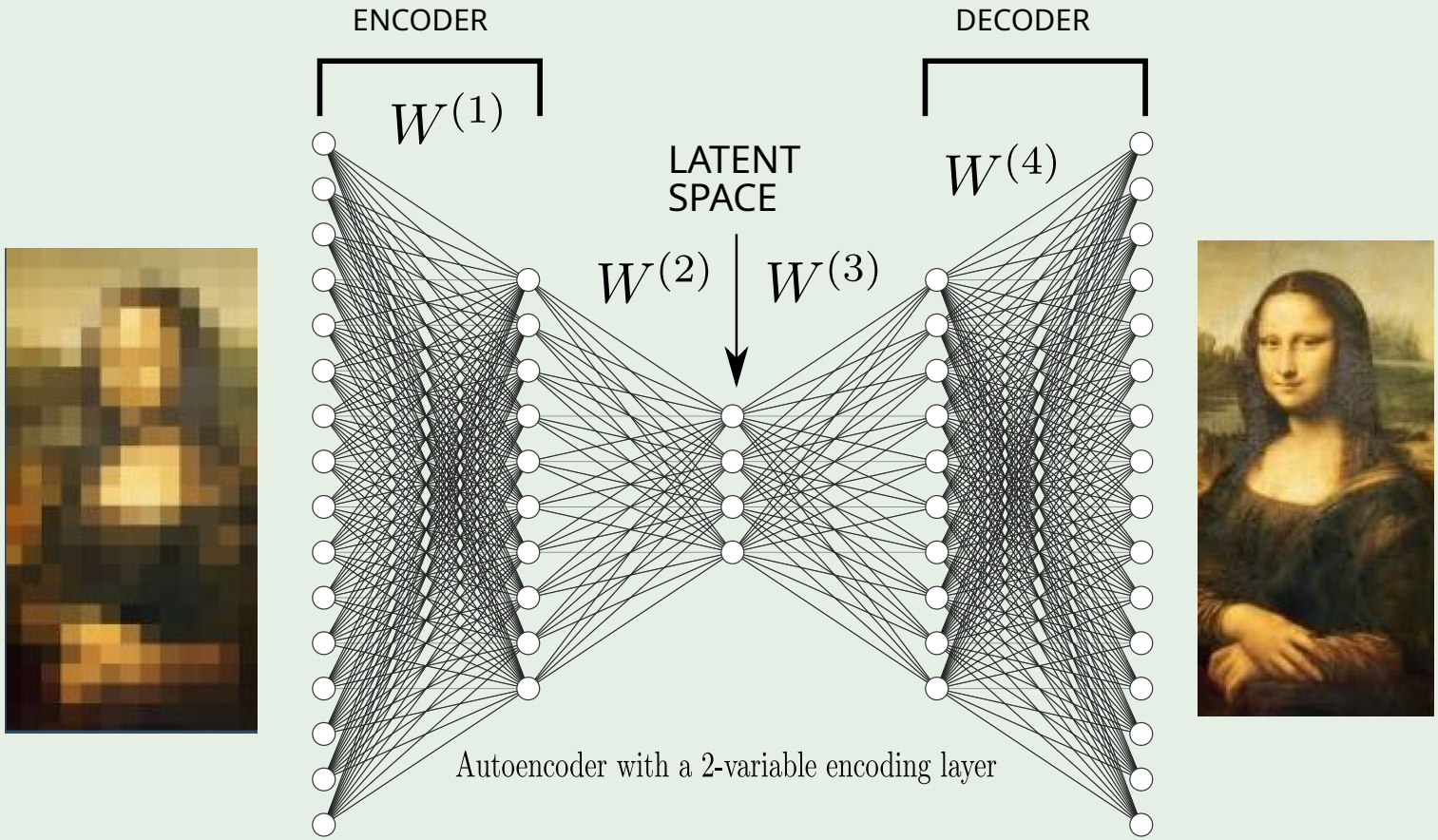
Introduction

From [1]

- "An autoencoder is a specific type of a neural network, which is mainly designed to encode the input into a compressed and meaningful representation, and then decode it back such that the reconstructed input is similar as possible to the original one."



At the following work [2]

Definition

- An $n/p/n$ autonecoder is defined as a t-tuple $n, p, m, \mathbb{F}, \mathbb{G}, \mathcal{A}, \mathcal{B}, \mathcal{X}, \Delta$ where
  1. $\mathbb{F}$ and $\mathbb{G}$ are sets.
  2. n and p are positive integers with $0 < p < n$.
  3. $\mathcal{A}$ is a class of functions from $\mathbb{G}^p$ to $\mathbb{F}^n$.
  4. $\mathcal{B}$ is a class of functions from $\mathbb{F}^n$ to $\mathbb{G}^p$.
  5. $\mathcal{X} = \{x_1, ..., x_m\}$ is a set of m (training) vectors in $\mathbb{F}^n$.
  6. Δ is a dissimilarity or distortion function over $\mathbb{F}^n$.

Basically

We have that

- For any $A \in \mathcal{A}$ and $B \in \mathcal{B}$, the autoencoder transforms an input vector $x \in F^n$ into an output vector$A \circ B(x) \in F^n$

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Thus, we have

- The corresponding autoencoder problem is to find $A \in \mathcal{A}$ and $B \in \mathcal{B}$, that minimize the overall distortion function:

$$\min E(A, B) = \min_{A,B} \sum_{t=1}^{m} E(x_t) = \min_{A,B} \sum_{t=1}^{m} \Delta(B \circ A(x_t), x_t)$$

And there is the other case

We can have another output y_t

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Not only that

- $p < n$ corresponds to the regime where the autoencoder tries to implement some form of compression or feature extraction.

Baldani and Hornik [3]

In 1989, they proposed an initial linear case no activation functions

$$E(A, B) = \sum_{1 \leq t \leq T} \|y_t - BAx_t\|$$

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There are several properties under these autoencoders

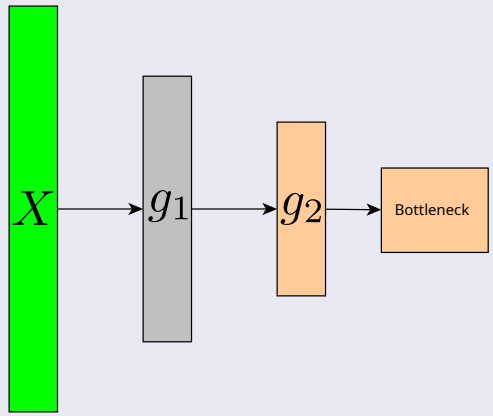
- But somethin interesting an optimal:
  - $E(A,B)$ is convex in the coefficient of B and attains minimum for B such that $BAA^T\Sigma_{XX} = A^T\Sigma_{XY}$

Outline

Basically, we have

Encoder

- The encoder is the part of the network which takes in the input and produces a lower Dimensional encoding



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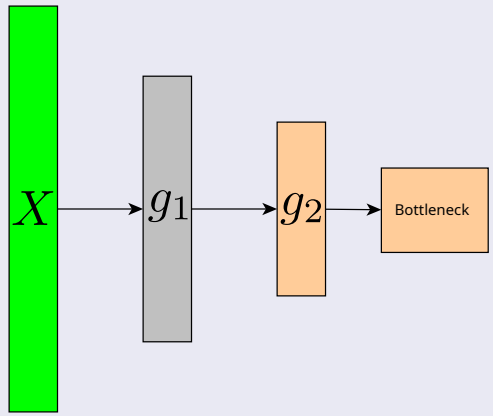


Something Notable

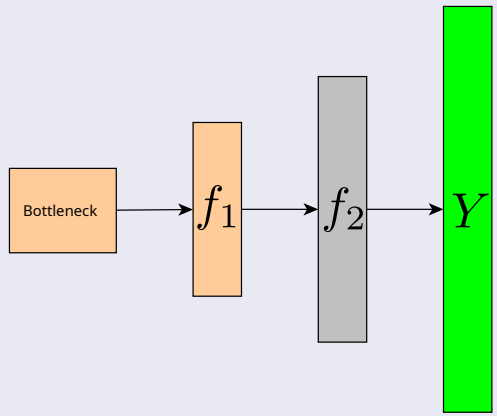
Bottleneck: It is the lower dimensional hidden layer where the encoding is produced.

- Note: Call it an embedding!!!

Then, we have that

Decoder

- The decoder takes in the encoding and recreates back the input.



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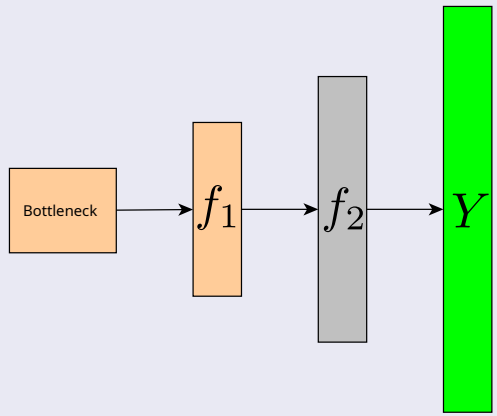
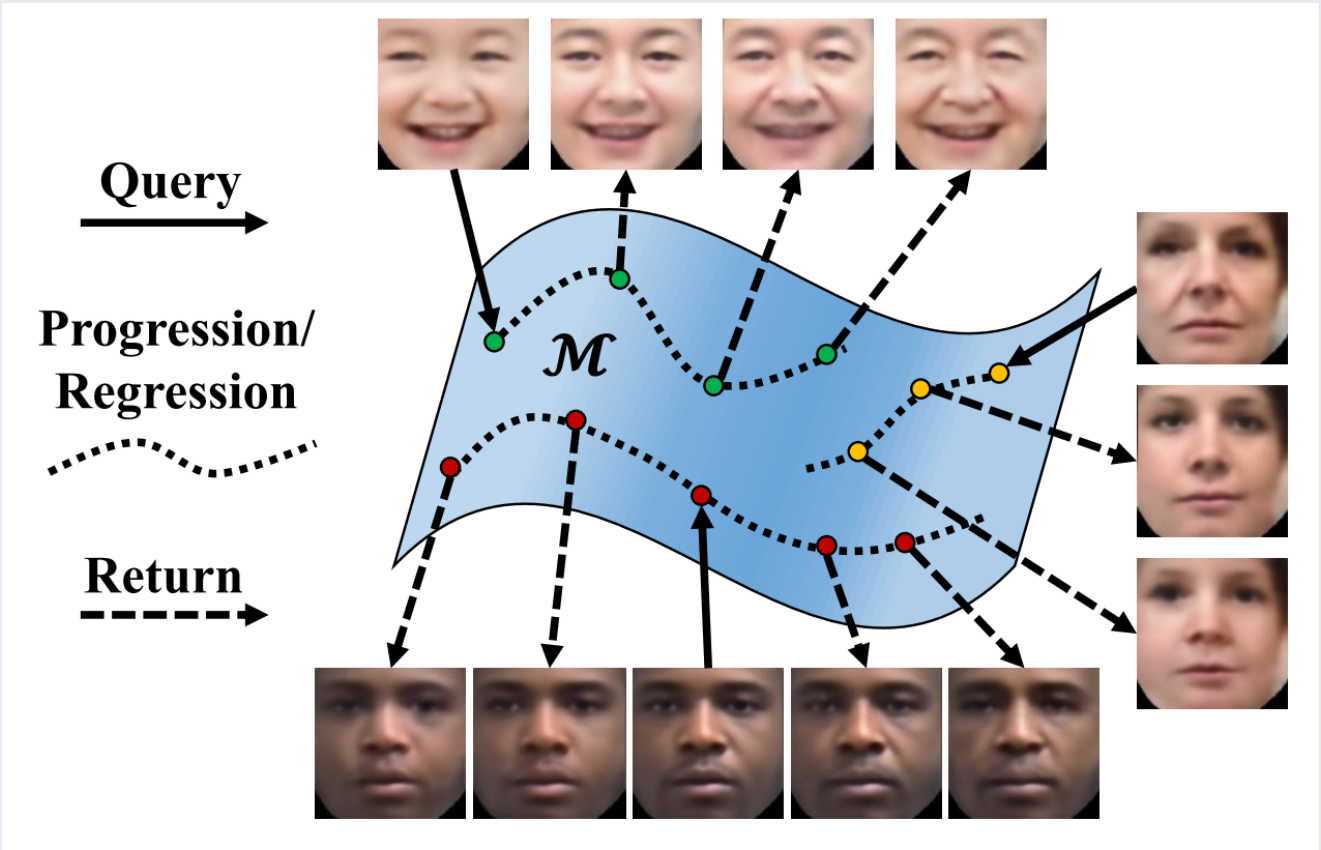


Remember the Transpose Convolution

- Yes, we can use it to implement the decoder.

Basically is Called a Manifold

Mapping x to a small dimension h from old to young



- Thanks to the Pytorch implementation by Mattan Serry, Hila Balahsan, and Dor Alt.

Autoencoders differ from General Data Compression

Autoencoders are data-specific

- i.e., only able to compress data similar to what they have been trained on

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- Which make general assumptions about "sound/images", but not about specific types of sounds/images
- Autoencoder for pictures of cats would do poorly in compressing pictures of trees
  - Because features it would learn would be cat-specific

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Autoencoders are lossy

- which means that the decompressed outputs will be degraded compared to the original inputs (similar to MP3 or JPEG compression).
- This differs from lossless arithmetic compression

And Actually, Autoncoders are Learn

Learning $g(f(\boldsymbol{x})) = \boldsymbol{x}$ everywhere is not useful

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Autoencoders are designed to be unable to copy perfectly

- Autoencoders learn useful properties of the data

Autoencoders learn useful properties of the data

- Being forced to prioritize which aspects of input should be copied

An important property

It can learn stochastic mappings

- Go beyond deterministic functions to mappings $p_{encoder}(h|x)$ and $p_{decoder}(x|h)$

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Now

- A little bit on the loss function...

Outline

Autoencoder is a feed-forward non-recurrent neural net

With an input layer, an output layer and one or more hidden layers

- Can be trained using the same techniques
- Compute gradients using back-propagation
  - Followed by minibatch gradient descent

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Unlike feedforward networks, can also be trained using Recirculation

- Compare activations on the input to activations of the reconstructed input
- More biologically plausible than back-prop but rarely used in ML

Autoencoder training using a loss function

We have Encoder f and Decoder g

- $f : X \to h$
- $g : h \to X$
- Thus, we have

$$\arg\min_{f,g} \|\boldsymbol{x} - (f \circ g)\,\boldsymbol{x}\|^2$$

Example

One hidden layer

- Takes input $\boldsymbol{x} \in \mathbb{R}^d$
- Maps into an output $\boldsymbol{h} \in \mathbb{R}^p$

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- $\boldsymbol{h} = \sigma_1 \left(W\boldsymbol{x} + \boldsymbol{b} \right) \rightarrow \boldsymbol{x}' = \sigma_2 \left(W'\boldsymbol{h} + \boldsymbol{b}' \right)$

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Trained to minimize reconstruction error

$$L\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \left\| \boldsymbol{x} - \boldsymbol{x}' \right\| = \left\| \boldsymbol{x} - \sigma_2 \left(W^t \sigma_1 \left(W\boldsymbol{x} + \boldsymbol{b} \right) + \boldsymbol{b}' \right) \right\|$$

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Undercomplete Autoencoder

Copying input to output sounds useless

- Imagine that we do not have interest in decoder output
- We hope $\boldsymbol{h}$ takes on useful properties

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Undercomplete autoencoder

- Constrain $\boldsymbol{h}$ to have lower dimension than $\boldsymbol{x}$
- Force it to capture most salient features of training data

Autoencoder with linear decoder + MSE is PCA

We have that

$$L\left(\boldsymbol{x}, g\left(f\left(\boldsymbol{x}\right)\right)\right) = \left\|x - g\left(f\left(\boldsymbol{x}\right)\right)\right\|^2$$

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Something Notable

- Where L is a loss function penalizing $g(f(\boldsymbol{x}))$ for being dissimilar from $\boldsymbol{x}$

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Thus

- When the decoder $\boldsymbol{g}$ is linear and L is the mean squared error, an undercomplete autoencoder learns to span the same subspace as PCA

$$g\left(\boldsymbol{x}\right) = W\boldsymbol{h} + \boldsymbol{b}$$

We have

In this case

- The autoencoder trained to perform the copying task has learned the principal subspace of the training data as a side-effect

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Autoencoders with nonlinear f and g

- They can learn more powerful nonlinear generalizations of PCA
- Something called Capacity

The capacity of a network

The capacity of a network refers to

- The range or scope of the types of functions that the model can approximate.
- Informally, a model's capacity is its ability to fit a wide variety of functions.

Encoder/Decoder Capacity

If encoder f and decoder g are allowed too much capacity

- Autoencoder can learn to perform the copying task without learning any useful information about distribution of data

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- Autoencoder with a one-dimensional code and a very powerful nonlinear encoder can learn to map $x(i)$ to code i.
- The decoder can learn to map these integer indices back to the values of specific training examples

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A notable problem

- Autoencoder trained for copying task fails to learn anything useful if f/g capacity is too great

Cases when Autoencoder Learning Fails

Where autoencoders fail to learn anything useful

- Capacity of encoder/decoder f/g is too high
  - Capacity controlled by depth
- Hidden code $\boldsymbol{h}$ has dimension equal to input $\boldsymbol{x}$
- Overcomplete case: where hidden code $\boldsymbol{h}$ has dimension greater than input $\boldsymbol{x}$
  - Even a linear encoder/decoder can learn to copy input to output without learning anything useful about data distribution

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What is regularization

L1 Regularization

- This method adds a penalty to the loss function for the sum of the absolute values of the model weights.

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Dropout

- This method randomly sets a fraction of the model's activations to zero during each training iteration.

Use regularization

Ideally

- choose code size (dimension of $\boldsymbol{h}$) small and capacity of encoder f and decoder g based on complexity of distribution modeled

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Regularized autoencoders provide the ability to do so

- Rather than limiting model capacity by keeping encoder/decoder shallow and code size small
- They use a loss function that encourages the model to have properties other than copy its input to output=

Regularized Autoencoder Properties

Regularized AEs have properties beyond copying input to output

- Sparsity of representation
- Smallness of the derivative of the representation
- Robustness to noise
- Robustness to missing inputs

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Regularized autoencoder can be nonlinear and overcomplete

- But still learn something useful about the data distribution even if model capacity is great enough to learn trivial identity function

Outline

Initializing Deep Learners

Autoencoders have many interesting applications

- As data compression, visualization, etc

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Something Notable

- Y. Bengio, P. Lamblin, D. Popovici, and H. Larochelle. Greedy layer-wise training of deep networks. In Advances in Neural Information Processing Systems, 2007.

They discovered something interesting

Something Notable

- They observed that autoencoders could be used as a way to "pre-train" neural networks.

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- They observed that autoencoders could be used as a way to "pre-train" neural networks.

With pretraining, the process of training a deep network is divided in a sequence of steps

1. Pretraining step: train a sequence of shallow autoencoders, greedily one layer at a time, using unsupervised data,
2. Fine-tuning step 1: train the last layer using supervised data,
3. Fine-tuning step 2: use backpropagation to fine-tune the entire network using supervised data.

Basically

The step 2 can be seen as the training of a Perceptron

- This can be done easily

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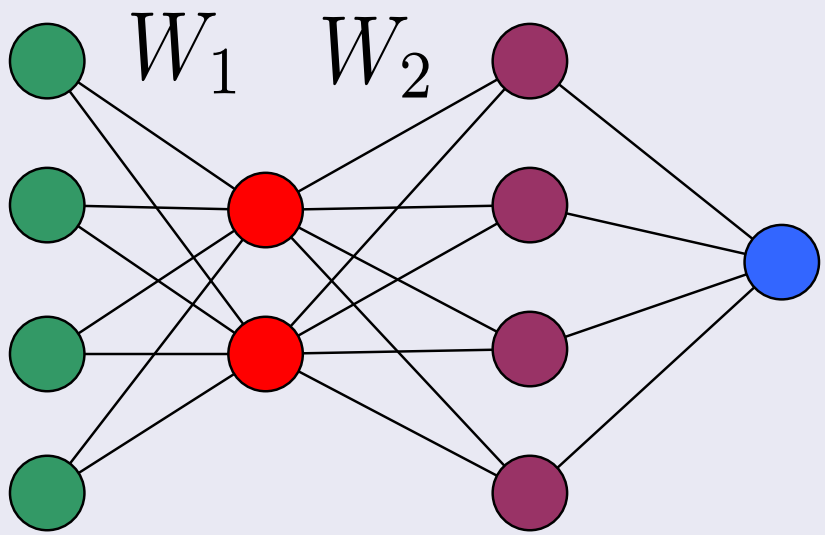
- This can be done easily

The Backpropagation of the entire network

- Also the classic procedure

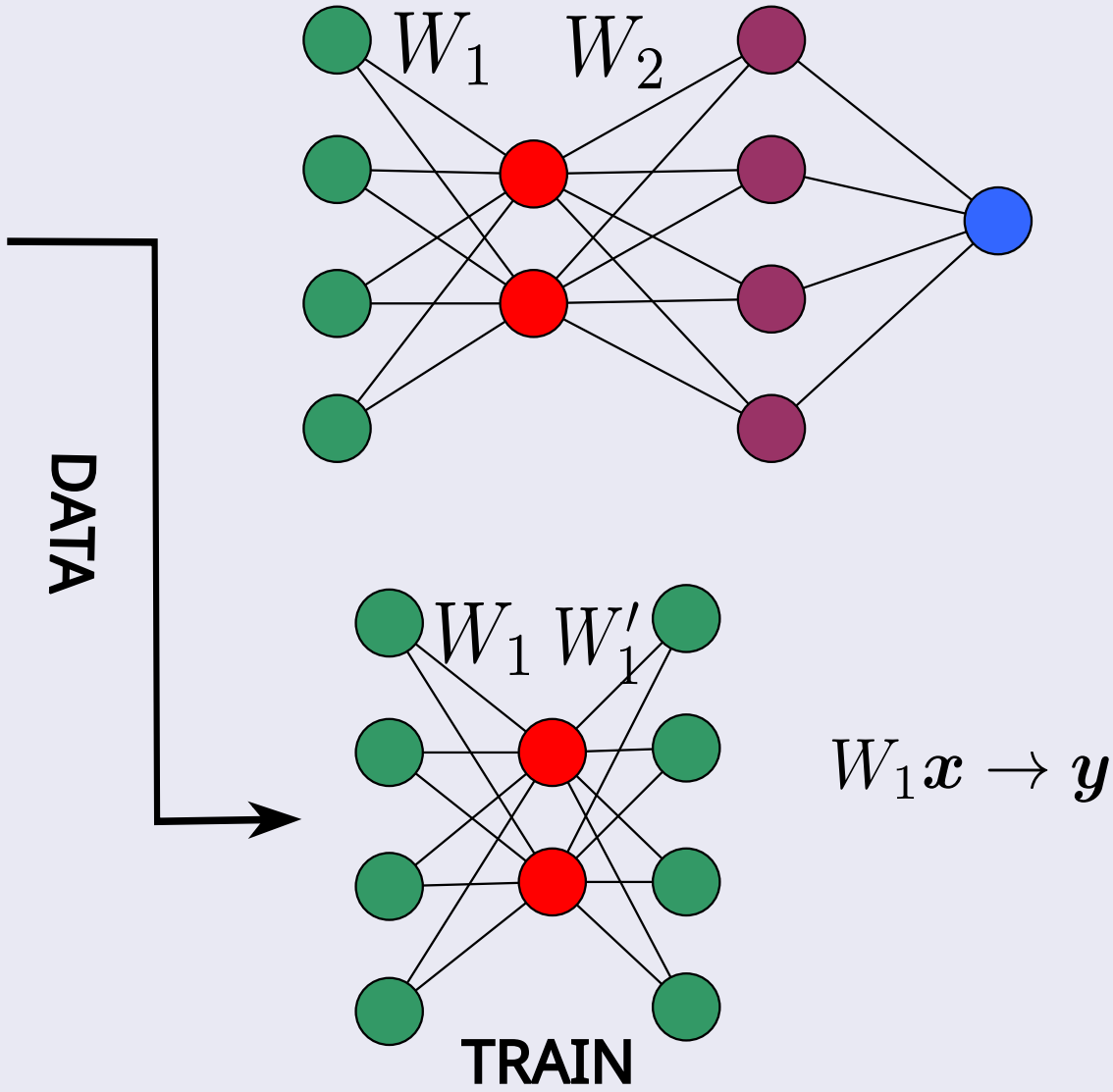
The First Step is the interesting one

We have a Feed Forward Architecture



First Pre-training, the first layer

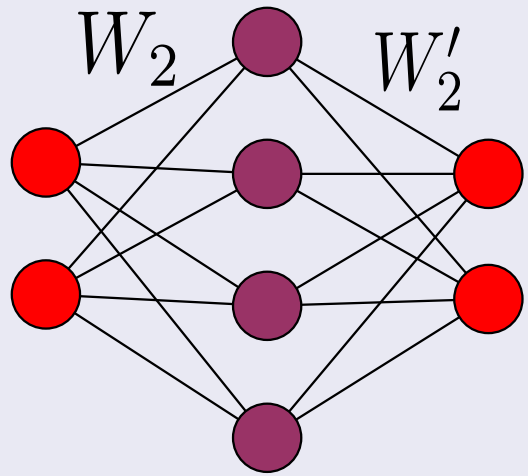
We have



Therefore, we have the final sub-step

We use the y to train another auto-encoder

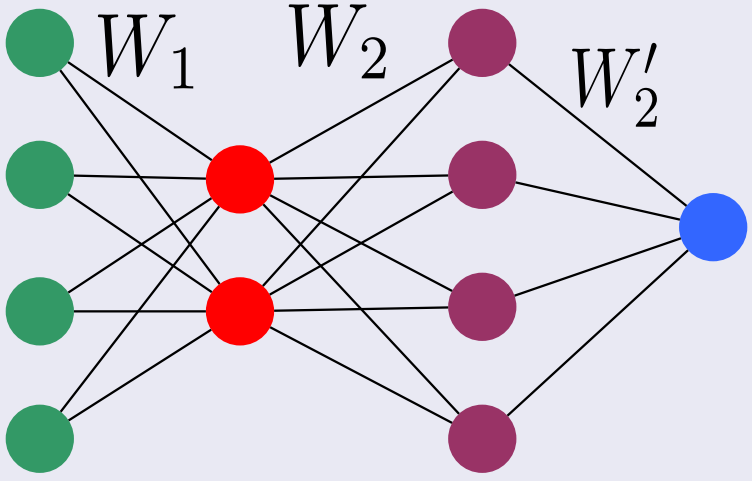
$$W_1 x \rightarrow y$$



TRAIN

Finally

We have that



Train with Labeled Samples

However

As Quality Data Sets become more widely avaible

- Google, Facebook, Microsoft and many others took charge of that...

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This efforts were abandoned

- Instead Transfer Learning [4] become a more popular idea
  - For initialization....

Outline

Sparse Autoencoders

Similar to the LASSO

$$\arg\min_{A,B} \sum_{t=1}^{m} \Delta\left(B \circ A\left(x_t\right), x_t\right) + \lambda \sum_{i} |a_i|$$

- where a_i is the activation at the i^{th} hidden layer and i iterates over all the hidden activation's.

Other Ways

KL-divergence

- We can assume the activation of each neuron acts as a Bernouli variable with probability p and tweak that probability.

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KL-divergence

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For each neuron j

- The calculated empirical probability is $\hat{p}_j = \frac{1}{m} \sum_i a_i (i)$ where i iterates over the samples in the batch:

$$\arg\min_{A,B} \sum_{t=1}^{m} \Delta \left(B \circ A \left(x_t \right), x_t \right) + \sum_i KL \left(p \| \hat{p} \right)$$

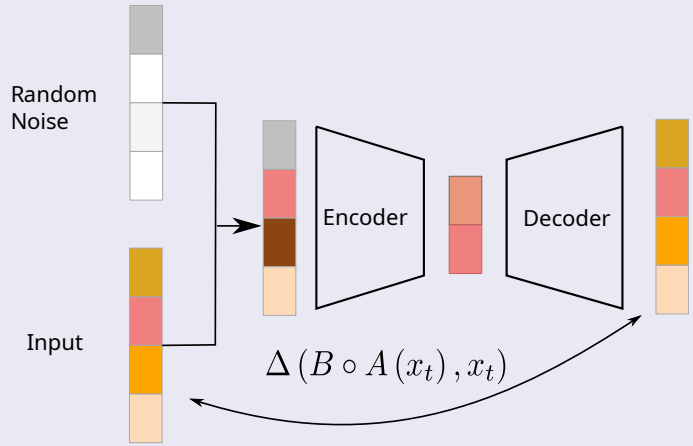
  - where the regularization term in it aims at matching p to $\hat{p}$.

Outline

Denoising Autoencoders

Note

- They can be viewed either as a regularization option, or as robust autoencoders which can be used for error correction.



Here, we have

We have that the input can be seen as

$$\widetilde{x} = x + N\left(0, \sigma I\right) \rightarrow p\left(\widetilde{x}|x\right) \sim N\left(x, \sigma I\right)$$

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An also

$$\widetilde{x} = \beta \odot x \rightarrow \beta \sim Ber\left(p\right)$$

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Contractive Autoencoders

Here, the desire is to reduce the effect of small perturbations

- On the feature extraction process.

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By forcing the encoder to avoid changes

- Not important for the reconstruction by the decoder.

Basically

Apply regularization into the hidden layer of the encoder

- Into the Jacobian matrix of the Hidden Layers of the Encoder

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- Into the Jacobian matrix of the Hidden Layers of the Encoder

Fromally, $J_{ji} = \nabla_{x_i} h_j (x_i)$

- Thus changes at the nodes h_j of a layer h.

Thus, we have

We try to minimize a Ridge regression on the Jacobian

$$\arg\min_{A,B} E\left(\Delta\left(x, B \circ A\left(x\right)\right)\right) + \lambda \left\| J_A\left(x\right)\right\|_2^2$$

Outline

The Paper

Around 2015 [5]

- An extraordinary network came to be
  - "U-Net: Convolutional Networks for Biomedical Image Segmentation" by Olaf Ronneberger, Philipp Fischer, and Thomas Brox

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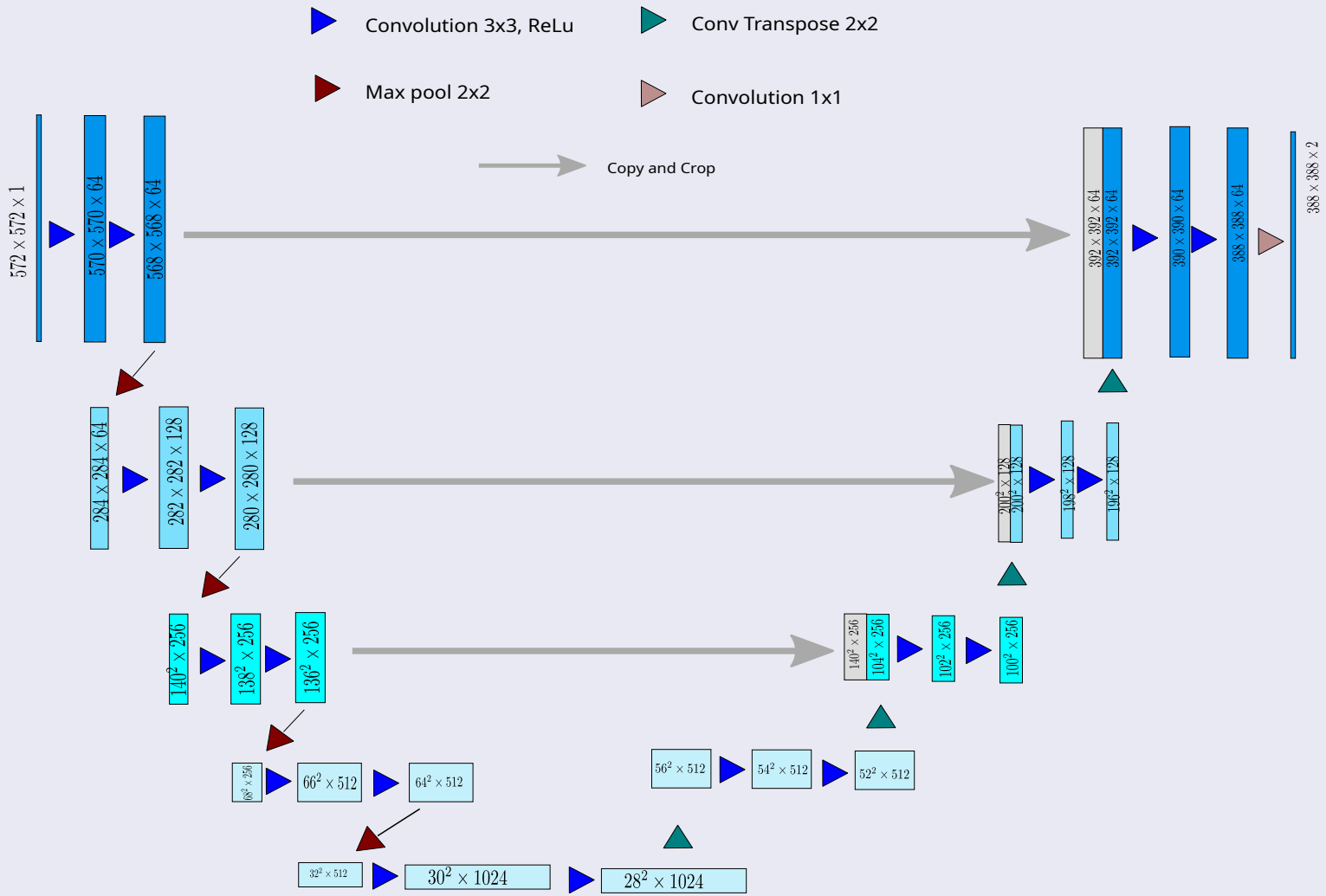
It won

1. The Grand Challenge for Computer-Automated Detection of Caries in Bitewing Radiography at ISBI 2015,
2. The Cell Tracking Challenge at ISBI 2015

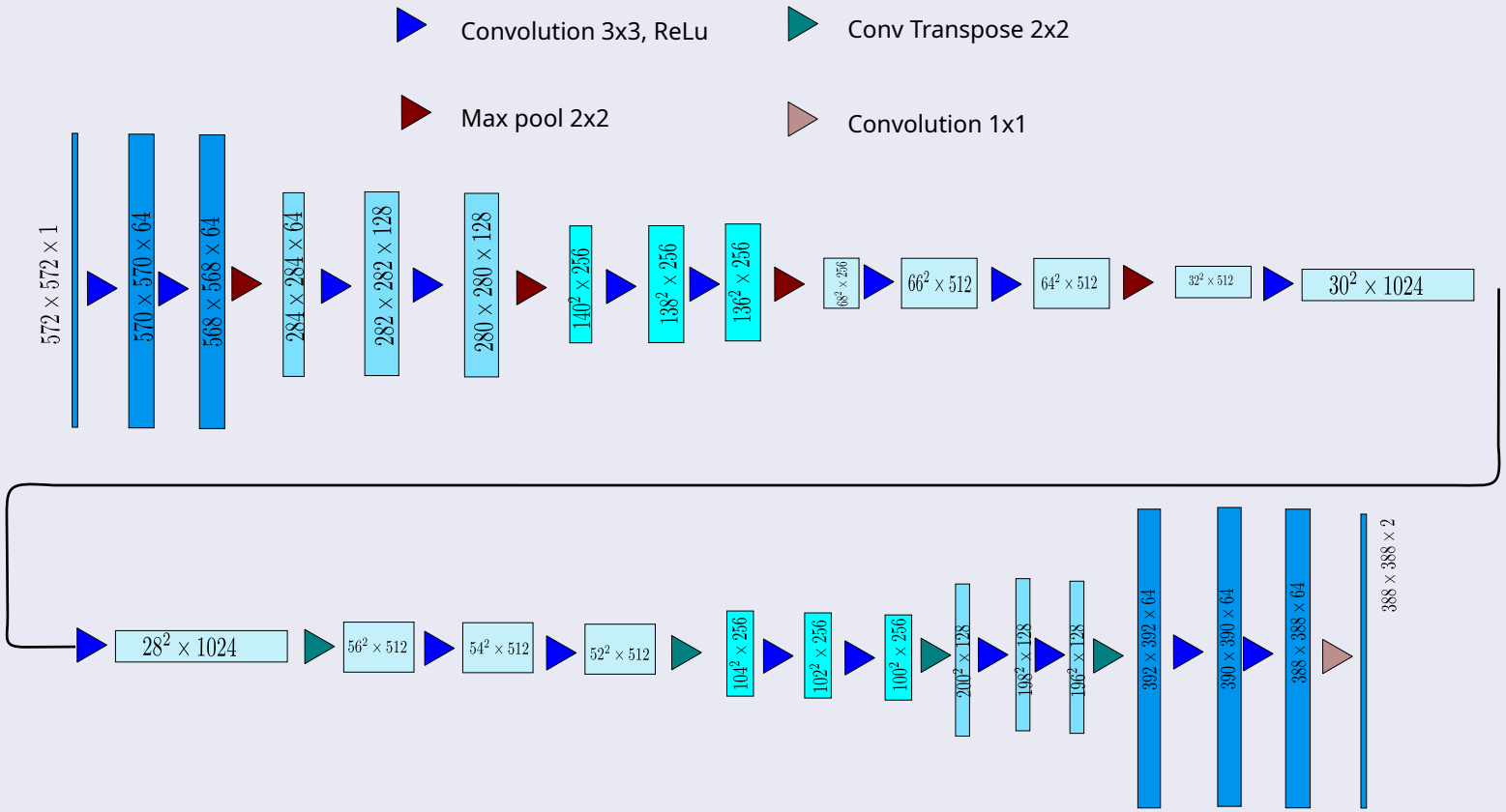
The Segmentation Architecture

We have (Imagen from [5])



Similarity with an Autoencoder

If we remove the extra passing of information, we finish with an autoencoder



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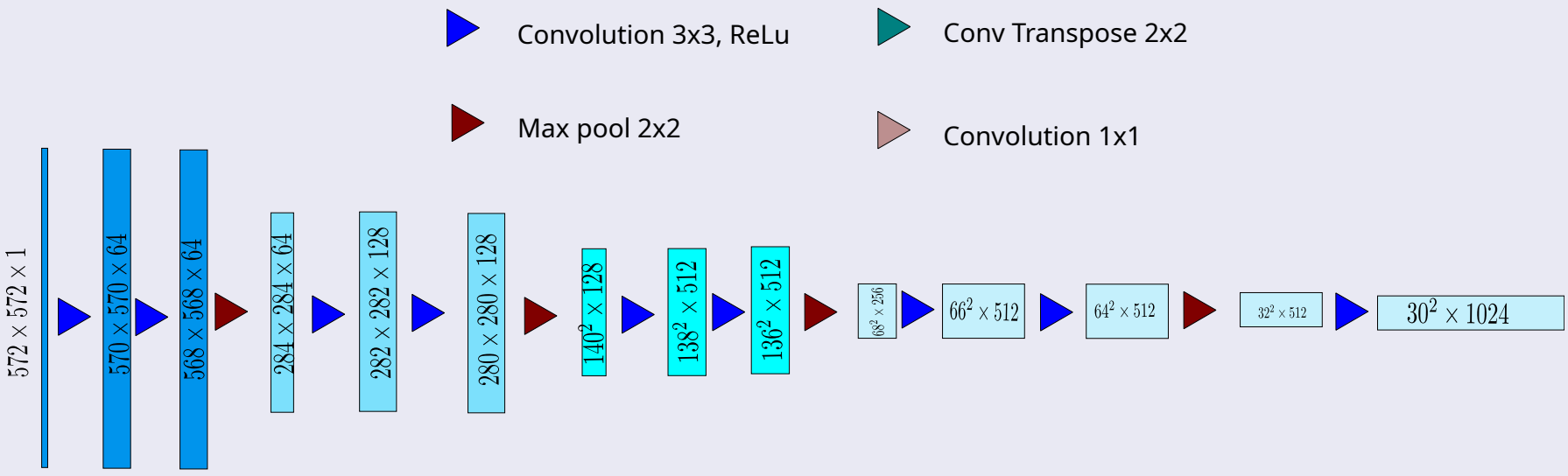
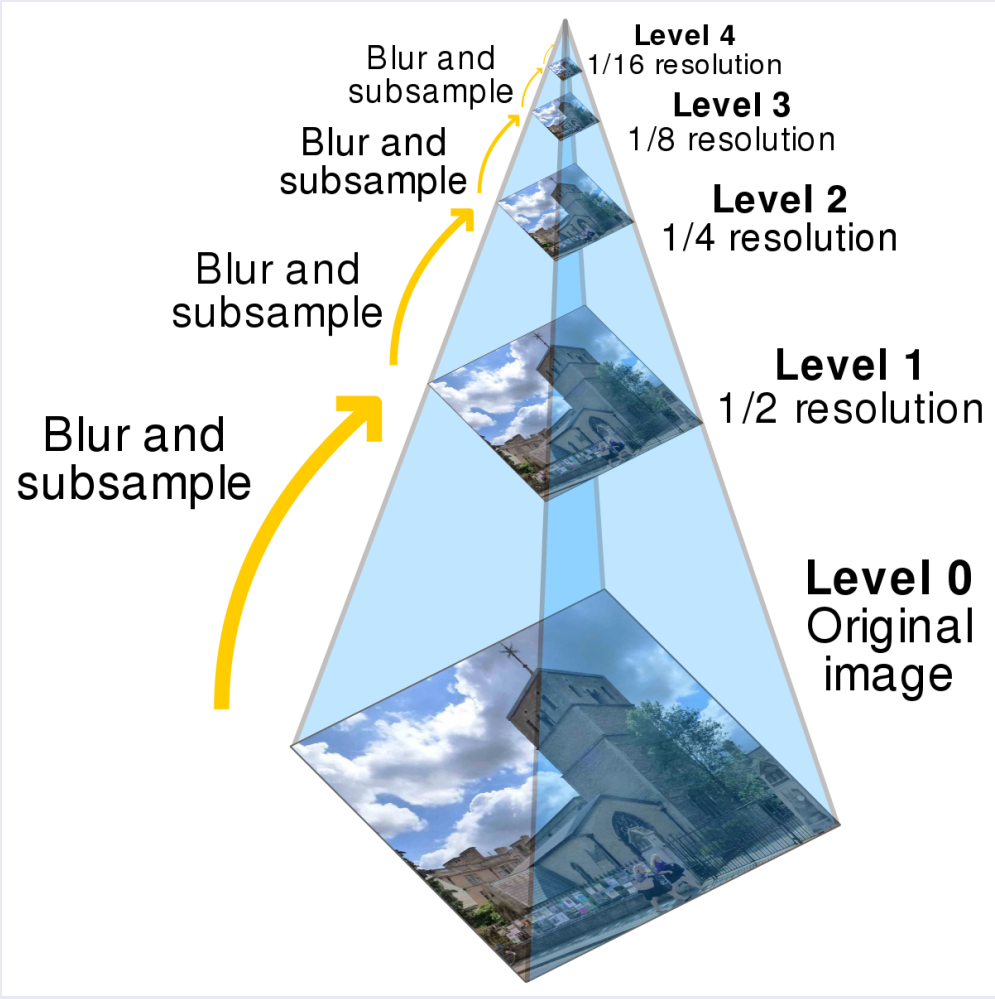
At the encoder part



If you think about this

It is our Image Pyramid of old computer vision



Clearly

We can train this pyramide/encoder with data

- Yes our old backpropagation a.k.a automatic differentiation

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At the center of this is the Convolution for multiple filters

$$Y_i^{(l)}(x,y) = B_i^{(l)}(x,y) + \sum_{j=1}^{m_1^{(l-1)}} \sum_{u=-ks}^{ks} \sum_{v=-ks}^{ks} Y_j^{(l-1)}(i-u, j-v) K_{ij}^{(l)}(u,v)$$

Basically

We take the j filter of the C_{out} dimension

- Then for each filter j you apply the convolution to each $Image_k$

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We take the j filter of the C_{out} dimension

- Then for each filter j you apply the convolution to each $Image_k$

Then you simply add the images result of such convolution

- And Add Pointwise the bias $b_{C_{out_j}}$

Outline

The Variational Autoencoders [6]

It is based on the Maximum a Posteriori Idea under a Random Process

- A value $x^{(i)}$ is generated from some likelihood distribution $p_\Theta(x|z)$ with a prior $p_\Theta(z)$

$$p_\Theta(z|x) \approx p_\Theta(x|z)\, p_\Theta(z)$$

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$$p_\Theta(z|x) \approx p_\Theta(x|z)\, p_\Theta(z)$$

We ask $p_\Theta(x|z)$ and $p_\Theta(z)$

1. They are coming from parametric families
2. They are differentiable almost everywhere w.r.t. Θ and z

However

When we have the following case

- The case where the integral of the marginal likelihood is intractable

$$p_{\Theta}(x) = \int p_{\Theta}(x|z)\, p_{\Theta}(z)\, dz$$

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$$p_\Theta(x) = \int p_\Theta(x|z)\, p_\Theta(z)\, dz$$

Also the **posterior density** is also intractable (No Expectation Maximization can be used)

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

However

When we have the following case

- The case where the integral of the marginal likelihood is intractable

$$p_{\Theta}(x) = \int p_{\Theta}(x|z)\, p_{\Theta}(z)\, dz$$

Also the **posterior density** is also intractable (No Expectation Maximization can be used)

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

These intractability's are quite common and appear in cases of moderately complicated likelihood functions

- For example Neural Networks...

More problems with sampling Bayesian Estimators

Gibbs Samplers, Metropolis-Hastings

- Have a serious problem, they are difficult to parallelize making them unusable for Deep Learning Applications.

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- Variational Bayes is such alternative

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- Have a serious problem, they are difficult to parallelize making them unusable for Deep Learning Applications.

We need another way to estimate the posterior of a Bayesian method

- Variational Bayes is such alternative

This is done by approximate $p(x|z)$ by the use of a tractable $q(x)$

- This is done by the use a trick in Variational Bayes.

Outline

We start with something simple

The classic

- The marginal likelihood is composed of a sum over the marginal likelihoods of individual datapoints:

$$\log p_\theta\left(\boldsymbol{x}_1, ..., \boldsymbol{x}_N\right) = \sum_{i=1}^{N} \log p_\theta\left(\boldsymbol{x}_i\right)$$

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- The marginal likelihood is composed of a sum over the marginal likelihoods of individual datapoints:

$$\log p_\theta\left(\boldsymbol{x}_1, ..., \boldsymbol{x}_N\right) = \sum_{i=1}^{N} \log p_\theta\left(\boldsymbol{x}_i\right)$$

Therefore, if we can maximize each $\log p_\theta\left(\boldsymbol{x}_i\right)$

- We maximize all $\log p_\theta\left(\boldsymbol{x}_1, ..., \boldsymbol{x}_N\right)$

Outline

The Variational Bound using the Kullback-Leibler (KL) Divergence

The best Variational Bayes approximation $q^* \in \mathcal{Q}$ is found by minimizing against the true $p(x)$

$$q^* = \arg\min_{q^* \in \mathcal{Q}} \left\{ KL(q \| p) = \int q(x) \log\left(\frac{q(x)}{p(x)}\right) dx \right\}$$

Properties of KL Divergence

Non-Negativity

- We have that $KL(q \| p) \geq 0$
- Equality holds if and only if : $q = p$ almost surely (i.e., the distributions are identical).

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Convexity in q

- The KL divergence is convex in q (for fixed p).
- This ensures that the optimization problem in variational inference (minimizing KL divergence) has a unique global minimum, making it tractable for gradient-based methods.

Furthermore

We actually cannot minimize the KL divergence exactly,

- but we can minimize a function that is equal to it up to a constant

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- but we can minimize a function that is equal to it up to a constant

An application of the Jensen's inequality for probability distributions

- When f is concave

$$f\left(E\left[x\right]\right) \geq E\left[f\left(x\right)\right]$$

Using it we get the maximizing the Evidence Lower Bound (ELBO)

Going back to the problem of maximizing $\log p_\theta(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$

$$
\begin{aligned}
\log p(x) &= \log \int_z p(x, z) \\
&= \log \int_z p(x, z) \frac{q(z)}{q(z)} \\
&= \log \left[E_q \left[\frac{p(x, Z)}{q(z)} \right] \right] \\
&\geq E_q \left[\log \left(\frac{p(x, Z)}{q(z)} \right) \right] \\
&= E_q [\log p(x, Z)] - E_q [\log q(Z)]
\end{aligned}
$$

From minimization to maximization

Minimizing KL is equivalent to maximizing the lower bound on $\log p(x)$

$$ELBO(q) = E_q[\log p(x, Z)] - E_q[\log q(Z)]$$

- The Expectation Lower Bound (ELBO) which also appears at the Expectation Maximization

We can see this when looking at the Posterior probability

Note first that

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

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We can see how the ELBO is inserted into the KL divergence

$$\begin{aligned}
KL(q(z) \| p(z|x)) &= E_q\left[\log \frac{q(Z)}{p(Z|x)}\right] \\
&= E_q[\log q(Z)] - E_q[\log p(Z|x)] \\
&= E_q[\log q(Z)] - E_q\left[\log \frac{p(Z,x)}{p(x)}\right] \\
&= -\left(\underbrace{E_q[\log p(Z,x)] - E_q[\log q(Z)]}_{ELBO}\right) + \log p(x) \\
&= -E_q\left[\log \frac{p(Z,x)}{q(Z)}\right] + \log p(x)
\end{aligned}$$

Therefore

If we want to minimize the $KL(q(z) \| p(z|x))$

- We need to maximize the term $E_q[\log p(x, Z)] - E_q[\log q(Z)]$

Outline

Thus, we have

Something Notable

- The join likelihood is composed of a sum over the marginal likelihoods of individual datapoints

$$\log p_{\Theta}\left(z_1, z_2, z_3, ..., z_N\right) = \sum_{i=1}^{N} \log p_{\Theta}\left(z_i\right)$$

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Typically, this family does not contain the true posterior

- because the hidden variables are dependent.
  - A the Gaussian mixture model all of the cluster assignments z_i are dependent on each other and the cluster locations $\mu_{1:K}$ given the data $x_{1:n}$.
  - These dependencies are often what makes the posterior difficult to work with.

Some Notation

$p\left(z_j|z_{-j},x\right)$

- $p\left(z_j|z_1,...,z_{j-1},z_j,...,z_m,x\right)=p\left(z_j|z_{-j},x\right)$

Now, we optimize the ELBO for this factorized distribution

First, recall the chain rule and use it to decompose the joint

$$p\left(z_{1:m}, x_{1:n}\right) = p\left(x_{1:n}\right) \prod_{j=1}^{m} p\left(z_j | z_{1:j-1}, x_{1:n}\right)$$

- Notice that the z variables can occur in any order in this chain.

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Second, decompose the entropy of the variational distribution,

$$E\left[\log q\left(z_{1:m}\right)\right] = \sum_{j=1}^{m} E_j\left[\log q\left(z_j\right)\right]$$

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Second, decompose the entropy of the variational distribution,

$$E\left[\log q\left(z_{1:m}\right)\right] = \sum_{j=1}^{m} E_j\left[\log q\left(z_j\right)\right]$$

We know from the previous

$$KL\left(q\left(z\right) \| p\left(z|x\right)\right) = -E_q\left[\log \frac{p(Z,x)}{q(Z)}\right] + \log p\left(x\right)$$

$$KL\left(q\left(z\right) \| p\left(z|x\right)\right) = \log p\left(x\right) - \left[E_q\left[\log p\left(Z, x\right) - \log q\left(Z\right)\right]\right]$$

We have then

We know that

$$p\left(z_j|z_{1:j-1},x_{1:n}\right)=\frac{p\left(z_{1:j},x_{1:n}\right)}{p\left(z_{1:j-1},x_{1:n}\right)}$$

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We know that

$$p\left(z_j|z_{1:j-1},x_{1:n}\right)=\frac{p\left(z_{1:j},x_{1:n}\right)}{p\left(z_{1:j-1},x_{1:n}\right)}$$

Then if we multiply with $\frac{p(z_{1:j-1},x_{1:n})}{p(z_{1:j-1},x_{1:n})}$ the numerator can go out and seen as a constant

$$\mathcal{L}=\log p\left(x_{1:n}\right)-\sum_{j=1}^{m}\left(E\left[\log\frac{p\left(z_{1:j},x_{1:n}\right)}{p\left(z_{1:j-1},x_{1:n}\right)}\right]+\underbrace{E\left[p\left(z_{1:j-1},x_{1:n}\right)\right]}_{\text{const with respect to } z_j}-E_j\left[\log q\left(z_j\right)\right]\right)$$

Finally, we get

A final equation

$$\mathcal{L} \approx \log p\left(x_{1:n}\right) - \underbrace{\sum_{j=1}^{m}\left(E\left[\log p\left(z_j | z_{1:j-1}, x_{1:n}\right)\right] - E_j\left[\log q\left(z_j\right)\right]\right)}_{KL}$$

Now, Consider the ELBO as a function of $q(z_j)$

Employ the chain rule with the variable z_k as the last variable in the list

- This leads to the objective function

$$\begin{aligned}\mathcal{L} =& E\left[\log p\left(z_j|z_{-j},x\right)\right] - E_j\left[\log q\left(z_j\right)\right] + constant \\ \approx& E\left[\log p\left(z_j|z_{-j},x\right)\right] - E_j\left[\log q\left(z_j\right)\right]\end{aligned}$$

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Write this objective as a function of $q(z_k)$

$$\mathcal{L}\left[q\left(z_j\right)\right] \approx \int q\left(z_j\right)\log p\left(z_j|z_{-j},x\right)dz_j - \int q\left(z_j\right)\log q\left(z_j\right)dz_j$$

Therefore, we want

To maximize this quantity

$$\arg\max_{q_j} \left\{ \int q(z_j) \log p(z_j | z_{-j}, x)\, dz_j - \int q(z_j) \log q(z_j)\, dz_j \right\}$$

Now Optimize

Take the derivative with respect to $q(z_j)$

$$\frac{d\mathcal{L}[q(z_j)]}{dq(z_j)} = E_q[\log p(z_j|z_{-j}, x)] - \log q(z_j) - \underbrace{\frac{q(z_j)}{q(z_j)}}_{1} = 0$$

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This (and Lagrange multipliers) leads to an coordinate ascent for $q(z_j)$

$$q^*(z_j) \propto \exp\{E_q[\log p(z_j|z_{-j}, x)]\}$$

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Since the denominator of the conditional does not depend on z_j

$$q^*(z_j) \propto \exp\{E_q[\log p(z_j, z_{-j}, x)]\}$$

Some Remarks

We have that

- This coordinate ascent procedure convergences to a local maximum.
- The coordinate ascent update for $q(z_j)$ only depends on the other, fixed approximations $q(z_k), k \neq j$.

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- This coordinate ascent procedure convergences to a local maximum.
- The coordinate ascent update for $q(z_j)$ only depends on the other, fixed approximations $q(z_k), k \neq j$.

In addition

- While this determines the optimal $q(z_j)$, it is still not specified.
- Depending on what form we use, the coordinate update $q(z_j)$ might not be easy to work with.

Outline

We have that

Thus, from $\log p_\Theta(z_1, z_2, z_3, ..., z_N) = \sum_{i=1}^{N} \log p_\Theta(z_i)$,and knowing that KL is positive

$$\log p_\Theta(z_i) \geq -\int_{\mathcal{Z}} q_\phi(z) \log\left(\frac{p_\Theta(x, z_i)}{q_\phi(z)}\right) dx + \mathcal{T}(\Theta, \phi | z_i)$$

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The First Term has

- $\int_{\mathcal{Z}} q_\phi(z) \log\left(\frac{p_\Theta(x,z_i)}{q_\phi(z)}\right) dx = D_{KL}(p_\Theta(x, z_i) || q_\phi(z))$ is the KL Divergence of the approximate of the true posterior

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The Second Term

- $\mathcal{T}(\Theta, \phi | z_i)$ the variational lower bound on the marginal likelihood z_i

Now given that the $D_{KL}\left(p_{\Theta}\left(x, z_i\right)||q_{\phi}\left(z\right)\right)$ is positive

We can say

$$\log p_{\Theta}\left(z_i\right) \geq \mathcal{T}\left(\Theta, \phi | z_i\right) = E_{q_{\phi}(x|z)}\left[-\log q_{\phi}\left(x|z\right) + \log p_{\Theta}\left(z\right)\right]$$

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Actually is a KL on p_Θ and q_ϕ

$$-\log q_\phi\left(x|z\right) + \log p_\Theta\left(z\right) = \log\left(\frac{p_\Theta\left(z\right)}{q_\phi\left(x|z\right)}\right)$$

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Actually is a KL on p_Θ and q_ϕ

$$-\log q_\phi\left(x|z\right) + \log p_\Theta\left(z\right) = \log\left(\frac{p_\Theta\left(z\right)}{q_\phi\left(x|z\right)}\right)$$

Actually, we can simplify this last function by dropping the term $-\log q_\phi\left(x|z\right)$ because is already in the first term

$$\mathcal{T}\left(\Theta, \phi | z_i\right) \propto E_{q_\phi(x|z)}\left[\log p_\Theta\left(z\right)\right]$$

Therefore, we can generate a loss function combining both terms $\mathcal{L}(\Theta, \phi|z)$

As the following give that they are KL divergences i.e. maximization of this minimize the divergences

$$\mathcal{L}(\Theta, \phi|z_i) = -KL(p_\Theta(x, z)||q_\phi(z)) + E_{q_\phi(x|z_i)}[\log p_\Theta(z_i)]$$

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Thus, we want to derive $\mathcal{L}(\Theta, \phi|z_i)$

- w.r.t. both the variational parameters ϕ and generative parameters Θ.

Problem

Problem is that MCMC is not enough

- The usual (naïve) Monte Carlo gradient estimator for this type of problem is:

$$\begin{aligned}\nabla_{\phi} E_{q_{\phi}(x)}\left(\log p_{\Theta}\left(z_i\right)\right) &= E\left(\nabla_{q_{\phi}(x)} q_{\phi}\left(x\right) \log p_{\Theta}\left(z_i\right)\right) \\ &\approx \frac{1}{L}\sum_{l=1}^{L} \nabla_{q_{\phi}(x)} q_{\phi}\left(x_l\right) \log p_{\Theta}\left(z_i|x_l\right) \\ &\approx E_{\nabla_{q_{\phi}(x)} q_{\phi}(x_l)}\left[\log p_{\Theta}\left(z|x_l\right)\right]\end{aligned}$$

Problem with this first attempt of using this for maximization

Here, we have that $x \sim q_\phi(x|z_i)$, yes z_i is a hidden variable

- This gradient estimator exhibits exhibits very high variance and non practical

Outline

First, explicit re-parameterization Gradients

Suppose we would like to optimize an expectation $E_{q_\phi(x)}[f(x)]$

- A continuously differentiable function $f(z)$ w.r.t. the parameters of the distribution.

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We assume that we can find a standardization function $S_\phi\left(x\right) = \epsilon \sim q\left(\epsilon\right)$

- Such that you can do the following $x = S_\phi^{-1}\left(\epsilon\right)$

First, explicit re-parameterization Gradients

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- Such that you can do the following $x = S_\phi^{-1}(\epsilon)$

For example, for a Gaussian distribution $N(\mu, \sigma^2)$

- We can use the following function $S_{\mu,\sigma}(x) = \frac{x-\mu}{\sigma} \sim N(0,1)$ then we have we can sample $\epsilon \sim N(0,1)$

$$S_{\mu,\sigma}^{-1}(\epsilon) = \sigma \cdot \epsilon + \mu$$

Therefore, we can express the $E_{q_\phi(x)}\left[f\left(x\right)\right]$

As follow

$$E_{q_\phi(x)}\left[f\left(x\right)\right] = E_{q(\epsilon)}\left[f\left(S_\phi^{-1}\left(\epsilon\right)\right)\right]$$

Therefore, we can express the $E_{q_\phi(x)}\left[f\left(x\right)\right]$

As follow

$$E_{q_\phi(x)}\left[f\left(x\right)\right] = E_{q(\epsilon)}\left[f\left(S_\phi^{-1}\left(\epsilon\right)\right)\right]$$

This allows us to compute the gradient of the expectation as the expectation of the gradients by rule chain:

$$\begin{aligned}\nabla_\phi E_{q_\phi(x)}\left[f\left(x\right)\right] &= E_{q(\epsilon)}\left[\nabla_\phi f\left(S_{\mu,\sigma}^{-1}\left(\epsilon\right)\right)\right] \\ &= E_{q(\epsilon)}\left[\nabla_z f\left(S_{\mu,\sigma}^{-1}\left(\epsilon\right)\right)\nabla_\phi S_\phi^{-1}\left(\epsilon\right)\right]\end{aligned}$$

Therefore

An alternative was proposed to avoid the inverse of $S_\phi(x)$

- For this, we first we express the classic stuff

$$\nabla_\phi E_{q_\phi(x)}[f(x)] = E_{q_\phi(x)}[\nabla_x f(x) \nabla_\phi x]$$
$$\nabla_\phi x = \nabla_\phi S_\phi^{-1}(\epsilon)\Big|_{\epsilon = S_\phi(x)}$$

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It was proposed to compute $\nabla_\phi x$ by implicit differentiation

- Implicit differentiation makes use of the chain rule to differentiate a function which cannot be explicitly expressed in the form $y = f(x)$

$$\frac{df(y(x))}{dx} = \frac{df}{dy} \times \frac{dy}{dx}$$

Then

We apply the total gradient to the equality $S_\phi(x) = \epsilon$

- We finish with the following given that $S_\phi(x)$ depends on ϕ directly by the subscript and from x indirectly. Thus, $x = x(\phi)$:

$$\frac{dS_\phi(x)}{d\phi} = \frac{d\epsilon}{d\phi}$$

$$\frac{dS_\phi(x)}{dx} \times \frac{dx}{d\phi} + \frac{dS_\phi(x)}{d\phi} = 0$$

Then, we have that

Therefore, we have that

$$\frac{dx}{d\phi} = -\left(\frac{dS_\phi(x)}{dx}\right)^{-1} \times \frac{dS_\phi(x)}{d\phi}$$

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This expression for the gradient only requires differentiating the standardization function

- Basically we get the value and invert it, we do not need an explicit version of the inverse function, then derive it.

Example

Univariate Normal distribution $N(\mu, \sigma^2)$

- We have the standardization function $S_{\mu,\sigma}(x) = \frac{x-\mu}{\sigma} = \epsilon \sim N(0,1)$

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We have then, if we use the derivatives

$$\frac{dx}{d\mu} = -\left(\frac{dS_{\mu,\sigma}(x)}{dz}\right)^{-1} \times \frac{dS_{\mu,\sigma}(x)}{d\mu} = -\frac{-\frac{1}{\sigma}}{\frac{1}{\sigma}} = 1$$

$$\frac{dx}{d\sigma} = -\left(\frac{dS_{\mu,\sigma}(x)}{dz}\right)^{-1} \times \frac{dS_{\mu,\sigma}(x)}{d\sigma} = \frac{-\frac{(x-\mu)}{\sigma^2}}{\frac{1}{\sigma}} = \frac{(x-\mu)}{\sigma} \sim N(0,1)$$

If we compare against inverting and deriving

We have the following inverse of the function

$$z = S_{\mu,\sigma}^{-1}(x) = \mu + \sigma\epsilon$$

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Then, we have that with $\epsilon \sim N(0,1)$

$$\frac{dz}{d\mu} = 1, \qquad \frac{dz}{d\sigma} = \epsilon$$

Outline

We have that

The essential parameterization trick is quite simple

- Let x be a continuous random variable and $x \sim q_\phi(x|z)$ a conditional distribution

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- Let x be a continuous random variable and $x \sim q_\phi(x|z)$ a conditional distribution

It is possible to extend $S_\phi(x) = \epsilon$

$$g_{\phi,z}(x) = \epsilon$$

- with $\epsilon \sim p(\epsilon)$ and $g_\phi(\cdot)$ is some vector valued function parameterized by ϕ, z

This parameterization is useful for our case

It can be used to rewrite an expectation w.r.t $q_\phi(x|z)$

- Such that the Monte Carlo estimate of the expectation is differentiable w.r.t. ϕ

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- Such that the Monte Carlo estimate of the expectation is differentiable w.r.t. ϕ

We want the following

- Given the mapping $g_{\phi,z}(x) = \epsilon$ (Here, x is a vector and $dx = \prod_i dx_i$ are infinitesimals)

$$q_\phi(x|z) \approx g_{\phi,z}(x)$$

Now, we can do the following

Given that the error is a small variation, we can say that in an small area

$$q_\phi(x|z)\prod_i dx_i = p(x)\prod_i d\epsilon_i$$

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Given that the error is a small variation, we can say that in an small area

$$q_\phi(x|z)\prod_i dx_i = p(x)\prod_i d\epsilon_i$$

Therefore

$$\int q_\phi(x|z) f(x)\,dx = \int p(x) f(x)\,dx = \int p(x) f(g_{\phi,z}(x))\,dx$$

We can then construct then a variational estimation

We have that

$$\int q_\phi(x|z) f(x) dx = \frac{1}{L} \sum_{l=1}^{L} f(g_{\phi,z}(x)) \text{ with } \epsilon_l \sim p(\epsilon)$$

Therefore, we have

Using the previous ideas

$$\nabla_\phi E_{q_\phi(x)}\left[f\left(g_{\phi,z}\left(x\right)\right)\right] = E_{q_\phi(x)}\left[\nabla_x f\left(g_{\phi,z}\left(x\right)\right)\frac{dx}{d\phi,z}\right]$$

$$\frac{dx}{d\phi,z} = -\left(\frac{dg_{\phi,z}\left(x\right)}{dx}\right)^{-1} \times \frac{dg_{\phi,z}\left(x\right)}{d\phi,z}$$

Outline

Therefore

We have that

$$\widetilde{\mathcal{L}}^{A}\left(\Theta,\phi|z_i\right)\approx\mathcal{L}\left(\Theta,\phi|z_i\right)$$

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$$\widetilde{\mathcal{L}}^{A}\left(\Theta,\phi|z_i\right)\approx\mathcal{L}\left(\Theta,\phi|z_i\right)$$

Thus, we use the estimation with $x_{i,l}=g_{\phi}\left(\epsilon_{i,l}\right)$ and $\epsilon_l\sim p\left(\epsilon\right)$

$$\widetilde{\mathcal{L}}^{A}\left(\Theta,\phi|z_i\right)=\frac{1}{L}\sum_{l=1}^{L}\left[\log p_{\Theta}\left(z_i,x_{i,l}\right)-\log q_{\phi}\left(x_{i,l}|z_i\right)\right]$$

Therefore

We have that

$$\widetilde{\mathcal{L}}^{A}\left(\Theta,\phi|z_i\right)\approx\mathcal{L}\left(\Theta,\phi|z_i\right)$$

Thus, we use the estimation with $x_{i,l}=g_{\phi}\left(\epsilon_{i,l}\right)$ and $\epsilon_l\sim p\left(\epsilon\right)$

$$\widetilde{\mathcal{L}}^{A}\left(\Theta,\phi|z_i\right)=\frac{1}{L}\sum_{l=1}^{L}\left[\log p_{\Theta}\left(z_i,x_{i,l}\right)-\log q_{\phi}\left(x_{i,l}|z_i\right)\right]$$

Actually, if $p\left(x\right)$ is seen as a normalization factor

$$\log\left(\frac{p_{\Theta}\left(z|x\right)}{q_{\phi}\left(x\right)}\right)=\log\left(\frac{p_{\Theta}\left(z,x\right)}{p\left(z\right)q_{\phi}\left(x\right)}\right)\approx\log\left(\frac{p_{\Theta}\left(z,x\right)}{q_{\phi}\left(x|z\right)}\right)$$

In this was, we have

We can say that

$$\log\left(\frac{p_\Theta\left(z_i, x_{i,l}\right)}{q_\phi\left(x_{i,l}|z_i\right)}\right) \approx \log p_\Theta\left(z_i, x_{i,l}\right) - \log q_\phi\left(x_{i,l}|z_i\right)$$

Final Algorithm

Minibatch version of the Auto-Encoding VB (AEVB) algorithm

- Initialize Parameters Θ, ϕ
- Repeat
- $X^M \leftarrow$ Random Mini-batch of M data points
- $\epsilon \leftarrow$ Random samples from noise distribution $p(\epsilon)$
- $g \leftarrow \nabla_{\Theta,\phi} \widetilde{\mathcal{L}}^A (\Theta, \phi | z_i)$ (Gradient Mini-batch estimator)
- Θ, ϕ update parameters using the gradient
- return Θ, ϕ

Outline

The original variational auto-encoder

It is a continuous latent variable model.

- The model is intended to learn a latent space $\mathcal{Z} = \mathbb{R}^t$ using a given set of samples $\{x_n\} \subseteq \mathcal{Y} = \mathbb{R}^d$
- Such that $t \ll d$

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- Such that $t \ll d$

Therefore

- The model consists of the generative model $p(x|z)$ given a fixed prior $p(z)$

Bernoulli MLP as decoder

In this case, let $p_\Theta(x|z)$ be a multivariate Bernoulli

- The probability is calculated using a fully connected neural network with a single layer

$$\log p(x|z) = \sum_{i=1}^{D} x_i \log y_i + (1 - x_i) \log (1 - y_i)$$

  - where $\boldsymbol{y} = f_\sigma(W_2 \tanh(W_1 z + b_1) + b_2)$ with f_σ is the sigmoidal function
  - with $\Theta = \{W_1, W_2, b_1, b_2\}$ are the weight and biases of the MLP

Gaussian MLP as encoder

We have the following function

$$\begin{aligned}
\log p(z|x) &= \log N\left(\mu, \sigma^2 I\right) \\
\text{where } \mu &= W_4 h + b_4 \\
\log \sigma^2 &= W_5 h + b_5 \\
h &= \tanh\left(W_3 x + b_3\right)
\end{aligned}$$

We have then

Let the prior over isotropic multivariate Gaussian

$$p_{\Theta}(z) = N(0, I)$$

- Note that in this case, the prior lacks parameters.

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Note

- Note the true posterior $p_\Theta(z|x)$ is in this case intractable.

Now for our estimation

We have then the following

$$\log q_\phi(\boldsymbol{z}|\boldsymbol{x}) = \log N\left(\boldsymbol{\mu}, \sigma^2 I\right)$$

- where the mean and s.d. of the approximate posterior, $\boldsymbol{\mu}$ and σ , are outputs of the encoding MLP, i.e. nonlinear functions of data point $\boldsymbol{x}$ and the variational parameters ϕ

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Then, we sample $z_{i,l} \sim q_\phi(z|x_i)$ using the fact that we have a diagonal covariance $\sigma^2 I$

$$z_{i,l} = \mu_i + \sigma_i \odot \epsilon_l \text{ and } \epsilon_l \sim N(0, I)$$

Then, we have that

In this model both

- $p_\Theta(z)$ and $q_\phi(z|x_i)$ are Gaussian

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- $p_\Theta(z)$ and $q_\phi(z|x_i)$ are Gaussian

The resulting estimator for this model comes from the classic where the l is the meaning of multiple samples of z_i

$$\mathcal{L}(\Theta, \phi|x_i) = D_{KL}(q_\phi(z|x_i)||p_\Theta(z)) + \underbrace{\frac{1}{L}\sum_{l=1}^{L} -\log p_\theta(x_i|z_{i,l})}_{E[-\log p_\theta(x_i|z_i)]}$$

- Basically the negative of $-\int_{\mathcal{Z}} q_\phi(z) \log\left(\frac{p_\Theta(x,z_i)}{q_\phi(z)}\right) dx + \mathcal{T}(\Theta, \phi|z_i)$ which we want to maximize but when minimizing we take the negative.

Therefore

We have that $q_\phi(z|x_i) = N(z|\mu(x), \sigma^2(x) I)$

- Where at the encoder

$$\begin{aligned} \mu &= W_4 x + b_4 \\ \log \sigma^2 &= W_5 x + b_5 \end{aligned}$$

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The prior of $p(z) \approx N(z|0, I)$

- Then, the KL divergence is

$$D_{KL}(q_\phi(z|x) || p_\Theta(z)) = E_{q_\phi(z|x)}\left[\log \frac{q_\phi(z|x)}{p_\Theta(z)}\right]$$

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$$D_{KL}(q_\phi(z|x)||p_\Theta(z)) = E_{q_\phi(z|x)}\left[\log \frac{q_\phi(z|x)}{p_\Theta(z)}\right]$$

Expand the logarithm

$$\log \frac{q_\phi(z|x)}{p_\Theta(z)} = \log q_\phi(z|x) - \log p_\Theta(z)$$

Given that we have Gaussian's

Assume the encoder outputs a diagonal Gaussian distribution

$$\log q_\phi(\boldsymbol{z}|\boldsymbol{x}) = -\frac{1}{2}\left(d\log 2\pi + d\log\sigma^2 + \frac{\|\boldsymbol{z}-\boldsymbol{\mu}\|^2}{\sigma^2}\right)$$

$$p_\Theta(\boldsymbol{z}) = -\frac{1}{2}\boldsymbol{z}^T\boldsymbol{z} - \frac{d}{2}\log 2\pi$$

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$$p_\Theta(\boldsymbol{z}) = -\frac{1}{2}\boldsymbol{z}^T\boldsymbol{z} - \frac{d}{2}\log 2\pi$$

Putting all together, we have

$$D_{KL}\left(q_\phi(z|x_i)\,||p_\Theta(z)\right) = E_{q_\phi(z|x_i)}\left[-\frac{1}{2}d\log 2\pi - \frac{1}{2}d\log\sigma^2 - \frac{1}{2}\frac{\|\boldsymbol{z}-\boldsymbol{\mu}\|^2}{\sigma^2} + \frac{1}{2}z^T z + \frac{d}{2}\log 2\pi\right]$$

We have the following equality's on the Expectation

We have the following

$$E_{q_\phi(z|x_i)}\left[\|\boldsymbol{z}-\boldsymbol{\mu}\|^2\right] = E_{q_\phi(z|x_i)}\left[tr\left(\left[\boldsymbol{z}-\boldsymbol{\mu}\right]\left[\boldsymbol{z}-\boldsymbol{\mu}\right]^T\right)\right] = tr\left(\sigma^2 I\right) = d\sigma^2$$

$$E_{q_\phi(z|x_i)}\left[z^T z\right] = \mu^T\mu + tr\left(\sigma I\right) = \mu^T\mu + d\sigma^2$$

Therefore, we apply the expected value

We have the following

$$D_{KL}\left(q_\phi\left(z|x_i\right)||p_\Theta\left(z\right)\right) = -\frac{1}{2}\log 2\pi - \frac{1}{2}\log\sigma^2 - \frac{1}{2}\frac{d\sigma^2}{\sigma^2} + \frac{1}{2}\mu^T\mu + \frac{1}{2}d\sigma^2 + \frac{d}{2}\log 2\pi$$

$$\approx -\frac{1}{2}d\log\sigma^2 - \frac{d}{2} + \frac{1}{2}\sum_{i=1}^{d}\mu_i^2 + \frac{1}{2}d\sigma^2$$

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Which can be seen as with $\sigma_i^2 = \sigma^2$

$$D_{KL}\left(q_\phi\left(z|x_i\right)||p_\Theta\left(z\right)\right) = -\frac{1}{2}\sum_{i=1}^{d}\left(\log\sigma_i^2 + 1 - \frac{1}{2}\mu_i^2 + \sigma_i^2\right)$$

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$$D_{KL}\left(q_\phi\left(z|x_i\right)||p_\Theta\left(z\right)\right) = -\frac{1}{2}\log 2\pi - \frac{1}{2}\log\sigma^2 - \frac{1}{2}\frac{d\sigma^2}{\sigma^2} + \frac{1}{2}\mu^T\mu + \frac{1}{2}d\sigma^2 + \frac{d}{2}\log 2\pi$$

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Finally, what we want to minimize this the ELBO will be maximized

$$\mathcal{L}\left(\Theta,\phi|x_i\right) = \underbrace{-\frac{1}{2}\sum_{i=1}^{d}\left(1+\log\left(\sigma_i^2\right)-\left(\mu_i\right)^2-\left(\sigma_i\right)^2\right)}_{D_{KL}\left(q_\phi(z|x_i)||p_\Theta(z)\right)} + \underbrace{\frac{1}{L}\sum_{l=1}^{L}-\log p_\theta\left(x_i|z_{i,l}\right)}_{E[-\log p_\theta(x|z)]}$$

Now what about the real Loss function?

We can do the following if we think that $E\left[\log p_\theta\left(x|z\right)\right]$ is the reconstruction log of the data i.e $x \sim p_\theta\left(x|z\right)$

- We can see that $p_\theta\left(x|z\right)$, if it is modeled as a Bernoulli distribution because you rebuild it or not

$$p_\theta\left(x|z\right) = p^x\left(1-p\right)^{1-x}$$

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Where we use $p = \sigma\left(z\right)$ the output of the decoder

$$p_\theta\left(x|z\right) = \sigma\left(z\right)^x\left(1-\sigma\left(z\right)\right)^{1-x} \Rightarrow -\log p_\theta\left(x|z\right) = -x\log\left(\sigma\left(z\right)\right) - \left(1-x\right)\log\left(1-\sigma\left(z\right)\right)$$

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Therefore when you take a minibatch or the $E\left[-\log p_\theta\left(x_i|z_i\right)\right]$

$$E\left[-\log p_\theta\left(x|z\right)\right] = BCE\left[\sigma\left(z\right), x\right]$$

Therefore the final Loss function is

Two parts the divergence and the binary cross entropy

$$\mathcal{L}\left(\Theta,\phi|x_i\right)=\underbrace{-\frac{1}{2}\sum_{i=1}^{d}\left(1+\log\left(\sigma_i^2\right)-\left(\mu_i\right)^2-\left(\sigma_i\right)^2\right)}_{D_{KL}\left(q_\phi(z|x_i)||p_\Theta(z)\right)}+\underbrace{BCE\left[\sigma\left(z\right),x\right]}_{E[-\log p_\theta(x|z)]}$$

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A last comment is the following, this model is not exactly a generative model but

- the $q(z|x)$ (simple and tractable posteriors) must close enough to $N(0, I)$.
- We can sample from $N(0, I)$ to get a input for the decoder and get some generated sample.

Given the inception of the Variational part

It is coming from the work of [7]

- Bishop, C.M.: Pattern Recognition and Machine Learning (Information Science and Statistics). Springer-Verlag, Berlin, Heidelberg (2006)

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Variational Autoencoder (VAE)

- VAE are generative models that attempt to describe data generation through a probabilistic distribution.

Outline

Outline

Generative Model

At the encoder part

- The posterior distribution $q_\phi(x|z_i)$ which is derived by the encoder

Generative Model

At the encoder part

- The posterior distribution $q_\phi(x|z_i)$ which is derived by the encoder

Thus, we have

- This is regularized towards a continuous and complete distribution in the shape of the predefined prior of the latent variables $p_\Theta(x)$.

Therefore

Once trained

- One can simply samples random variables from the the same prior, and feed it to the decoder.

Therefore

Once trained

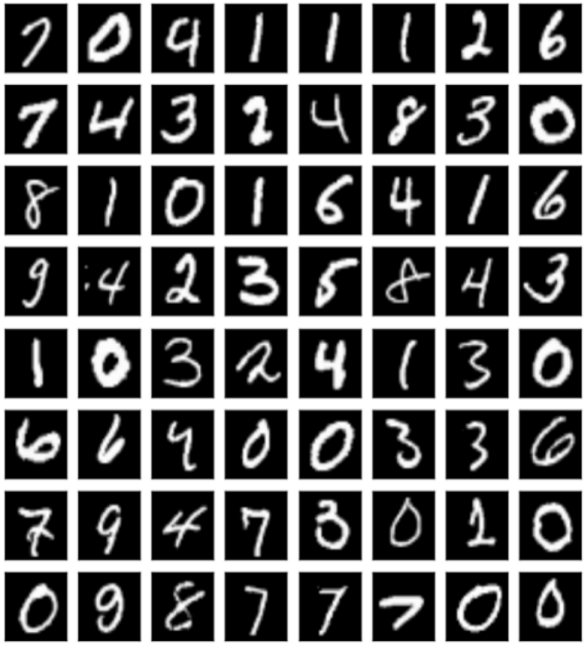
- One can simply samples random variables from the the same prior, and feed it to the decoder.

Since the decoder was trained generate x from $p_\Theta(x_i|z)$

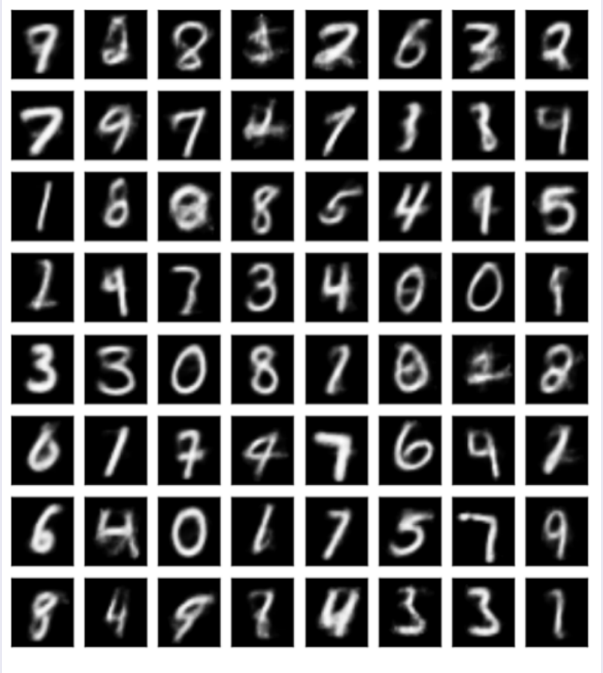
- It would generate a meaningful generated sample

Example

Original Images vs the generated



Sample from the original MNIST dataset



VAE generated MNIST IMAGES

Outline

Consider N images $\{X_l\}_{l=1}^{N}$, with $X_l \in \mathbb{R}^{N_x \times N_y \times C}$

We introduce the decoder

- To introduce the image decoder (generative model) in its simplest form, we first consider a decoder with $L = 2$ layers.

Code Entry $\Downarrow$

$$Layer\ 2: \widetilde{S}^{n,2} = \sum_{k_2=1}^{K_2} D^{k_2,2} * S^{n,k_2,2} \tag{1}$$

$$Unpool: S^{n,1} = \text{unpool}\left(\widetilde{S}^{n,2}\right) \tag{2}$$

$$Layer\ 1: \widetilde{S}^{n,1} = \sum_{k_1=1}^{K_1} D^{k_1,2} * S^{n,k_1,2} \tag{3}$$

$$\text{Data Generation: } X_l \sim N\left(\widetilde{S}^{n,1}, \alpha_0^{-1} I\right) \tag{4}$$

Notation

The following are 3D tensors

- $D^{k_l,l}$
- $S^{n,l}$
- $\widetilde{S}^{n,l}$

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2D Activation Maps

- $S^{n,k,l}$ as slices of 3D tensors $S^{n,l}$

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2D Activation Maps

- $S^{n,k,l}$ as slices of 3D tensors $S^{n,l}$

Finally

- $D^{k,l} * S^{n,k,l} =$ each of the K_{l-1} "slices" of $D^{k_l,l}$ is convolved with the spatially-dependent $S^{n,k,l}$

Meaning for equation (4)

It indicates

1. $E[X_l] = \widetilde{S}^{n,1}$
2. $X_l - E(X_l)$ is iid zero mean Gaussina with preccision α_0

The Stochastic Unpooling

$S^{n,k_l,l}$ is partitioned into contiguous $p_x \times p_y$ pooling blocks

- $z_{i,j}^{n,k,1} \in \{0,1\}^{p_x p_y}$ be a vector of $p_x p_y - 1$ zeros and a single one.

The Stochastic Unpooling

$S^{n,k_l,l}$ is partitioned into contiguous $p_x \times p_y$ pooling blocks

- $z_{i,j}^{n,k,1} \in \{0,1\}^{p_x p_y}$ be a vector of $p_x p_y - 1$ zeros and a single one.

$z_{i,j}^{n,k,1}$ corresponds to pooling bloock (i,j) in $S^{n,k_1,1}$

- The location of the non-zero element of $z_{i,j}^{n,k,1}$ identifies the location of the single non-zero element in the corresponding pooling block of $S^{n,k_1,1}$.

Therefore

The non-zero element in pooling block (i, j)

- $S^{n,k_1,1}$ is set to $\widetilde{S}_{i,j}^{n,k_1,2}$

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- $S^{n,k_1,1}$ is set to $\widetilde{S}_{i,j}^{n,k_1,2}$

Thus, we have the following multinomial for the unpooling

$$z_{i,j}^{n,k_1,1} \sim \text{Mult}\left(1; \frac{1}{p_x p_y}, ..., \frac{1}{p_x p_y}\right)$$

Finally, the Encoder

Something Notable

Code Entry $\Downarrow$

$$Layer\ 1{:}\widetilde{C}^{n,k_1,1} = X_l *_s F^{k_1,1} \tag{5}$$

$$Pool\ {:}C^{n,1} \sim pool \tag{6}$$

$$Layer\ 2{:}\widetilde{C}^{n,k_2,2} = C^{n,1} *_s F^{k_2,2} \tag{7}$$

$$\text{Data Generation:} s_n \sim N\left(\mu_0 \widetilde{C}^{n,2}, diag\left(\sigma_\phi\left[\widetilde{C}^{n,2}\right]\right)\right) \tag{8}$$

This was trained in a semisupervised way

By using a loss function

$$\mathcal{L}_{\phi,\alpha,\psi}(X,Y) = \xi\left\{E_{q_\phi(s|X)}\left[\log p_\psi(Y|s)\right]\right\} + \underbrace{E_{q_\phi(s,z|X)}\left[\log p_\alpha(X,s,z) - \log q_\phi(s,z|X)\right]}_{\mathcal{U}_{\phi,\alpha}(X)}$$

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$$\begin{aligned}\mathcal{L}_{\phi,\alpha,\psi}(X,Y) =& \xi\left\{E_{q_\phi(s|X)}\left[\log p_\psi(Y|s)\right]\right\} \\ &+ \underbrace{E_{q_\phi(s,z|X)}\left[\log p_\alpha(X,s,z) - \log q_\phi(s,z|X)\right]}_{\mathcal{U}_{\phi,\alpha}(X)}\end{aligned}$$

The lower bound for the entire dataset is then

$$\mathcal{J}_{\phi,\alpha,\psi} = \sum_{(X,Y)\in\mathcal{D}_c} \mathcal{L}_{\phi,\alpha,\psi}(X,Y) + \sum_{X\in\mathcal{D}_u} \mathcal{U}_{\phi,\alpha}(X)$$

Benchmark for Classic

We have

Table 1: Classification error (%) and testing time (ms per image) on benchmarks.

Method	MNIST		CIFAR-10		CIFAR-100		Caltech 101		Caltech 256	
	test error	test time	test error	test time	test error	test time	test error	test time	test error	test time
Gibbs [8]	0.37	3.1	8.21	10.4	34.33	10.4	12.87	50.4	29.50	52.3
MCEM [8]	0.45	0.8	9.04	1.1	35.92	1.1	13.51	8.8	30.13	8.9
VAE-d	0.42	**0.007**	10.74	**0.02**	37.96	**0.02**	14.79	**0.3**	32.18	**0.3**
VAE (Ours)	0.38	**0.007**	8.19	**0.02**	35.01	**0.02**	11.99	**0.3**	29.33	**0.3**

Method	ImageNet 2012			ImageNet Pretrained for			
	top-1 error	top-5 error	test time	Caltech 101		Caltech 256	
				test error	test time	test error	test time
MCEM [8]	37.9	16.1	14.4	6.85	14.1	22.10	14.2
VAE (Ours)	38.2	15.7	**1.0**	6.91	**0.9**	22.53	**0.9**

Other examples

We have a long list

- Autoencoders for classification
- Autoencoders for clustering
- Autoencoders for anomaly detection
- Autoencoders for recommendation systems


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