Advanced machine learning and data analysis for the physical sciences

Morten Hjorth-Jensen

Department of Physics and Center for Computing in Science Education, University of Oslo, Norway

March 27

Plans for the week March 24-28

1. Finalizing discussion on autoencoders and implementing Autoencoders with TensorFlow/Keras and PyTorch
2. Overview of generative models
3. Probability distributions and Markov Chain Monte Carlo simulations
4. Boltzmann machines and energy models
5. Reading recommendation: Goodfellow et al chapters 16 and 18.1 and 18.2. Chapter 17 gives a background to Monte Carlo Markov Chains.

Autoencoders: code examples

These examples here are based the codes from A. Geron's textbook. They can be easily modified and adapted to different data sets. The first example is a straightforward AE.

```python
import sys
assert sys.version_info >= (3, 5)

# Is this notebook running on Colab or Kaggle?
IS_COLAB = "google.colab" in sys.modules
IS_KAGGLE = "kaggle_secrets" in sys.modules

# Scikit-Learn >=0.20 is required
import sklearn
assert sklearn.__version__ >= "0.20"

# TensorFlow >= 2.0 is required
```

```python
import tensorflow as tf
from tensorflow import keras
assert tf.__version__ >= "2.0"

if not tf.config.list_physical_devices('GPU'):
    print("No GPU was detected. LSTMs and CNNs can be very slow without a GPU.")
    if IS_COLAB:
        print("Go to Runtime > Change runtime and select a GPU hardware accelerator.")
    if IS_KAGGLE:
        print("Go to Settings > Accelerator and select GPU.")

# Common imports
import numpy as np
import os

# to make this notebook's output stable across runs
np.random.seed(42)
tf.random.set_seed(42)

# To plot pretty figures
import matplotlib as mpl
import matplotlib.pyplot as plt
mpl.rc('axes', labelsize=14)
mpl.rc('xtick', labelsize=12)
mpl.rc('ytick', labelsize=12)

# Where to save the figures
PROJECT_ROOT_DIR = "."
CHAPTER_ID = "autoencoders"
IMAGES_PATH = os.path.join(PROJECT_ROOT_DIR, "images", CHAPTER_ID)
os.makedirs(IMAGES_PATH, exist_ok=True)

def save_fig(fig_id, tight_layout=True, fig_extension="png", resolution=300):
    path = os.path.join(IMAGES_PATH, fig_id + "." + fig_extension)
    print("Saving figure", fig_id)
    if tight_layout:
        plt.tight_layout()
    plt.savefig(path, format=fig_extension, dpi=resolution)

def plot_image(image):
    plt.imshow(image, cmap="binary")
    plt.axis("off")


np.random.seed(4)

def generate_3d_data(m, w1=0.1, w2=0.3, noise=0.1):
    angles = np.random.rand(m) * 3 * np.pi / 2 - 0.5
    data = np.empty((m, 3))
    data[:, 0] = np.cos(angles) + np.sin(angles)/2 + noise * np.random.randn(m) / 2
    data[:, 1] = np.sin(angles) * 0.7 + noise * np.random.randn(m) / 2
    data[:, 2] = data[:, 0] * w1 + data[:, 1] * w2 + noise * np.random.randn(m)
    return data

X_train = generate_3d_data(60)
X_train = X_train - X_train.mean(axis=0, keepdims=0)


np.random.seed(42)
tf.random.set_seed(42)
```

```
encoder = keras.models.Sequential([keras.layers.Dense(2, input_shape=[3])])
decoder = keras.models.Sequential([keras.layers.Dense(3, input_shape=[2])])
autoencoder = keras.models.Sequential([encoder, decoder])

autoencoder.compile(loss="mse", optimizer=keras.optimizers.SGD(learning_rate=1.5))

codings = encoder.predict(X_train)
fig = plt.figure(figsize=(4,3))
plt.plot(codings[:,0], codings[:, 1], "b.")
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18, rotation=0)
plt.grid(True)
save_fig("linear_autoencoder_pca_plot")
plt.show()
```

More advanced features, stacked AEs

```
# You can select the so-called fashion data as well, here we just use the MNIST standard set
#(X_train_full, y_train_full), (X_test, y_test) = keras.datasets.fashion_mnist.load_data()
(X_train_full, y_train_full), (X_test, y_test) = keras.datasets.mnist.load_data()
X_train_full = X_train_full.astype(np.float32) / 255
X_test = X_test.astype(np.float32) / 255
X_train, X_valid = X_train_full[:-5000], X_train_full[-5000:]
y_train, y_valid = y_train_full[:-5000], y_train_full[-5000:]
```

We can now train all layers at once by building a stacked AE with 3 hidden layers and 1 output layer (i.e., 2 stacked Autoencoders).

```
def rounded_accuracy(y_true, y_pred):
    return keras.metrics.binary_accuracy(tf.round(y_true), tf.round(y_pred))
tf.random.set_seed(42)
np.random.seed(42)

stacked_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(30, activation="selu"),
])
stacked_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
stacked_ae = keras.models.Sequential([stacked_encoder, stacked_decoder])
stacked_ae.compile(loss="binary_crossentropy",
                   optimizer=keras.optimizers.SGD(learning_rate=1.5), metrics=[rounded_accuracy])
history = stacked_ae.fit(X_train, X_train, epochs=20,
                         validation_data=(X_valid, X_valid))
```

This function processes a few test images through the autoencoder and displays the original images and their reconstructions.

```
def show_reconstructions(model, images=X_valid, n_images=5):
    reconstructions = model.predict(images[:n_images])
    fig = plt.figure(figsize=(n_images * 1.5, 3))
    for image_index in range(n_images):
        plt.subplot(2, n_images, 1 + image_index)
        plot_image(images[image_index])
        plt.subplot(2, n_images, 1 + n_images + image_index)
        plot_image(reconstructions[image_index])
show_reconstructions(stacked_ae)
save_fig("reconstruction_plot")
```

Then visualize

```
np.random.seed(42)
from sklearn.manifold import TSNE
X_valid_compressed = stacked_encoder.predict(X_valid)
tsne = TSNE()
X_valid_2D = tsne.fit_transform(X_valid_compressed)
X_valid_2D = (X_valid_2D - X_valid_2D.min()) / (X_valid_2D.max() - X_valid_2D.min())
plt.scatter(X_valid_2D[:, 0], X_valid_2D[:, 1], c=y_valid, s=10, cmap="tab10")
plt.axis("off")
plt.show()
```

And visualize in a nicer way

```
# adapted from https://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html
plt.figure(figsize=(10, 8))
cmap = plt.cm.tab10
plt.scatter(X_valid_2D[:, 0], X_valid_2D[:, 1], c=y_valid, s=10, cmap=cmap)
image_positions = np.array([[1., 1.]])
for index, position in enumerate(X_valid_2D):
    dist = np.sum((position - image_positions) ** 2, axis=1)
    if np.min(dist) > 0.02: # if far enough from other images
        image_positions = np.r_[image_positions, [position]]
        imagebox = mpl.offsetbox.AnnotationBbox(
            mpl.offsetbox.OffsetImage(X_valid[index], cmap="binary"),
            position, bboxprops={"edgecolor": cmap(y_valid[index]), "lw": 2})
        plt.gca().add_artist(imagebox)
plt.axis("off")
save_fig("fashion_mnist_visualization_plot")
plt.show()
```

Using Convolutional Layers Instead of Dense Layers

```
tf.random.set_seed(42)
np.random.seed(42)

conv_encoder = keras.models.Sequential([
    keras.layers.Reshape([28, 28, 1], input_shape=[28, 28]),
    keras.layers.Conv2D(16, kernel_size=3, padding="SAME", activation="selu"),
    keras.layers.MaxPool2D(pool_size=2),
    keras.layers.Conv2D(32, kernel_size=3, padding="SAME", activation="selu"),
    keras.layers.MaxPool2D(pool_size=2),
    keras.layers.Conv2D(64, kernel_size=3, padding="SAME", activation="selu"),
    keras.layers.MaxPool2D(pool_size=2)
])
conv_decoder = keras.models.Sequential([
    keras.layers.Conv2DTranspose(32, kernel_size=3, strides=2, padding="VALID", activation="selu"
                                 input_shape=[3, 3, 64]),
    keras.layers.Conv2DTranspose(16, kernel_size=3, strides=2, padding="SAME", activation="selu"),
    keras.layers.Conv2DTranspose(1, kernel_size=3, strides=2, padding="SAME", activation="sigmoid"
    keras.layers.Reshape([28, 28])
])
conv_ae = keras.models.Sequential([conv_encoder, conv_decoder])

conv_ae.compile(loss="binary_crossentropy", optimizer=keras.optimizers.SGD(learning_rate=1.0),
                metrics=[rounded_accuracy])
history = conv_ae.fit(X_train, X_train, epochs=5,
                      validation_data=(X_valid, X_valid))
```

```
conv_encoder.summary()
conv_decoder.summary()
```

```
show_reconstructions(conv_ae)
plt.show()
```

Recurrent Autoencoders

```
recurrent_encoder = keras.models.Sequential([
    keras.layers.LSTM(100, return_sequences=True, input_shape=[28, 28]),
    keras.layers.LSTM(30)
])
recurrent_decoder = keras.models.Sequential([
    keras.layers.RepeatVector(28, input_shape=[30]),
    keras.layers.LSTM(100, return_sequences=True),
    keras.layers.TimeDistributed(keras.layers.Dense(28, activation="sigmoid"))
])
recurrent_ae = keras.models.Sequential([recurrent_encoder, recurrent_decoder])
recurrent_ae.compile(loss="binary_crossentropy", optimizer=keras.optimizers.SGD(0.1),
                     metrics=[rounded_accuracy])
history = recurrent_ae.fit(X_train, X_train, epochs=10, validation_data=(X_valid, X_valid))
```

```
show_reconstructions(recurrent_ae)
plt.show()
```

Stacked denoising Autoencoder with Gaussian noise

```
tf.random.set_seed(42)
np.random.seed(42)

denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.GaussianNoise(0.2),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(30, activation="selu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
denoising_ae = keras.models.Sequential([denoising_encoder, denoising_decoder])
```

```
denoising_ae.compile(loss="binary_crossentropy", optimizer=keras.optimizers.SGD(learning_rate=1.0)
                     metrics=[rounded_accuracy])
history = denoising_ae.fit(X_train, X_train, epochs=10,
                           validation_data=(X_valid, X_valid))
```

```
tf.random.set_seed(42)
np.random.seed(42)

noise = keras.layers.GaussianNoise(0.2)
show_reconstructions(denoising_ae, noise(X_valid, training=True))
plt.show()
```

And using dropout

```
tf.random.set_seed(42)
np.random.seed(42)

dropout_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(30, activation="selu")
])
dropout_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
dropout_ae = keras.models.Sequential([dropout_encoder, dropout_decoder])
dropout_ae.compile(loss="binary_crossentropy", optimizer=keras.optimizers.SGD(learning_rate=1.0),
                   metrics=[rounded_accuracy])
history = dropout_ae.fit(X_train, X_train, epochs=10,
                         validation_data=(X_valid, X_valid))
```

```
tf.random.set_seed(42)
np.random.seed(42)

dropout = keras.layers.Dropout(0.5)
show_reconstructions(dropout_ae, dropout(X_valid, training=True))
save_fig("dropout_denoising_plot", tight_layout=False)
```

PyTorch example

We will continue with the MNIST database, which has 60000 training examples and a test set of 10000 handwritten numbers. The images have only one color channel and have a size of 28×28 pixels. We start by uploading the data set.

```
# import the Torch packages
# transforms are used to preprocess the images, e.g. crop, rotate, normalize, etc
import torch
from torchvision import datasets,transforms

# specify the data path in which you would like to store the downloaded files
# ToTensor() here is used to convert data type to tensor
```

```
train_dataset = datasets.MNIST(root='./mnist_data/', train=True, transform=transforms.ToTensor(),
test_dataset = datasets.MNIST(root='./mnist_data/', train=False, transform=transforms.ToTensor(),
print(train_dataset)
batchSize=128

#only after packed in DataLoader, can we feed the data into the neural network iteratively
train_loader = torch.utils.data.DataLoader(dataset=train_dataset, batch_size=batchSize, shuffle=Tr
test_loader = torch.utils.data.DataLoader(dataset=test_dataset, batch_size=batchSize, shuffle=Fals
```

We visualize the images here using the *imshow* function function and the *make_grid* function from PyTorch to arrange and display them.

```
# package we used to manipulate matrix
import numpy as np
# package we used for image processing
from matplotlib import pyplot as plt
from torchvision.utils import make_grid

def imshow(img):
    npimg = img.numpy()
    #transpose: change array axis to correspond to the plt.imshow() function
    plt.imshow(np.transpose(npimg, (1, 2, 0)))
    plt.show()

# load the first 16 training samples from next iteration
# [:16,:,:,:] for the 4 dimension of examples, first dimension take first 16, other dimension tak
# arrange the image in grid
examples, _ = next(iter(train_loader))
example_show=make_grid(examples[:16,:,:,:], 4)

# then display them
imshow(example_show)
```

Our autoencoder consists of two parts, see also the TensorFlow example above. The encoder and decoder parts are represented by two fully connected feed forward neural networks where we use the standard Sigmoid function. In the encoder part we reduce the dimensionality of the image from $28 \times 28 = 784$ pixels to first $16 \times 16 = 256$ pixels and then to 128 pixels. The 128 pixel representation is then used to define the representation of the input and the input to the decoder part. The latter attempts to reconstruct the images.

```
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

# Network Parameters
num_hidden_1 = 256  # 1st layer num features
num_hidden_2 = 128  # 2nd layer num features (the latent dim)
num_input = 784  # MNIST data input (img shape: 28*28)


# Building the encoder
class Autoencoder(nn.Module):
    def __init__(self, x_dim, h_dim1, h_dim2):
        super(Autoencoder, self).__init__()
        # encoder part
        self.fc1 = nn.Linear(x_dim, h_dim1)
        self.fc2 = nn.Linear(h_dim1, h_dim2)
        # decoder part
        self.fc3 = nn.Linear(h_dim2, h_dim1)
        self.fc4 = nn.Linear(h_dim1, x_dim)

    def encoder(self, x):
        x = torch.sigmoid(self.fc1(x))
        x = torch.sigmoid(self.fc2(x))
        return x

    def decoder(self, x):
        x = torch.sigmoid(self.fc3(x))
        x = torch.sigmoid(self.fc4(x))
        return x

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x

# When initializing, it will run __init__() function as above
model = Autoencoder(num_input, num_hidden_1, num_hidden_2)
```

We define here the cost/loss function and the optimizer we employ (Adam here).

```
# define loss function and parameters
optimizer = optim.Adam(model.parameters())
epoch = 100
# MSE loss will calculate Mean Squared Error between the inputs
loss_function = nn.MSELoss()

print('====Training start====')
for i in range(epoch):
    train_loss = 0
    for batch_idx, (data, _) in enumerate(train_loader):
        # prepare input data
        inputs = torch.reshape(data,(-1, 784)) # -1 can be any value.
        # set gradient to zero
        optimizer.zero_grad()
        # feed inputs into model
        recon_x = model(inputs)
        # calculating loss
        loss = loss_function(recon_x, inputs)
        # calculate gradient of each parameter
        loss.backward()
        train_loss += loss.item()
        # update the weight based on the gradient calculated
        optimizer.step()
    if i%10==0:
        print('====> Epoch: {} Average loss: {:.9f}'.format(i, train_loss ))
print('====Training finish====')
```

As we have trained the network, we will now reconstruct various test samples to see if the model can generalize to data which were not included in the training set.

```
# load 16 images from testset
inputs, _ = next(iter(test_loader))
inputs_example = make_grid(inputs[:16,:,:,:],4)
imshow(inputs_example)

#convert from image to tensor
#inputs=inputs.cuda()
inputs=torch.reshape(inputs,(-1,784))

# get the outputs from the trained model
outputs=model(inputs)

#convert from tensor to image
outputs=torch.reshape(outputs,(-1,1,28,28))
outputs=outputs.detach().cpu()

#show the output images
outputs_example = make_grid(outputs[:16,:,:,:],4)
imshow(outputs_example)
```

After training the auto-encoder, we can now use the model to reconstruct some images. In order to reconstruct different training images, the model has learned to recognize how the image looks like and describe it in the 128-dimensional latent space. In other words, the visual information of images is compressed and encoded in the 128-dimensional representations. As we assume that samples from the same categories should be more visually similar than those from different classes, the representations can then be used for image recognition, i.e., handwritten digit images recognition in our case.

One simple way to recognize images is to randomly select ten training samples from each class and annotate them with the corresponding label. Then given the test data, we can predict which classes they belong to by finding the most similar labelled training samples to them.

```
# get 100 image-label pairs from training set
x_train, y_train = next(iter(train_loader))

# 10 classes, 10 samples per class, 100 in total
candidates = np.random.choice(batchSize, 10*10)

# randomly select 100 samples
x_train = x_train[candidates]
y_train = y_train[candidates]

# display the selected samples and print their labels

imshow(make_grid(x_train[:100,:,:,:],10))
print(y_train.reshape(10, 10))

# get 100 image-label pairs from test set
x_test, y_test = next(iter(train_loader))
candidates_test = np.random.choice(batchSize, 10*10)

x_test = x_test[candidates_test]
y_test = y_test[candidates_test]

# display the selected samples and print their labels
```

```
imshow(make_grid(x_test[:100,:,:,:],10))

print(y_test.reshape(10, 10))


# compute the representations of training and test samples
#h_train=model.encoder(torch.reshape(x_train.cuda(),(-1,784)))
#h_test=model.encoder(torch.reshape(x_test.cuda(),(-1,784)))
h_train=model.encoder(torch.reshape(x_train,(-1,784)))
h_test=model.encoder(torch.reshape(x_test,(-1,784)))

# find the nearest training samples to each test instance, in terms of MSE
MSEs = np.mean(np.power(np.expand_dims(h_test.detach().cpu(), axis=1) - np.expand_dims(h_train.det
neighbours = MSEs.argmin(axis=1)
predicts = y_train[neighbours]

# print(np.stack([y_test, predicts], axis=1))
print('Recognition accuracy according to the learned representation is %.1f%%' % (100 * (y_test ==
```

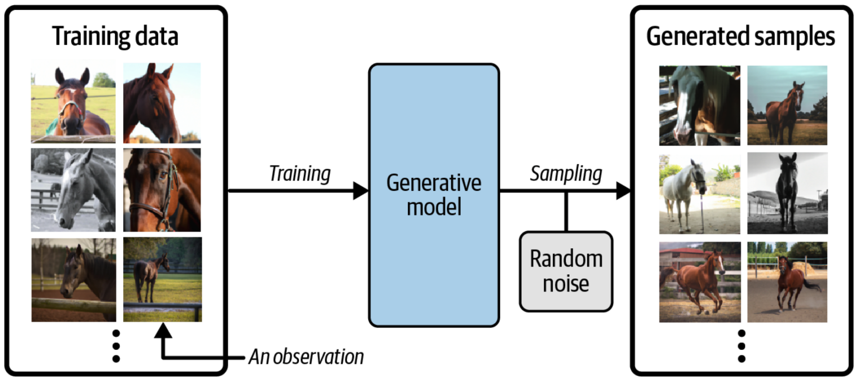
What Is Generative Modeling?

Generative modeling can be broadly defined as follows:

Generative modeling is a branch of machine learning that involves training a model to produce new data that is similar to a given dataset.

What does this mean in practice? Suppose we have a dataset containing photos of horses. We can train a generative model on this dataset to capture the rules that govern the complex relationships between pixels in images of horses. Then we can sample from this model to create novel, realistic images of horses that did not exist in the original dataset.

Example of generative modeling, taken from Generative Deeep Learning by David Foster



Generative Modeling

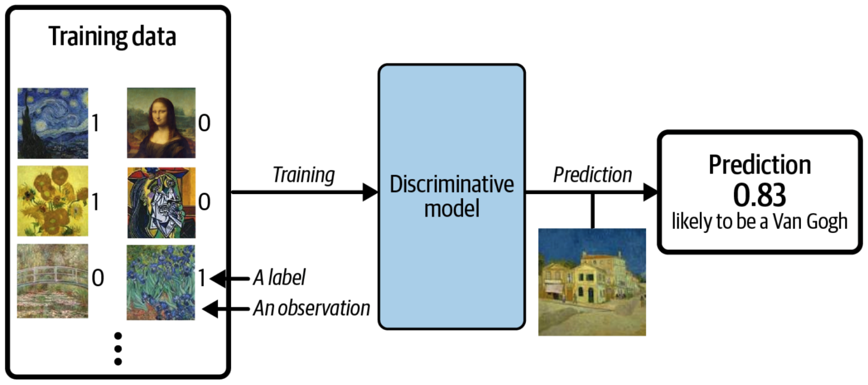
In order to build a generative model, we require a dataset consisting of many examples of the entity we are trying to generate. This is known as the training data, and one such data point is called an observation.

Each observation consists of many features. For an image generation problem, the features are usually the individual pixel values; for a text generation problem, the features could be individual words or groups of letters. It is our goal to build a model that can generate new sets of features that look as if they have been created using the same rules as the original data. Conceptually, for image generation this is an incredibly difficult task, considering the vast number of ways that individual pixel values can be assigned and the relatively tiny number of such arrangements that constitute an image of the entity we are trying to generate.

Generative Versus Discriminative Modeling

In order to truly understand what generative modeling aims to achieve and why this is important, it is useful to compare it to its counterpart, discriminative modeling. If you have studied machine learning, most problems you will have faced will have most likely been discriminative in nature.

Example of discriminative modeling, taken from Generative Deeep Learning by David Foster

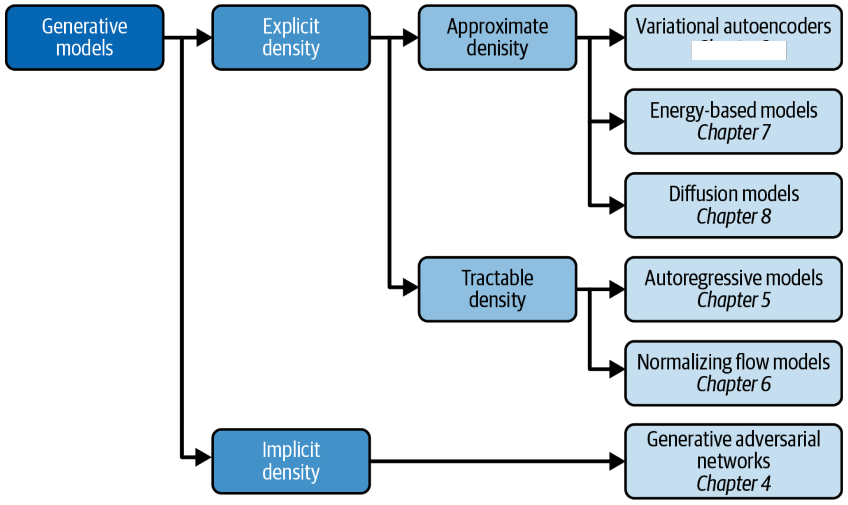


Discriminative Modeling

When performing discriminative modeling, each observation in the training data has a label. For a binary classification problem such as our data could be labeled as ones and zeros. Our model then learns how to discriminate between these two groups and outputs the probability that a new observation has label 1 or 0

In contrast, generative modeling doesn't require the dataset to be labeled because it concerns itself with generating entirely new data (for example an image), rather than trying to predict a label for say a given image.

Taxonomy of generative deep learning, taken from Generative Deep Learning by David Foster


Generative models
Explicit density
Approximate denisity
Variational autoencoders
Energy-based models Chapter 7
Diffusion models Chapter 8
Tractable density
Autoregressive models Chapter 5
Normalizing flow models Chapter 6
Implicit density
Generative adversarial networks Chapter 4

Statistics and Bayes' theorem

A central theorem in statistics is Bayes' theorem. This theorem plays a similar role as the good old Pythagoras' theorem in geometry. Bayes' theorem is extremely simple to derive. But to do so we need some basic axioms from statistics.

Assume we have two domains of events $X = [x_0, x_1, \dots, x_{n-1}]$ and $Y = [y_0, y_1, \dots, y_{n-1}]$.

We define also the likelihood for X and Y as $p(X)$ and $p(Y)$ respectively. The likelihood of a specific event x_i (or y_i) is then written as $p(X = x_i)$ or just $p(x_i) = p_i$.

Union of events is given by.

$$p(X \cup Y) = p(X) + p(Y) - p(X \cap Y).$$

The product rule (aka joint probability) is given by.

$$p(X \cup Y) = p(X, Y) = p(X|Y)p(Y) = p(Y|X)p(X),$$

where we read $p(X|Y)$ as the likelihood of obtaining X given Y.

If we have independent events then $p(X,Y) = p(X)p(Y)$.

Marginal Probability

The marginal probability is defined in terms of only one of the set of variables X, Y. For a discrete probability we have

$$p(X) = \sum_{i=0}^{n-1} p(X, Y = y_i) = \sum_{i=0}^{n-1} p(X|Y = y_i)p(Y = y_i) = \sum_{i=0}^{n-1} p(X|y_i)p(y_i).$$

Conditional Probability

The conditional probability, if $p(Y) > 0$, is

$$p(X|Y) = \frac{p(X,Y)}{p(Y)} = \frac{p(X,Y)}{\sum_{i=0}^{n-1} p(Y|X = x_i)p(x_i)}.$$

Bayes' Theorem

If we combine the conditional probability with the marginal probability and the standard product rule, we have

$$p(X|Y) = \frac{p(X,Y)}{p(Y)},$$

which we can rewrite as

$$p(X|Y) = \frac{p(X,Y)}{\sum_{i=0}^{n-1} p(Y|X = x_i)p(x_i)} = \frac{p(Y|X)p(X)}{\sum_{i=0}^{n-1} p(Y|X = x_i)p(x_i)},$$

which is Bayes' theorem. It allows us to evaluate the uncertainty in in X after we have observed Y. We can easily interchange X with Y.

Interpretations of Bayes' Theorem

The quantity $p(Y|X)$ on the right-hand side of the theorem is evaluated for the observed data Y and can be viewed as a function of the parameter space represented by X. This function is not necesseraly normalized and is normally called the likelihood function.

The function $p(X)$ on the right hand side is called the prior while the function on the left hand side is the called the posterior probability. The denominator on the right hand side serves as a normalization factor for the posterior distribution.

Let us try to illustrate Bayes' theorem through an example.

Example of Usage of Bayes' theorem

Let us suppose that you are undergoing a series of mammography scans in order to rule out possible breast cancer cases. We define the sensitivity for a positive event by the variable X. It takes binary values with $X = 1$ representing a positive event and $X = 0$ being a negative event. We reserve Y as a classification parameter for either a negative or a positive breast cancer confirmation. (Short note on wordings: positive here means having breast cancer, although none of us would consider this being a positive thing).

We let $Y = 1$ represent the the case of having breast cancer and $Y = 0$ as not.

Let us assume that if you have breast cancer, the test will be positive with a probability of 0.8, that is we have

$$p(X = 1|Y = 1) = 0.8.$$

This obviously sounds scary since many would conclude that if the test is positive, there is a likelihood of 80% for having cancer. It is however not correct, as the following Bayesian analysis shows.

Doing it correctly

If we look at various national surveys on breast cancer, the general likelihood of developing breast cancer is a very small number. Let us assume that the prior probability in the population as a whole is

$$p(Y = 1) = 0.004.$$

We need also to account for the fact that the test may produce a false positive result (false alarm). Let us here assume that we have

$$p(X = 1|Y = 0) = 0.1.$$

Using Bayes' theorem we can then find the posterior probability that the person has breast cancer in case of a positive test, that is we can compute

$$p(Y = 1|X = 1) = \frac{p(X = 1|Y = 1)p(Y = 1)}{p(X = 1|Y = 1)p(Y = 1) + p(X = 1|Y = 0)p(Y = 0)} = \frac{0.8 \times 0.004}{0.8 \times 0.004 + 0.1 \times 0.996} = 0.031.$$

That is, in case of a positive test, there is only a 3% chance of having breast cancer!

Maximum Likelihood Estimation (MLE)

We assume now that the various variables are stochastically distributed and **Independent and Identically Distrubuted** (iid).

In statistics, maximum likelihood estimation (MLE) is a method of estimating the parameters of an assumed probability distribution, given some observed data.

This is achieved by maximizing a likelihood function so that, under the assumed statistical model, the observed data is the most probable. The probability is then written in terms of the products of the individual probabilities.

However, computing the derivatives of a product function is cumbersome and can easily lead to overflow and/or underflowproblems, with potentials for loss of numerical precision.

In practice, it is more convenient to maximize the logarithm of the PDF because it is a monotonically increasing function of the argument. Alternatively, and this will be our option, we will minimize the negative of the logarithm since this is a monotonically decreasing function.

Note also that maximization/minimization of the logarithm of the PDF is equivalent to the maximization/minimization of the function itself.

Probability distributions and normalization constants

See whiteboard notes

Markov Chain Monte Carlo

See whiteboard notes

Boltzmann Machines

Why use a generative model rather than the more well known discriminative deep neural networks (DNN)?

- Discriminitave methods have several limitations: They are mainly supervised learning methods, thus requiring labeled data. And there are tasks they cannot accomplish, like drawing new examples from an unknown probability distribution.
- A generative model can learn to represent and sample from a probability distribution. The core idea is to learn a parametric model of the probability distribution from which the training data was drawn. As an example
    1. A model for images could learn to draw new examples of cats and dogs, given a training dataset of images of cats and dogs.
    2. Generate a sample of an ordered or disordered Ising model phase, having been given samples of such phases.
    3. Model the trial function for Monte Carlo calculations
- Both use gradient-descent based learning procedures for minimizing cost functions
- Energy based models don't use backpropagation and automatic differentiation for computing gradients, instead turning to Markov Chain Monte Carlo methods.

- DNNs often have several hidden layers. A restricted Boltzmann machine has only one hidden layer, however several RBMs can be stacked to make up Deep Belief Networks, of which they constitute the building blocks.

History: The RBM was developed by amongst others Geoffrey Hinton, called by some the "Godfather of Deep Learning", working with the University of Toronto and Google.

A BM is what we would call an undirected probabilistic graphical model with stochastic continuous or discrete units.

It is interpreted as a stochastic recurrent neural network where the state of each unit(neurons/nodes) depends on the units it is connected to. The weights in the network represent thus the strength of the interaction between various units/nodes.

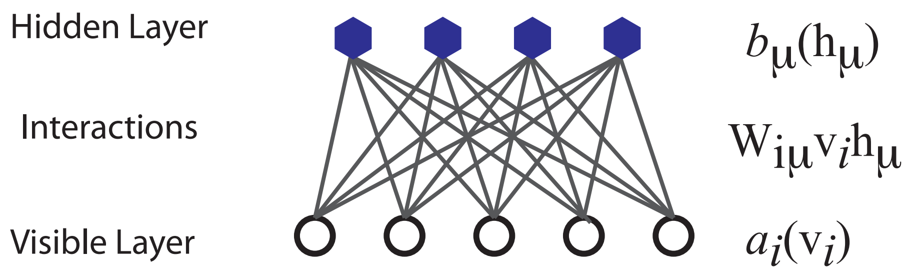
It turns into a Hopfield network if we choose deterministic rather than stochastic units. In contrast to a Hopfield network, a BM is a so-called generative model. It allows us to generate new samples from the learned distribution.

A standard BM network is divided into a set of observable and visible units $\hat{x}$ and a set of unknown hidden units/nodes $\hat{h}$.

Additionally there can be bias nodes for the hidden and visible layers. These biases are normally set to 1.

BMs are stackable, meaning they cwe can train a BM which serves as input to another BM. We can construct deep networks for learning complex PDFs. The layers can be trained one after another, a feature which makes them popular in deep learning

However, they are often hard to train. This leads to the introduction of so-called restricted BMs, or RBMS. Here we take away all lateral connections between nodes in the visible layer as well as connections between nodes in the hidden layer. The network is illustrated in the figure below.



The network

The network layers:

1. A function $\mathbf{x}$ that represents the visible layer, a vector of M elements (nodes). This layer represents both what the RBM might be given as training input, and what we want it to be able to reconstruct. This might for example be the pixels of an image, the spin values of the Ising model, or coefficients representing speech.

2. The function $\mathbf{h}$ represents the hidden, or latent, layer. A vector of N elements (nodes). Also called "feature detectors".

The goal of the hidden layer is to increase the model's expressive power. We encode complex interactions between visible variables by introducing additional, hidden variables that interact with visible degrees of freedom in a simple manner, yet still reproduce the complex correlations between visible degrees in the data once marginalized over (integrated out).

The network parameters, to be optimized/learned:

1. $\mathbf{a}$ represents the visible bias, a vector of same length as $\mathbf{x}$.

2. $\mathbf{b}$ represents the hidden bias, a vector of same lenght as $\mathbf{h}$.

3. W represents the interaction weights, a matrix of size $M \times N$.

Joint distribution

The restricted Boltzmann machine is described by a Boltzmann distribution

$$P_{rbm}(\mathbf{x},\mathbf{h}) = \frac{1}{Z} e^{-\frac{1}{T_0}E(\mathbf{x},\mathbf{h})}, \tag{1}$$

where Z is the normalization constant or partition function, defined as

$$Z = \int \int e^{-\frac{1}{T_0} E(\mathbf{x},\mathbf{h})} d\mathbf{x} d\mathbf{h}. \tag{2}$$

It is common to ignore T_0 by setting it to one.

Network Elements, the energy function

The function $E(\mathbf{x}, \mathbf{h})$ gives the **energy** of a configuration (pair of vectors) $(\mathbf{x}, \mathbf{h})$. The lower the energy of a configuration, the higher the probability of it. This function also depends on the parameters $\mathbf{a}$, $\mathbf{b}$ and W. Thus, when we adjust them during the learning procedure, we are adjusting the energy function to best fit our problem.

Defining different types of RBMs

There are different variants of RBMs, and the differences lie in the types of visible and hidden units we choose as well as in the implementation of the energy function $E(\mathbf{x}, \mathbf{h})$. The connection between the nodes in the two layers is given by the weights w_{ij}.

Binary-Binary RBM: RBMs were first developed using binary units in both the visible and hidden layer. The corresponding energy function is defined as follows:

$$E(\mathbf{x}, \mathbf{h}) = -\sum_i^M x_i a_i - \sum_j^N b_j h_j - \sum_{i,j}^{M,N} x_i w_{ij} h_j, \tag{3}$$

where the binary values taken on by the nodes are most commonly 0 and 1.

Gaussian-Binary RBM: Another varient is the RBM where the visible units are Gaussian while the hidden units remain binary:

$$E(\mathbf{x}, \mathbf{h}) = \sum_i^M \frac{(x_i - a_i)^2}{2\sigma_i^2} - \sum_j^N b_j h_j - \sum_{i,j}^{M,N} \frac{x_i w_{ij} h_j}{\sigma_i^2}. \tag{4}$$

1. RBMs are Useful when we model continuous data (i.e., we wish $\mathbf{x}$ to be continuous)
2. Requires a smaller learning rate, since there's no upper bound to the value a component might take in the reconstruction

Other types of units include:

1. Softmax and multinomial units
2. Gaussian visible and hidden units

3. Binomial units
4. Rectified linear units

Cost function

When working with a training dataset, the most common training approach is maximizing the log-likelihood of the training data. The log likelihood characterizes the log-probability of generating the observed data using our generative model. Using this method our cost function is chosen as the negative log-likelihood. The learning then consists of trying to find parameters that maximize the probability of the dataset, and is known as Maximum Likelihood Estimation (MLE). Denoting the parameters as $\boldsymbol{\theta} = a_1, ..., a_M, b_1, ..., b_N, w_{11}, ..., w_{MN}$, the log-likelihood is given by

$$\begin{aligned} \mathcal{L}(\{\theta_i\}) &= \langle \text{log} P_\theta(\boldsymbol{x}) \rangle_{data} & (5) \\ &= -\langle E(\boldsymbol{x}; \{\theta_i\}) \rangle_{data} - \text{log} Z(\{\theta_i\}), & (6) \end{aligned}$$

where we used that the normalization constant does not depend on the data, $\langle \text{log} Z(\{\theta_i\}) \rangle = \text{log} Z(\{\theta_i\})$ Our cost function is the negative log-likelihood, $\mathcal{C}(\{\theta_i\}) = -\mathcal{L}(\{\theta_i\})$

Optimization / Training

The training procedure of choice often is Stochastic Gradient Descent (SGD). It consists of a series of iterations where we update the parameters according to the equation

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta \nabla \mathcal{C}(\boldsymbol{\theta}_k) \tag{7}$$

at each k-th iteration. There are a range of variants of the algorithm which aim at making the learning rate η more adaptive so the method might be more efficient while remaining stable.

We now need the gradient of the cost function in order to minimize it. We find that

$$\begin{aligned} \frac{\partial \mathcal{C}(\{\theta_i\})}{\partial \theta_i} &= \langle \frac{\partial E(\boldsymbol{x}; \theta_i)}{\partial \theta_i} \rangle_{data} + \frac{\partial \text{log} Z(\{\theta_i\})}{\partial \theta_i} & (8) \\ &= \langle O_i(\boldsymbol{x}) \rangle_{data} - \langle O_i(\boldsymbol{x}) \rangle_{model}, & (9) \end{aligned}$$

where in order to simplify notation we defined the "operator"

$$O_i(\boldsymbol{x}) = \frac{\partial E(\boldsymbol{x}; \theta_i)}{\partial \theta_i}, \tag{10}$$

and used the statistical mechanics relationship between expectation values and the log-partition function:

$$\langle O_i(\boldsymbol{x}) \rangle_{model} = \text{Tr} P_\theta(\boldsymbol{x}) O_i(\boldsymbol{x}) = -\frac{\partial \text{log} Z(\{\theta_i\})}{\partial \theta_i}. \tag{11}$$

The data-dependent term in the gradient is known as the positive phase of the gradient, while the model-dependent term is known as the negative phase of the gradient. The aim of the training is to lower the energy of configurations that are near observed data points (increasing their probability), and raising the energy of configurations that are far from observed data points (decreasing their probability).

The gradient of the negative log-likelihood cost function of a Binary-Binary RBM is then

$$\begin{aligned}
\frac{\partial \mathcal{C}(w_{ij}, a_i, b_j)}{\partial w_{ij}} =& \langle x_i h_j \rangle_{data} - \langle x_i h_j \rangle_{model} && (12)\\
\frac{\partial \mathcal{C}(w_{ij}, a_i, b_j)}{\partial a_{ij}} =& \langle x_i \rangle_{data} - \langle x_i \rangle_{model} && (13)\\
\frac{\partial \mathcal{C}(w_{ij}, a_i, b_j)}{\partial b_{ij}} =& \langle h_i \rangle_{data} - \langle h_i \rangle_{model}. && (14)\\
& && (15)
\end{aligned}$$

To get the expectation values with respect to the *data*, we set the visible units to each of the observed samples in the training data, then update the hidden units according to the conditional probability found before. We then average over all samples in the training data to calculate expectation values with respect to the data.

Kullback-Leibler relative entropy

When the goal of the training is to approximate a probability distribution, as it is in generative modeling, another relevant measure is the **Kullback-Leibler divergence**, also known as the relative entropy or Shannon entropy. It is a non-symmetric measure of the dissimilarity between two probability density functions p and q. If p is the unkown probability which we approximate with q, we can measure the difference by

$$\text{KL}(p||q) = \int_{-\infty}^{\infty} p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} d\boldsymbol{x}. \tag{16}$$

Thus, the Kullback-Leibler divergence between the distribution of the training data $f(\boldsymbol{x})$ and the model distribution $p(\boldsymbol{x}|\boldsymbol{\theta})$ is

$$\begin{aligned}
\text{KL}(f(\boldsymbol{x})||p(\boldsymbol{x}|\boldsymbol{\theta})) =& \int_{-\infty}^{\infty} f(\boldsymbol{x}) \log \frac{f(\boldsymbol{x})}{p(\boldsymbol{x}|\boldsymbol{\theta})} d\boldsymbol{x} && (17)\\
=& \int_{-\infty}^{\infty} f(\boldsymbol{x}) \log f(\boldsymbol{x}) d\boldsymbol{x} - \int_{-\infty}^{\infty} f(\boldsymbol{x}) \log p(\boldsymbol{x}|\boldsymbol{\theta}) d\boldsymbol{x} && (18)\\
=& \langle \log f(\boldsymbol{x}) \rangle_{f(\boldsymbol{x})} - \langle \log p(\boldsymbol{x}|\boldsymbol{\theta}) \rangle_{f(\boldsymbol{x})} && (19)\\
=& \langle \log f(\boldsymbol{x}) \rangle_{data} + \langle E(\boldsymbol{x}) \rangle_{data} + \log Z && (20)\\
=& \langle \log f(\boldsymbol{x}) \rangle_{data} + \mathcal{C}_{LL}. && (21)
\end{aligned}$$

The first term is constant with respect to $\boldsymbol{\theta}$ since $f(\boldsymbol{x})$ is independent of $\boldsymbol{\theta}$. Thus the Kullback-Leibler Divergence is minimal when the second term is minimal. The second term is the log-likelihood cost function, hence minimizing the Kullback-Leibler divergence is equivalent to maximizing the log-likelihood.

To further understand generative models it is useful to study the gradient of the cost function which is needed in order to minimize it using methods like stochastic gradient descent.

The partition function is the generating function of expectation values, in particular there are mathematical relationships between expectation values and the log-partition function. In this case we have

$$\langle \frac{\partial E(\boldsymbol{x};\theta_i)}{\partial \theta_i} \rangle_{model} = \int p(\boldsymbol{x}|\boldsymbol{\theta}) \frac{\partial E(\boldsymbol{x};\theta_i)}{\partial \theta_i} d\boldsymbol{x} = -\frac{\partial \log Z(\theta_i)}{\partial \theta_i}. \tag{22}$$

Here $\langle \cdot \rangle_{model}$ is the expectation value over the model probability distribution $p(\boldsymbol{x}|\boldsymbol{\theta})$.

Setting up for gradient descent calculations

Using the previous relationship we can express the gradient of the cost function as

$$\frac{\partial \mathcal{C}_{LL}}{\partial \theta_i} = \langle \frac{\partial E(\boldsymbol{x};\theta_i)}{\partial \theta_i} \rangle_{data} + \frac{\partial \log Z(\theta_i)}{\partial \theta_i} \tag{23}$$

$$= \langle \frac{\partial E(\boldsymbol{x};\theta_i)}{\partial \theta_i} \rangle_{data} - \langle \frac{\partial E(\boldsymbol{x};\theta_i)}{\partial \theta_i} \rangle_{model} \tag{24}$$

$$\tag{25}$$

This expression shows that the gradient of the log-likelihood cost function is a **difference of moments**, with one calculated from the data and one calculated from the model. The data-dependent term is called the **positive phase** and the model-dependent term is called the **negative phase** of the gradient. We see now that minimizing the cost function results in lowering the energy of configurations $\boldsymbol{x}$ near points in the training data and increasing the energy of configurations not observed in the training data. That means we increase the model's probability of configurations similar to those in the training data.

The gradient of the cost function also demonstrates why gradients of unsupervised, generative models must be computed differently from for those of for example FNNs. While the data-dependent expectation value is easily calculated based on the samples $\boldsymbol{x}_i$ in the training data, we must sample from the model in order to generate samples from which to caclulate the model-dependent term. We sample from the model by using MCMC-based methods. We can not sample from the model directly because the partition function Z is generally intractable.

As in supervised machine learning problems, the goal is also here to perform well on **unseen** data, that is to have good generalization from the training data. The distribution $f(x)$ we approximate is not the **true** distribution we wish to estimate, it is limited to the training data. Hence, in unsupervised training as well it is important to prevent overfitting to the training data. Thus it is common to add regularizers to the cost function in the same manner as we discussed for say linear regression.

Mathematical details

Because we are restricted to potential functions which are positive it is convenient to express them as exponentials, so that

$$\phi_C(\boldsymbol{x}_C) = e^{-E_C(\boldsymbol{x}_C)} \tag{26}$$

where $E(\boldsymbol{x}_C)$ is called an *energy function*, and the exponential representation is the *Boltzmann distribution.* The joint distribution is defined as the product of potentials.

The joint distribution of the random variables is then

$$\begin{aligned} p(\boldsymbol{x}) =& \frac{1}{Z}\prod_C \phi_C(\boldsymbol{x}_C) \\ =& \frac{1}{Z}\prod_C e^{-E_C(\boldsymbol{x}_C)} \\ =& \frac{1}{Z} e^{-\sum_C E_C(\boldsymbol{x}_C)} \\ =& \frac{1}{Z} e^{-E(\boldsymbol{x})}. \end{aligned} \tag{27}$$

$$p_{BM}(\boldsymbol{x},\boldsymbol{h}) = \frac{1}{Z_{BM}} e^{-\frac{1}{T}E_{BM}(\boldsymbol{x},\boldsymbol{h})}, \tag{28}$$

with the partition function

$$Z_{BM} = \int\int e^{-\frac{1}{T}E_{BM}(\tilde{\boldsymbol{x}},\tilde{\boldsymbol{h}})} d\tilde{\boldsymbol{x}} d\tilde{\boldsymbol{h}}. \tag{29}$$

T is a physics-inspired parameter named temperature and will be assumed to be 1 unless otherwise stated. The energy function of the Boltzmann machine determines the interactions between the nodes and is defined

$$\begin{aligned} E_{BM}(\boldsymbol{x},\boldsymbol{h}) =& -\sum_{i,k}^{M,K} a_i^k \alpha_i^k(x_i) - \sum_{j,l}^{N,L} b_j^l \beta_j^l(h_j) - \sum_{i,j,k,l}^{M,N,K,L} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(h_j) \\ & - \sum_{i,m=i+1,k}^{M,M,K} \alpha_i^k(x_i) v_{im}^k \alpha_m^k(x_m) - \sum_{j,n=j+1,l}^{N,N,L} \beta_j^l(h_j) u_{jn}^l \beta_n^l(h_n). \end{aligned} \tag{30}$$

Here $\alpha_i^k(x_i)$ and $\beta_j^l(h_j)$ are one-dimensional transfer functions or mappings from the given input value to the desired feature value. They can be arbitrary functions of the input variables and are independent of the parameterization (parameters referring to weight and biases), meaning they are not affected by training of the model. The indices k and l indicate that there can be multiple transfer functions per variable. Furthermore, a_i^k and b_j^l are the visible and hidden bias. w_{ij}^{kl} are weights of the **inter-layer** connection terms which connect visible and hidden units. v_{im}^k and u_{jn}^l are weights of the **intra-layer** connection terms which connect the visible units to each other and the hidden units to each other, respectively.

We remove the intra-layer connections by setting v_{im} and u_{jn} to zero. The expression for the energy of the RBM is then

$$E_{RBM}(\boldsymbol{x},\boldsymbol{h}) = -\sum_{i,k}^{M,K} a_i^k \alpha_i^k(x_i) - \sum_{j,l}^{N,L} b_j^l \beta_j^l(h_j) - \sum_{i,j,k,l}^{M,N,K,L} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(h_j). \tag{31}$$

resulting in

$$\begin{aligned}
P_{RBM}(\boldsymbol{x}) =& \int P_{RBM}(\boldsymbol{x},\tilde{\boldsymbol{h}}) d\tilde{\boldsymbol{h}} \\
=& \frac{1}{Z_{RBM}} \int e^{-E_{RBM}(\boldsymbol{x},\tilde{\boldsymbol{h}})} d\tilde{\boldsymbol{h}} \\
=& \frac{1}{Z_{RBM}} \int e^{\sum_{i,k} a_i^k \alpha_i^k(x_i) + \sum_{j,l} b_j^l \beta_j^l(\tilde{h}_j) + \sum_{i,j,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(\tilde{h}_j)} d\tilde{\boldsymbol{h}} \\
=& \frac{1}{Z_{RBM}} e^{\sum_{i,k} a_i^k \alpha_i^k(x_i)} \int \prod_j^N e^{\sum_l b_j^l \beta_j^l(\tilde{h}_j) + \sum_{i,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(\tilde{h}_j)} d\tilde{\boldsymbol{h}} \\
=& \frac{1}{Z_{RBM}} e^{\sum_{i,k} a_i^k \alpha_i^k(x_i)} \bigg(\int e^{\sum_l b_1^l \beta_1^l(\tilde{h}_1) + \sum_{i,k,l} \alpha_i^k(x_i) w_{i1}^{kl} \beta_1^l(\tilde{h}_1)} d\tilde{h}_1 \\
& \times \int e^{\sum_l b_2^l \beta_2^l(\tilde{h}_2) + \sum_{i,k,l} \alpha_i^k(x_i) w_{i2}^{kl} \beta_2^l(\tilde{h}_2)} d\tilde{h}_2 \\
& \times ... \\
& \times \int e^{\sum_l b_N^l \beta_N^l(\tilde{h}_N) + \sum_{i,k,l} \alpha_i^k(x_i) w_{iN}^{kl} \beta_N^l(\tilde{h}_N)} d\tilde{h}_N \bigg) \\
=& \frac{1}{Z_{RBM}} e^{\sum_{i,k} a_i^k \alpha_i^k(x_i)} \prod_j^N \int e^{\sum_l b_j^l \beta_j^l(\tilde{h}_j) + \sum_{i,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(\tilde{h}_j)} d\tilde{h}_j
\end{aligned} \tag{32}$$

Similarly

$$
\begin{aligned}
P_{RBM}(\boldsymbol{h}) =& \frac{1}{Z_{RBM}} \int e^{-E_{RBM}(\tilde{\boldsymbol{x}},\boldsymbol{h})} d\tilde{\boldsymbol{x}} \\
=& \frac{1}{Z_{RBM}} e^{\sum_{j,l} b_j^l \beta_j^l(h_j)} \prod_i^M \int e^{\sum_k a_i^k \alpha_i^k(\tilde{x}_i) + \sum_{j,k,l} \alpha_i^k(\tilde{x}_i) w_{ij}^{kl} \beta_j^l(h_j)} d\tilde{x}_i
\end{aligned}
\tag{33}
$$

Using Bayes theorem

$$
\begin{aligned}
P_{RBM}(\boldsymbol{h}|\boldsymbol{x}) =& \frac{P_{RBM}(\boldsymbol{x},\boldsymbol{h})}{P_{RBM}(\boldsymbol{x})} \\
=& \frac{\frac{1}{Z_{RBM}} e^{\sum_{i,k} a_i^k \alpha_i^k(x_i) + \sum_{j,l} b_j^l \beta_j^l(h_j) + \sum_{i,j,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(h_j)}}{\frac{1}{Z_{RBM}} e^{\sum_{i,k} a_i^k \alpha_i^k(x_i)} \prod_j^N \int e^{\sum_l b_j^l \beta_j^l(\tilde{h}_j) + \sum_{i,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(\tilde{h}_j)} d\tilde{h}_j} \\
=& \prod_j^N \frac{e^{\sum_l b_j^l \beta_j^l(h_j) + \sum_{i,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(h_j)}}{\int e^{\sum_l b_j^l \beta_j^l(\tilde{h}_j) + \sum_{i,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(\tilde{h}_j)} d\tilde{h}_j}
\end{aligned}
\tag{34}
$$

Similarly

$$
\begin{aligned}
P_{RBM}(\boldsymbol{x}|\boldsymbol{h}) =& \frac{P_{RBM}(\boldsymbol{x},\boldsymbol{h})}{P_{RBM}(\boldsymbol{h})} \\
=& \prod_i^M \frac{e^{\sum_k a_i^k \alpha_i^k(x_i) + \sum_{j,k,l} \alpha_i^k(x_i) w_{ij}^{kl} \beta_j^l(h_j)}}{\int e^{\sum_k a_i^k \alpha_i^k(\tilde{x}_i) + \sum_{j,k,l} \alpha_i^k(\tilde{x}_i) w_{ij}^{kl} \beta_j^l(h_j)} d\tilde{x}_i}
\end{aligned}
\tag{35}
$$

The original RBM had binary visible and hidden nodes. They were showned to be universal approximators of discrete distributions. It was also shown that adding hidden units yields strictly improved modelling power. The common choice of binary values are 0 and 1. However, in some physics applications, -1 and 1 might be a more natural choice. We will here use 0 and 1.

$$
E_{BB}(\boldsymbol{x},\mathbf{h}) = -\sum_i^M x_i a_i - \sum_j^N b_j h_j - \sum_{i,j}^{M,N} x_i w_{ij} h_j. \tag{36}
$$

$$
p_{BB}(\boldsymbol{x},\boldsymbol{h}) = \frac{1}{Z_{BB}} e^{\sum_i^M a_i x_i + \sum_j^N b_j h_j + \sum_{ij}^{M,N} x_i w_{ij} h_j} \tag{37}
$$

$$
= \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a} + \boldsymbol{b}^T \boldsymbol{h} + \boldsymbol{x}^T \boldsymbol{W} \boldsymbol{h}} \tag{38}
$$

with the partition function

$$
Z_{BB} = \sum_{\boldsymbol{x},\boldsymbol{h}} e^{\boldsymbol{x}^T \boldsymbol{a} + \boldsymbol{b}^T \boldsymbol{h} + \boldsymbol{x}^T \boldsymbol{W} \boldsymbol{h}}. \tag{39}
$$

Marginal Probability Density Functions

In order to find the probability of any configuration of the visible units we derive the marginal probability density function.

$$
\begin{aligned}
p_{BB}(\boldsymbol{x}) =& \sum_{\boldsymbol{h}} p_{BB}(\boldsymbol{x}, \boldsymbol{h}) && (40)\\
=& \frac{1}{Z_{BB}} \sum_{\boldsymbol{h}} e^{\boldsymbol{x}^T \boldsymbol{a} + \boldsymbol{b}^T \boldsymbol{h} + \boldsymbol{x}^T \boldsymbol{W} \boldsymbol{h}}\\
=& \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a}} \sum_{\boldsymbol{h}} e^{\sum_j^N (b_j + \boldsymbol{x}^T \boldsymbol{w}_{*j}) h_j}\\
=& \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a}} \sum_{\boldsymbol{h}} \prod_j^N e^{(b_j + \boldsymbol{x}^T \boldsymbol{w}_{*j}) h_j}\\
=& \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a}} \Bigg(\sum_{h_1} e^{(b_1 + \boldsymbol{x}^T \boldsymbol{w}_{*1}) h_1} \times \sum_{h_2} e^{(b_2 + \boldsymbol{x}^T \boldsymbol{w}_{*2}) h_2} \times\\
& \dots \times \sum_{h_2} e^{(b_N + \boldsymbol{x}^T \boldsymbol{w}_{*N}) h_N} \Bigg)\\
=& \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a}} \prod_j^N \sum_{h_j} e^{(b_j + \boldsymbol{x}^T \boldsymbol{w}_{*j}) h_j}\\
=& \frac{1}{Z_{BB}} e^{\boldsymbol{x}^T \boldsymbol{a}} \prod_j^N (1 + e^{b_j + \boldsymbol{x}^T \boldsymbol{w}_{*j}}). && (41)
\end{aligned}
$$

A similar derivation yields the marginal probability of the hidden units

$$
p_{BB}(\boldsymbol{h}) = \frac{1}{Z_{BB}} e^{\boldsymbol{b}^T \boldsymbol{h}} \prod_i^M (1 + e^{a_i + \boldsymbol{w}_{i*}^T \boldsymbol{h}}). \tag{42}
$$

Conditional Probability Density Functions

We derive the probability of the hidden units given the visible units using Bayes' rule

$$\begin{aligned}
p_{BB}(\boldsymbol{h}|\boldsymbol{x}) =& \frac{p_{BB}(\boldsymbol{x},\boldsymbol{h})}{p_{BB}(\boldsymbol{x})} \\
=& \frac{\frac{1}{Z_{BB}} e^{\boldsymbol{x}^T\boldsymbol{a}+\boldsymbol{b}^T\boldsymbol{h}+\boldsymbol{x}^T\boldsymbol{W}\boldsymbol{h}}}{\frac{1}{Z_{BB}} e^{\boldsymbol{x}^T\boldsymbol{a}} \prod_j^N (1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}})} \\
=& \frac{e^{\boldsymbol{x}^T\boldsymbol{a}} e^{\sum_j^N (b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j})h_j}}{e^{\boldsymbol{x}^T\boldsymbol{a}} \prod_j^N (1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}})} \\
=& \prod_j^N \frac{e^{(b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j})h_j}}{1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}}} \\
=& \prod_j^N p_{BB}(h_j|\boldsymbol{x}). \qquad (43)
\end{aligned}$$

From this we find the probability of a hidden unit being "on" or "off":

$$\begin{aligned}
p_{BB}(h_j=1|\boldsymbol{x}) =& \frac{e^{(b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j})h_j}}{1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}}} \qquad (44) \\
=& \frac{e^{(b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j})}}{1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}}} \qquad (45) \\
=& \frac{1}{1+e^{-(b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j})}}, \qquad (46)
\end{aligned}$$

and

$$p_{BB}(h_j=0|\boldsymbol{x}) = \frac{1}{1+e^{b_j+\boldsymbol{x}^T\boldsymbol{w}_{*j}}}. \qquad (47)$$

Similarly we have that the conditional probability of the visible units given the hidden are

$$\begin{aligned}
p_{BB}(\boldsymbol{x}|\boldsymbol{h}) =& \prod_i^M \frac{e^{(a_i+\boldsymbol{w}_{i*}^T\boldsymbol{h})x_i}}{1+e^{a_i+\boldsymbol{w}_{i*}^T\boldsymbol{h}}} \qquad (48) \\
=& \prod_i^M p_{BB}(x_i|\boldsymbol{h}). \qquad (49)
\end{aligned}$$

$$\begin{aligned}
p_{BB}(x_i=1|\boldsymbol{h}) =& \frac{1}{1+e^{-(a_i+\boldsymbol{w}_{i*}^T\boldsymbol{h})}} \qquad (50) \\
p_{BB}(x_i=0|\boldsymbol{h}) =& \frac{1}{1+e^{a_i+\boldsymbol{w}_{i*}^T\boldsymbol{h}}}. \qquad (51)
\end{aligned}$$

Gaussian-Binary Restricted Boltzmann Machines

Inserting into the expression for $E_{RBM}(\boldsymbol{x}, \boldsymbol{h})$ in equation results in the energy

$$\begin{aligned} E_{GB}(\boldsymbol{x}, \boldsymbol{h}) =& \sum_i^M \frac{(x_i - a_i)^2}{2\sigma_i^2} - \sum_j^N b_j h_j - \sum_{ij}^{M,N} \frac{x_i w_{ij} h_j}{\sigma_i^2} \\ =& || \frac{\boldsymbol{x} - \boldsymbol{a}}{2\boldsymbol{\sigma}} ||^2 - \boldsymbol{b}^T \boldsymbol{h} - (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W} \boldsymbol{h}. \end{aligned} \tag{52}$$

Joint Probability Density Function

$$\begin{aligned} p_{GB}(\boldsymbol{x}, \boldsymbol{h}) =& \frac{1}{Z_{GB}} e^{-|| \frac{\boldsymbol{x} - \boldsymbol{a}}{2\boldsymbol{\sigma}} ||^2 + \boldsymbol{b}^T \boldsymbol{h} + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W} \boldsymbol{h}} \\ =& \frac{1}{Z_{GB}} e^{- \sum_i^M \frac{(x_i - a_i)^2}{2\sigma_i^2} + \sum_j^N b_j h_j + \sum_{ij}^{M,N} \frac{x_i w_{ij} h_j}{\sigma_i^2}} \\ =& \frac{1}{Z_{GB}} \prod_{ij}^{M,N} e^{- \frac{(x_i - a_i)^2}{2\sigma_i^2} + b_j h_j + \frac{x_i w_{ij} h_j}{\sigma_i^2}}, \end{aligned} \tag{53}$$

with the partition function given by

$$Z_{GB} = \int \sum_{\tilde{\boldsymbol{h}}}^{\tilde{\boldsymbol{H}}} e^{-|| \frac{\tilde{\boldsymbol{x}} - \boldsymbol{a}}{2\boldsymbol{\sigma}} ||^2 + \boldsymbol{b}^T \tilde{\boldsymbol{h}} + (\frac{\tilde{\boldsymbol{x}}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W} \tilde{\boldsymbol{h}}} d\tilde{\boldsymbol{x}}. \tag{54}$$

Marginal Probability Density Functions

We proceed to find the marginal probability densitites of the Gaussian-binary RBM. We first marginalize over the binary hidden units to find $p_{GB}(\boldsymbol{x})$

$$\begin{aligned} p_{GB}(\boldsymbol{x}) =& \sum_{\tilde{\boldsymbol{h}}}^{\tilde{\boldsymbol{H}}} p_{GB}(\boldsymbol{x}, \tilde{\boldsymbol{h}}) \\ =& \frac{1}{Z_{GB}} \sum_{\tilde{\boldsymbol{h}}}^{\tilde{\boldsymbol{H}}} e^{-|| \frac{\boldsymbol{x} - \boldsymbol{a}}{2\boldsymbol{\sigma}} ||^2 + \boldsymbol{b}^T \tilde{\boldsymbol{h}} + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W} \tilde{\boldsymbol{h}}} \\ =& \frac{1}{Z_{GB}} e^{-|| \frac{\boldsymbol{x} - \boldsymbol{a}}{2\boldsymbol{\sigma}} ||^2} \prod_j^N (1 + e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}). \end{aligned} \tag{55}$$

We next marginalize over the visible units. This is the first time we marginalize over continuous values. We rewrite the exponential factor dependent on $\boldsymbol{x}$ as a Gaussian function before we integrate in the last step.

$$
\begin{aligned}
p_{GB}(\boldsymbol{h}) =& \int p_{GB}(\tilde{\boldsymbol{x}}, \boldsymbol{h}) d\tilde{\boldsymbol{x}} \\
=& \frac{1}{Z_{GB}} \int e^{-||\frac{\tilde{\boldsymbol{x}}-\boldsymbol{a}}{2\boldsymbol{\sigma}}||^2 + \boldsymbol{b}^T\boldsymbol{h} + (\frac{\tilde{\boldsymbol{x}}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W}\boldsymbol{h}} d\tilde{\boldsymbol{x}} \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \int \prod_i^M e^{-\frac{(\tilde{x}_i - a_i)^2}{2\sigma_i^2} + \frac{\tilde{x}_i \boldsymbol{w}_{i*}^T \boldsymbol{h}}{\sigma_i^2}} d\tilde{\boldsymbol{x}} \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \Bigg(\int e^{-\frac{(\tilde{x}_1 - a_1)^2}{2\sigma_1^2} + \frac{\tilde{x}_1 \boldsymbol{w}_{1*}^T \boldsymbol{h}}{\sigma_1^2}} d\tilde{x}_1 \\
& \times \int e^{-\frac{(\tilde{x}_2 - a_2)^2}{2\sigma_2^2} + \frac{\tilde{x}_2 \boldsymbol{w}_{2*}^T \boldsymbol{h}}{\sigma_2^2}} d\tilde{x}_2 \\
& \times \ldots \\
& \times \int e^{-\frac{(\tilde{x}_M - a_M)^2}{2\sigma_M^2} + \frac{\tilde{x}_M \boldsymbol{w}_{M*}^T \boldsymbol{h}}{\sigma_M^2}} d\tilde{x}_M \Bigg) \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \int e^{-\frac{(\tilde{x}_i - a_i)^2 - 2\tilde{x}_i \boldsymbol{w}_{i*}^T \boldsymbol{h}}{2\sigma_i^2}} d\tilde{x}_i \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \int e^{-\frac{\tilde{x}_i^2 - 2\tilde{x}_i (a_i + \tilde{x}_i \boldsymbol{w}_{i*}^T \boldsymbol{h}) + a_i^2}{2\sigma_i^2}} d\tilde{x}_i \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \int e^{-\frac{\tilde{x}_i^2 - 2\tilde{x}_i (a_i + \boldsymbol{w}_{i*}^T \boldsymbol{h}) + (a_i + \boldsymbol{w}_{i*}^T \boldsymbol{h})^2 - (a_i + \boldsymbol{w}_{i*}^T \boldsymbol{h})^2 + a_i^2}{2\sigma_i^2}} d\tilde{x}_i \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \int e^{-\frac{(\tilde{x}_i - (a_i + \boldsymbol{w}_{i*}^T \boldsymbol{h}))^2 - a_i^2 - 2a_i \boldsymbol{w}_{i*}^T \boldsymbol{h} - (\boldsymbol{w}_{i*}^T \boldsymbol{h})^2 + a_i^2}{2\sigma_i^2}} d\tilde{x}_i \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M e^{\frac{2a_i \boldsymbol{w}_{i*}^T \boldsymbol{h} + (\boldsymbol{w}_{i*}^T \boldsymbol{h})^2}{2\sigma_i^2}} \int e^{-\frac{(\tilde{x}_i - a_i - \boldsymbol{w}_{i*}^T \boldsymbol{h})^2}{2\sigma_i^2}} d\tilde{x}_i \\
=& \frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \sqrt{2\pi\sigma_i^2} e^{\frac{2a_i \boldsymbol{w}_{i*}^T \boldsymbol{h} + (\boldsymbol{w}_{i*}^T \boldsymbol{h})^2}{2\sigma_i^2}}.
\end{aligned}
\tag{56}
$$

Conditional Probability Density Functions

We finish by deriving the conditional probabilities.

$$\begin{aligned}
p_{GB}(\boldsymbol{h}|\boldsymbol{x}) =& \frac{p_{GB}(\boldsymbol{x},\boldsymbol{h})}{p_{GB}(\boldsymbol{x})} \\
=& \frac{\frac{1}{Z_{GB}} e^{-||\frac{\boldsymbol{x}-\boldsymbol{a}}{2\boldsymbol{\sigma}}||^2 + \boldsymbol{b}^T\boldsymbol{h} + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{W}\boldsymbol{h}}}{\frac{1}{Z_{GB}} e^{-||\frac{\boldsymbol{x}-\boldsymbol{a}}{2\boldsymbol{\sigma}}||^2} \prod_j^N (1 + e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}})} \\
=& \prod_j^N \frac{e^{(b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}) h_j}}{1 + e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}} \\
=& \prod_j^N p_{GB}(h_j|\boldsymbol{x}). \qquad (57)
\end{aligned}$$

The conditional probability of a binary hidden unit h_j being on or off again takes the form of a sigmoid function

$$\begin{aligned}
p_{GB}(h_j = 1|\boldsymbol{x}) =& \frac{e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}}{1 + e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}} \\
=& \frac{1}{1 + e^{-b_j - (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}} \qquad (58) \\
p_{GB}(h_j = 0|\boldsymbol{x}) =& \frac{1}{1 + e^{b_j + (\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T \boldsymbol{w}_{*j}}}. \qquad (59)
\end{aligned}$$

The conditional probability of the continuous $\boldsymbol{x}$ now has another form, however.

$$
\begin{aligned}
p_{GB}(\boldsymbol{x}|\boldsymbol{h}) =& \frac{p_{GB}(\boldsymbol{x},\boldsymbol{h})}{p_{GB}(\boldsymbol{h})} \\
=& \frac{\frac{1}{Z_{GB}} e^{-||\frac{\boldsymbol{x}-\boldsymbol{a}}{2\boldsymbol{\sigma}}||^2+\boldsymbol{b}^T\boldsymbol{h}+(\frac{\boldsymbol{x}}{\boldsymbol{\sigma}^2})^T\boldsymbol{W}\boldsymbol{h}}}{\frac{1}{Z_{GB}} e^{\boldsymbol{b}^T\boldsymbol{h}} \prod_i^M \sqrt{2\pi\sigma_i^2} e^{\frac{2a_i\boldsymbol{w}_{i*}^T\boldsymbol{h}+(\boldsymbol{w}_{i*}^T\boldsymbol{h})^2}{2\sigma_i^2}}} \\
=& \prod_i^M \frac{1}{\sqrt{2\pi\sigma_i^2}} \frac{e^{-\frac{(x_i-a_i)^2}{2\sigma_i^2}+\frac{x_i\boldsymbol{w}_{i*}^T\boldsymbol{h}}{2\sigma_i^2}}}{e^{\frac{2a_i\boldsymbol{w}_{i*}^T\boldsymbol{h}+(\boldsymbol{w}_{i*}^T\boldsymbol{h})^2}{2\sigma_i^2}}} \\
=& \prod_i^M \frac{1}{\sqrt{2\pi\sigma_i^2}} \frac{e^{-\frac{x_i^2-2a_ix_i+a_i^2-2x_i\boldsymbol{w}_{i*}^T\boldsymbol{h}}{2\sigma_i^2}}}{e^{\frac{2a_i\boldsymbol{w}_{i*}^T\boldsymbol{h}+(\boldsymbol{w}_{i*}^T\boldsymbol{h})^2}{2\sigma_i^2}}} \\
=& \prod_i^M \frac{1}{\sqrt{2\pi\sigma_i^2}} e^{-\frac{x_i^2-2a_ix_i+a_i^2-2x_i\boldsymbol{w}_{i*}^T\boldsymbol{h}+2a_i\boldsymbol{w}_{i*}^T\boldsymbol{h}+(\boldsymbol{w}_{i*}^T\boldsymbol{h})^2}{2\sigma_i^2}} \\
=& \prod_i^M \frac{1}{\sqrt{2\pi\sigma_i^2}} e^{-\frac{(x_i-b_i-\boldsymbol{w}_{i*}^T\boldsymbol{h})^2}{2\sigma_i^2}} \\
=& \prod_i^M \mathcal{N}(x_i|b_i+\boldsymbol{w}_{i*}^T\boldsymbol{h},\sigma_i^2) \qquad (60) \\
\Rightarrow p_{GB}(x_i|\boldsymbol{h}) =& \mathcal{N}(x_i|b_i+\boldsymbol{w}_{i*}^T\boldsymbol{h},\sigma_i^2). \qquad (61)
\end{aligned}
$$

The form of these conditional probabilities explains the name "Gaussian" and the form of the Gaussian-binary energy function. We see that the conditional probability of x_i given $\boldsymbol{h}$ is a normal distribution with mean $b_i + \boldsymbol{w}_{i*}^T\boldsymbol{h}$ and variance σ_i^2.