Deep learning

7.2. Autoencoders

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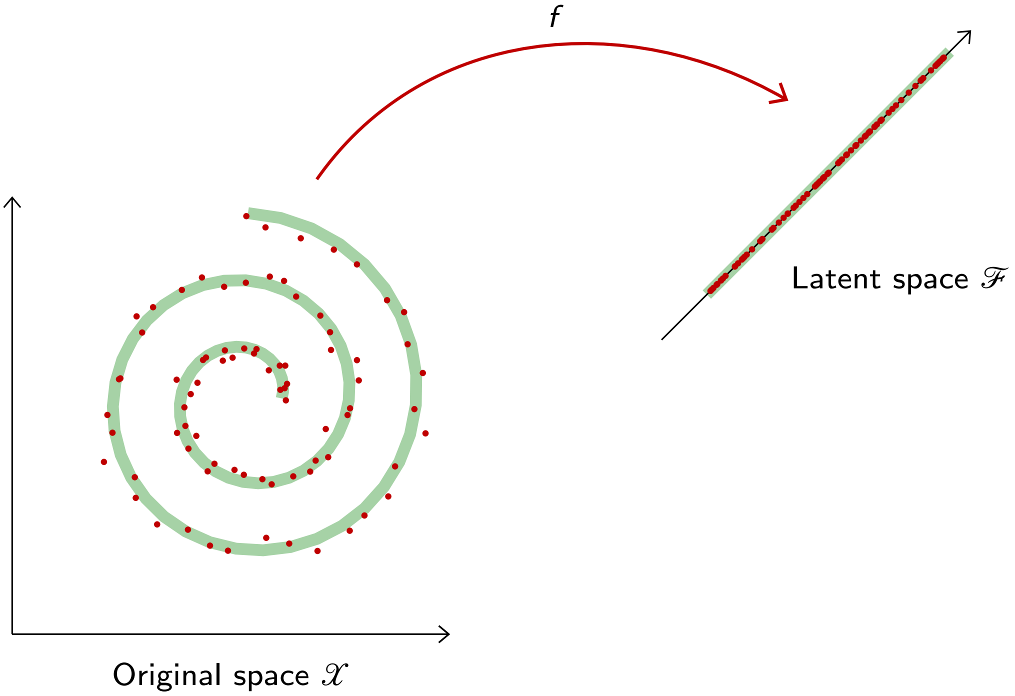
Many applications such as image synthesis, denoising, super-resolution, speech synthesis, compression, etc. require to go beyond classification and regression, and model explicitly a high dimension signal.

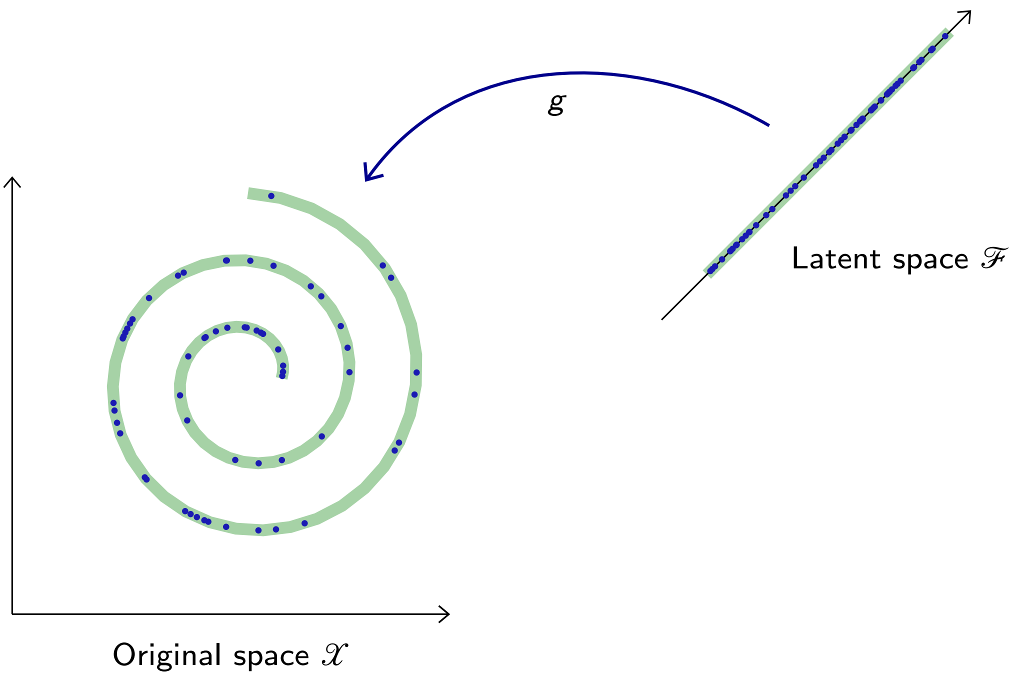
This modeling consists of finding “meaningful degrees of freedom” that describe the signal, and are of lesser dimension.



Notes

We consider this dataset of 2d points in the plan. The ultimate goal is to generate new points following the same distribution. These points are obviously lying on a 1d manifold (the green spiral), that is, there exists a mapping f which projects the points into to a so-called latent 1d space $\mathscr{F}$.

A way of generating new points would be to generate points in the latent space, and to then map them back to the original space with another mapping.



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When dealing with real-world signals, this objective involves the same theoretical and practical issues as for classification or regression: defining the right class of high-dimension models, and optimizing them.

Regarding synthesis, we saw that deep feed-forward architectures exhibit good generative properties, which motivates their use explicitly for that purpose.

Notes

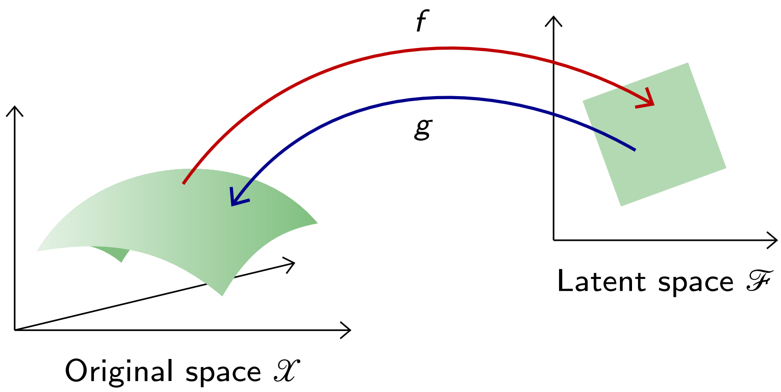
If we are given images of human faces, and we want to generate new ones, it makes sense to try to capture a small number of degrees of freedom such as morphological aspects (shape of the skull, color of the eyes, length of the nose, *etc.*) or geometrical dimensions (orientation in the image plan, illumination). Even though there may be many of them, there are definitely less than the resolution of the image.

It is reasonable to think that a proper way of synthesizing a human face would be to model a hundred dimensions, so that given those hundred dimensions, one would be able to generate one million pixels.

Autoencoders

An autoencoder maps a space to itself and is [close to] the identity on the data.

Dimension reduction can be achieved with an autoencoder composed of an **encoder** f from the original space $\mathscr{X}$ to a **latent** space $\mathscr{F}$, and a **decoder** g to map back to $\mathscr{X}$ (Bourlard and Kamp, 1988; Hinton and Zemel, 1994).



If the latent space is of lower dimension, the autoencoder has to capture a "good" parametrization, and in particular dependencies between components.

Notes

The original space $\mathscr{X}$ is of high dimension but the data (in green) lies on a manifold of much smaller dimension.

The encoder f maps the data to the latent space, which is of the dimension "guessed" by the human for the task. and the decoder g maps the data back to the original space.

Let q be the data distribution over $\mathscr{X}$. A good autoencoder could be characterized with the quadratic loss

$$\mathbb{E}_{X \sim q}\left[\|X - g \circ f(X)\|^2\right] \simeq 0.$$

Given two parametrized mappings $f(\cdot\,; w_f)$ and $g(\cdot\,; w_g)$, training consists of minimizing an empirical estimate of that loss

$$\hat{w}_f, \hat{w}_g = \underset{w_f, w_g}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \|x_n - g(f(x_n; w_f); w_g)\|^2 .$$

A simple example of such an autoencoder would be with both f and g linear, in which case the optimal solution is given by PCA. Better results can be achieved with more sophisticated classes of mappings, in particular deep architectures.

Notes

Given $x \in \mathscr{X}$, $f(x)$ is the projection in the latent space, and $g(f(x))$ is its reconstruction back to $\mathscr{X}$.

We can say that (f, g) is a good autoencoder when the expectation of the quadratic error between the original sample and its reconstructed version is small. This means that $g \circ f$ behaves live the identity on the original dataset.

Deep Autoencoders

A deep autoencoder combines an encoder composed of convolutional layers, with a decoder composed of transposed convolutions or other interpolating layers. *E.g.* for MNIST:

```
AutoEncoder (
  (encoder): Sequential (
    (0): Conv2d(1, 32, kernel_size=(5, 5), stride=(1, 1))
    (1): ReLU (inplace)
    (2): Conv2d(32, 32, kernel_size=(5, 5), stride=(1, 1))
    (3): ReLU (inplace)
    (4): Conv2d(32, 32, kernel_size=(4, 4), stride=(2, 2))
    (5): ReLU (inplace)
    (6): Conv2d(32, 32, kernel_size=(3, 3), stride=(2, 2))
    (7): ReLU (inplace)
    (8): Conv2d(32, 8, kernel_size=(4, 4), stride=(1, 1))
  )
  (decoder): Sequential (
    (0): ConvTranspose2d(8, 32, kernel_size=(4, 4), stride=(1, 1))
    (1): ReLU (inplace)
    (2): ConvTranspose2d(32, 32, kernel_size=(3, 3), stride=(2, 2))
    (3): ReLU (inplace)
    (4): ConvTranspose2d(32, 32, kernel_size=(4, 4), stride=(2, 2))
    (5): ReLU (inplace)
    (6): ConvTranspose2d(32, 32, kernel_size=(5, 5), stride=(1, 1))
    (7): ReLU (inplace)
    (8): ConvTranspose2d(32, 1, kernel_size=(5, 5), stride=(1, 1))
  )
)
```


Notes

A deep autoencoder is an autoencoder in which both the encoder and the decoder are deep models.

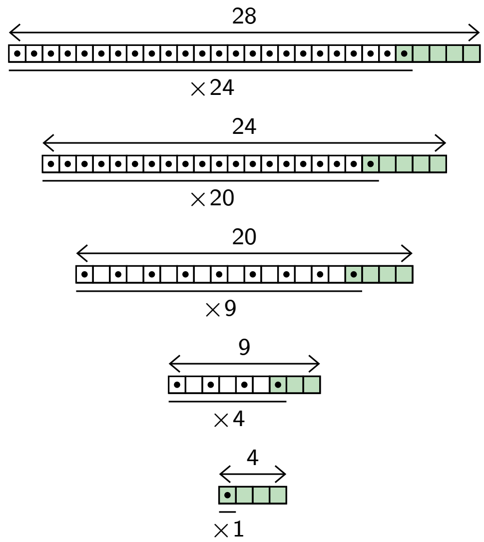
In this example, the latent space is of eight dimensions: at the end of the encoder, the output tensor is of size $8 \times 1 \times 1$.

The dimension reduction in the encoder is achieved with a stride of 2 in the convolutional layers.

The decoder performs the computation in the reserve order, each layer having its counterpart in the encoder.

Encoder

Tensor sizes / operations
$1 \times 28 \times 28$
`nn.Conv2d(1, 32, kernel_size=5, stride=1)`
$32 \times 24 \times 24$
`nn.Conv2d(32, 32, kernel_size=5, stride=1)`
$32 \times 20 \times 20$
`nn.Conv2d(32, 32, kernel_size=4, stride=2)`
$32 \times 9 \times 9$
`nn.Conv2d(32, 32, kernel_size=3, stride=2)`
$32 \times 4 \times 4$
`nn.Conv2d(32, 8, kernel_size=4, stride=1)`
$8 \times 1 \times 1$



Notes

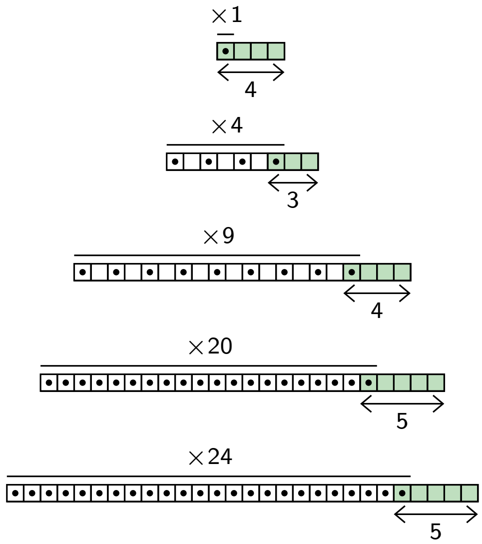
The table shows the successive size of the signal as it is processed by the encoder.

- The grid represents the dimension of the **input** tensor in the current layer, and accounts for both the height and the width, as images are squares;
- the dots • represent the locations where the filter is applied;
- the highlighted locations in green show the last locations where the filter could be applied, and show why the dimension is reduced.
- The double arrows above each grid is the dimension of the input tensor in the layer, while the number below the grid (preceded by $\times$) is the number of times the filter could be moved to perform the convolution.

In the end, the encoder processes a $1 \times 28 \times 28$ into a signal of size $8 \times 1 \times 1$.

Decoder

Tensor sizes / operations
$8 \times 1 \times 1$
`nn.ConvTranspose2d(8, 32, kernel_size=4, stride=1)`
$32 \times 4 \times 4$
`nn.ConvTranspose2d(32, 32, kernel_size=3, stride=2)`
$32 \times 9 \times 9$
`nn.ConvTranspose2d(32, 32, kernel_size=4, stride=2)`
$32 \times 20 \times 20$
`nn.ConvTranspose2d(32, 32, kernel_size=5, stride=1)`
$32 \times 24 \times 24$
`nn.ConvTranspose2d(32, 1, kernel_size=5, stride=1)`
$1 \times 28 \times 28$



Notes

The structure of the decoder is exactly the dual of the encoder.

- The grid represents the dimension of the **output** tensor in the current layer, and accounts for both the height and the width, as images are squares;
- the dots • represent the locations where the filter is applied;
- the highlighted locations in green show the last locations where the filter could be applied, and show why the dimension is increased.
- the number above the grid (preceded by ×) is the number of times the filter could be moved to perform the transposed convolution, while the double arrow below each grid is the resulted dimension of the output tensor.

Training is achieved with quadratic loss and Adam

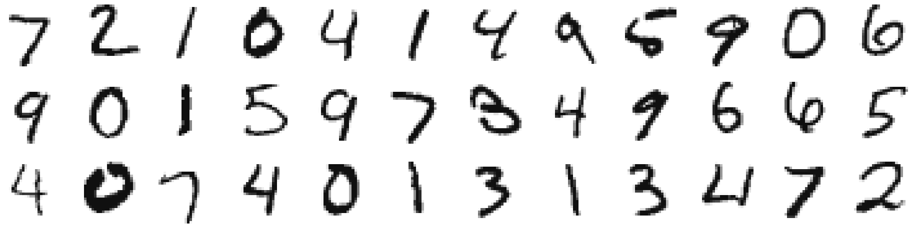
```
model = AutoEncoder(nb_channels, embedding_dim)

optimizer = optim.Adam(model.parameters(), lr = 1e-3)

for epoch in range(args.nb_epochs):
    for input in train_input.split(batch_size):
        z = model.encode(input)
        output = model.decode(z)
        loss = 0.5 * (output - input).pow(2).sum() / input.size(0)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```


Notes

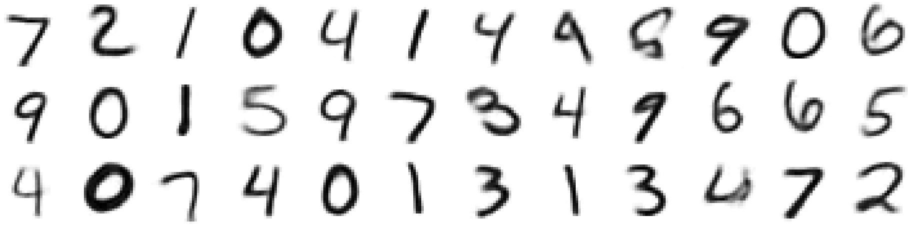
`embedding_dim` is the number of channels at the end of the encoder (8 in the previous slides).

Note that during training, the labels of the samples are not used. The goal is to model the density of the distribution of the data (unsupervised training).

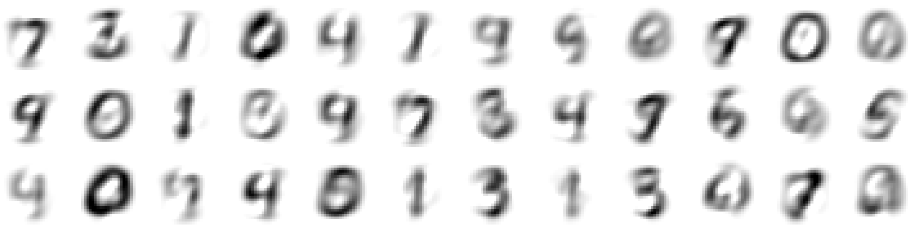
X (original samples)



$g \circ f(X)$ (CNN, $d = 8$)



$g \circ f(X)$ (PCA, $d = 8$)



Notes

The top images are some examples of original MNIST images.

The middle images are the outputs of the corresponding original images as reconstructed when they go thought the encoder and decoder.

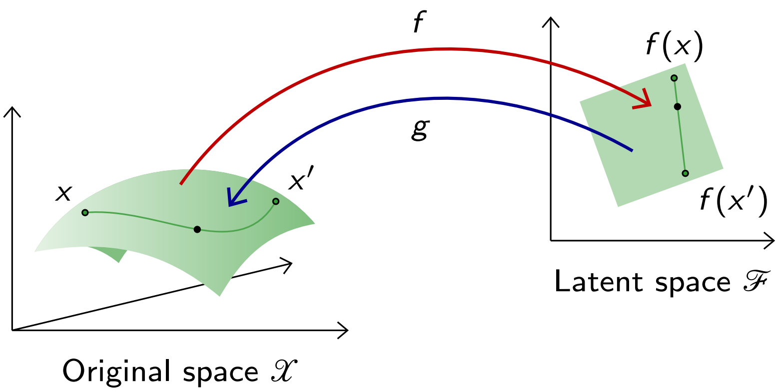
As a comparison, we show the projection with PCA, by equalizing the dimension of the latent space.

As expected, when the written digit is very unusual (bent "nine", half-made digit, rotated digit) the reconstructed image is wrong. Some statistically unusual details such as holes in the lines are not reconstructed. Such details can be reconstructed with a latent space of 32 for instance.

This experiment shows that the MNIST dataset can be reduced to a 32d dimension space and be reconstructed very well.

To get an intuition of the latent representation, we can pick two samples x and x' at random and interpolate samples along the line in the latent space

$$\forall x, x' \in \mathscr{X}^2,\ \alpha \in [0,1],\quad \xi(x, x', \alpha) = g((1-\alpha)f(x) + \alpha f(x')).$$



Notes

Moving on a line in the latent space between $f(x)$ and $f(x')$ can be done with a convex combination of $f(x)$ and $f(x')$:

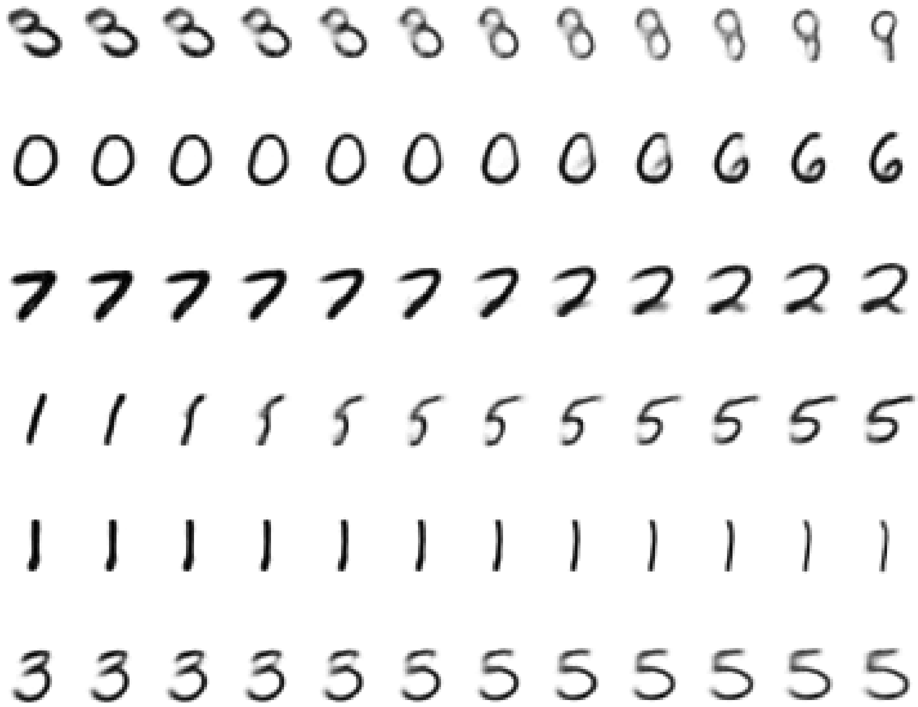
$$(1-\alpha)f(x) + \alpha f(x')$$

where $\alpha \in [0, 1]$:

- when $\alpha = 0$, we are at $f(x)$,
- when $\alpha = 1$, we are at $f(x')$,
- when $\alpha \in]0, 1[$, we are between $f(x)$ and $f(x')$.

PCA interpolation ($d = 32$)

Autoencoder interpolation ($d = 8$)

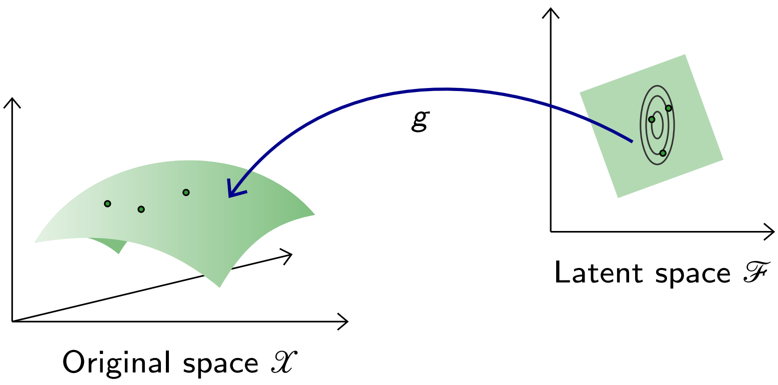


And we can assess the generative capabilities of the decoder g by introducing a [simple] density model q^Z over the latent space $\mathscr{F}$, sample there, and map the samples into the image space $\mathscr{X}$ with g.

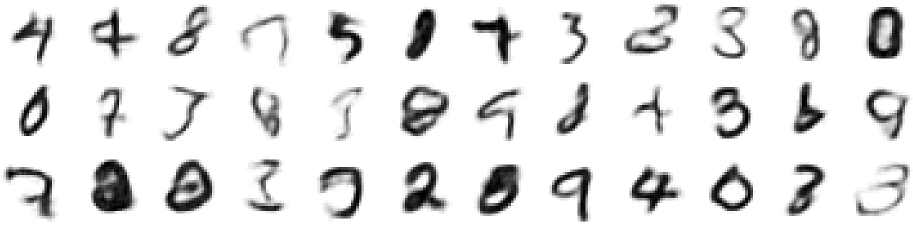
We can for instance use a Gaussian model with diagonal covariance matrix.

$$f(X) \sim \mathscr{N}(\hat{m}, \hat{\Delta})$$

where $\hat{m}$ is a vector and $\hat{\Delta}$ a diagonal matrix, both estimated on training data.



Autoencoder sampling ($d = 8$)



Autoencoder sampling ($d = 16$)

Autoencoder sampling ($d = 32$)

These results are unsatisfying, because the density model used on the latent space $\mathscr{F}$ is too simple and inadequate.

Building a "good" model amounts to our original problem of modeling an empirical distribution, although it may now be in a lower dimension space.

References

H. Bourlard and Y. Kamp. **Auto-association by multilayer perceptrons and singular value decomposition**. Biological Cybernetics, 59(4):291–294, 1988.

G. E. Hinton and R. S. Zemel. **Autoencoders, minimum description length and helmholtz free energy**. In Neural Information Processing Systems (NIPS), pages 3–10, 1994.