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Kullback – Leibler divergence

The **Kullback - Leibler divergence** or **relative entropy** ($D_{KL}(P\ ||\ Q)$) is a measure in information theory that describes the distance between two probability distributions.

The term divergence refers to a concept in statistical mathematics. It is a function that takes two probability distributions as input (p, q). There are some rules for divergence:

Let p and q be two probability distributions. Then:

$D(p, q)\ \geq\ 0$

$D(p, p) = 0$

As you can see, a divergence isn't necessarily symmetrical ($D(p,\ q)\ \neq\ D(q,\ p)$). Neither the KL divergence is. That's why we say $D_{KL}(P\ ||\ Q)$ is the KL divergence of Q with respect to P.

The KL divergence is the expectation of the logarithmic difference between the probabilities P and Q, where the expectation is taken using the probabilities of P:

$$D_{KL}(P\ ||\ Q) = E_{x \sim p}[log_b(P(x)) - log_b(Q(x))] = E_{x \sim p}[log_b(\frac{P(x)}{Q(x)})]$$

For discrete distributions it can be rewritten in the following formula:

$$D_{KL}(P\ ||\ Q) = \ \sum_{x \in X} P(x) log_b(\frac{P(x)}{Q(x)})$$

Where $P(x)$ and $Q(x)$ is the probability mass function of the random variables.

And for continuous distributions, the KL divergence is calculated using this integral:

$$D_{KL}(P\ ||\ Q) = \ \int_{x \in X} p(x) log_b(\frac{p(x)}{q(x)}) dx$$

Where $p(x)$ and $q(x)$ is the probability density function of the random variables.

The higher the relative entropy of Q with respect to P, the more distinguish the distributions. Let's see this in an example.

Example

Let $B \sim Bin(250, 0.008)$ and $P \sim Pois(2)$.

In [10]:
```
import numpy as np
import math
import matplotlib.pyplot as plt
from scipy.stats import poisson, binom

green = '#57cc99'
blue = '#22577a'
red = '#e56b6f'

line_thickness = 3

  = 250
```

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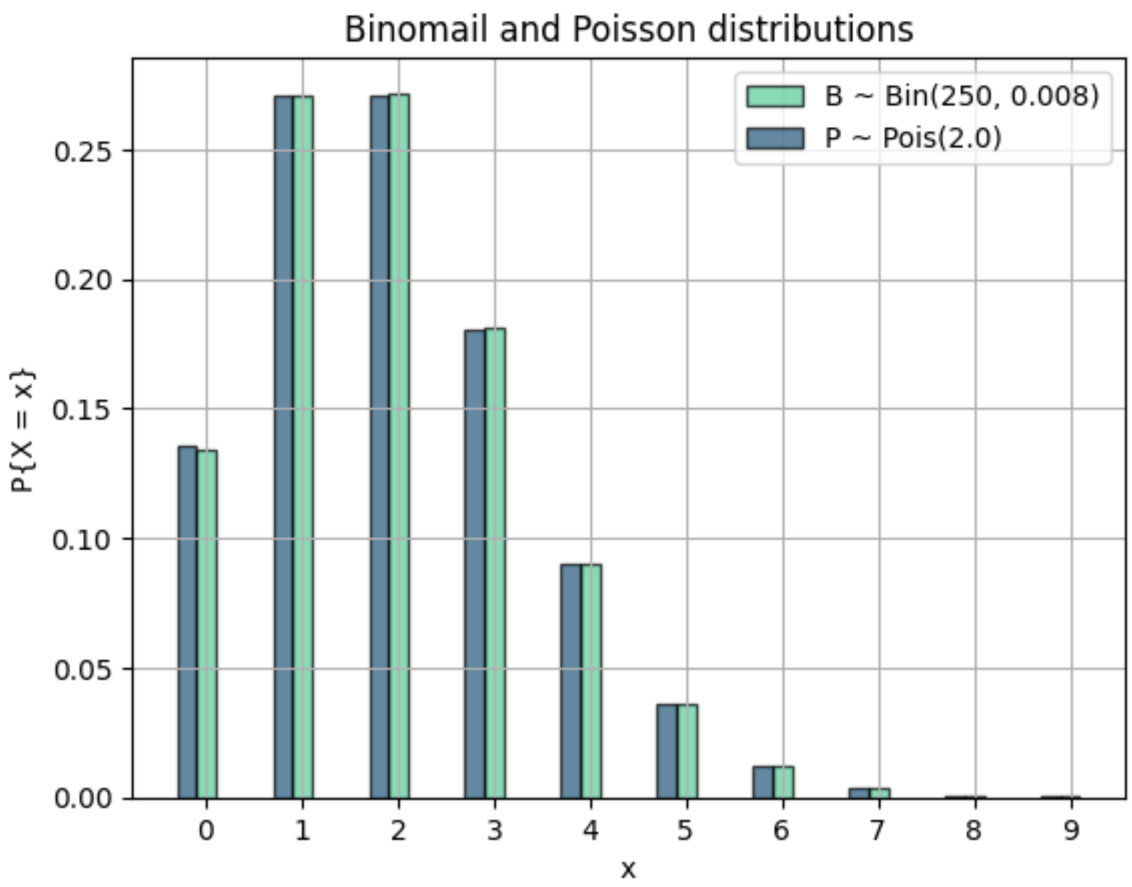
```
p = 0.008
mu = n * p

width = 0.2

x_values = np.arange(0, 10)

binomial_pmf = binom.pmf(x_values, n, p)
poisson_pmf = poisson.pmf(x_values, mu)

fig, ax = plt.subplots()

ax.bar(x_values, binomial_pmf, width, label='B ~ Bin({}, {})'.format(n, p), color=green, alpha=0.7, edgecolor='black')
ax.bar(x_values - width, poisson_pmf, width, label='P ~ Pois({})'.format(mu), color=blue, alpha=0.7, edgecolor='black')

ax.set_xticks(x_values)
ax.set_xlabel('x')
ax.set_ylabel('P{X = x}')
ax.set_title("Binomail and Poisson distributions")
ax.legend()
plt.grid(True)
plt.show()
```



Now let's calculate the KL divergence without using the library functions.

In [11]:
```
def relative_entropy(P, Q):
    res = 0
    for x in range(0, len(P)):
        res += P[x] * math.log(P[x] / Q[x])
    return res

print("D(B || P) =", relative_entropy(binomial_pmf, poisson_pmf))
print("D(P || B) =", relative_entropy(poisson_pmf, binomial_pmf))
```

```
D(B || P) = 2.094332797227328e-05
D(P || B) = 1.0766381413449403e-05
```

Let's recalculate it this time using library functions.

In [12]:
```
print("D(B || P) =", np.sum(binomial_pmf * np.log(binomial_pmf / poisson_pmf)))
print("D(P || B) =", np.sum(poisson_pmf * np.log(poisson_pmf / binomial_pmf)))
```

```
D(B || P) = 2.0943327972273254e-05
D(P || B) = 1.0766381413449322e-05
```

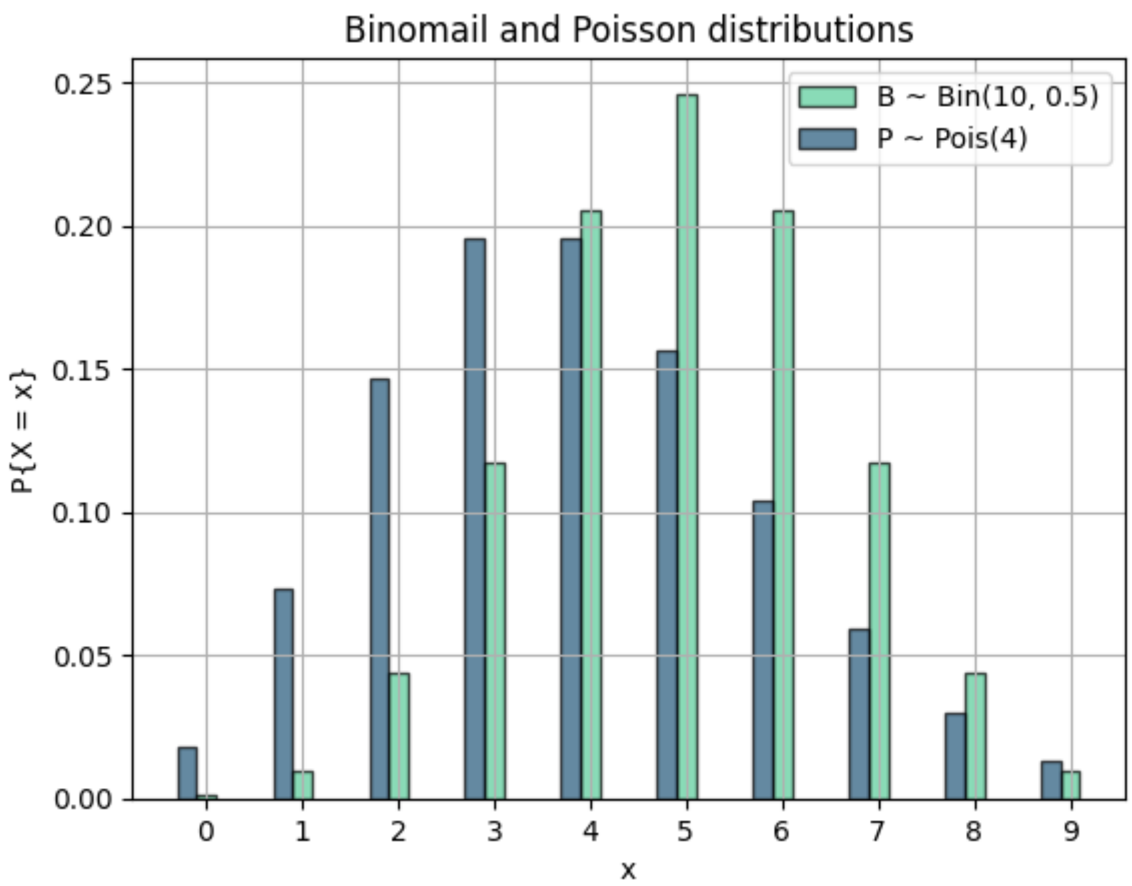
As you can see, the KL divergence is not symmetrical since $D_{KL}(B \ P) \neq D_{KL}(P \ B)$.

In this example, the KL divergence value is relatively low because B and P random variables have really close distributions. Let's see another example that has higher KL divergence:

In [13]:
```
n = 10
p = 0.5
mu = 4

binomial_pmf = binom.pmf(x_values, n, p)
poisson_pmf = poisson.pmf(x_values, mu)

fig, ax = plt.subplots()
```

Processing math: 96%

```
ax.bar(x_values, binomial_pmf, width, label='B ~ Bin({}, {})'.format(n, p), color=green, alpha=0.7, edgecolor='black')
ax.bar(x_values - width, poisson_pmf, width, label='P ~ Pois({})'.format(mu), color=blue, alpha=0.7, edgecolor='black')

ax.set_xticks(x_values)
ax.set_xlabel('x')
ax.set_ylabel('P{X = x}')
ax.set_title("Binomail and Poisson distributions")
ax.legend()
plt.grid(True)
plt.show()

print("D(B || P) =", relative_entropy(binomial_pmf, poisson_pmf))
print("D(P || B) =", relative_entropy(poisson_pmf, binomial_pmf))
```




```
D(B || P) = 0.21867216891725103
D(P || B) = 0.2787591791935817
```

As it can be seen, the KL divergence is much higher now, meaning the distributions are distant.

Cross - entropy

Cross - entropy is another measure in information theory between two probability distributions. The cross-entropy of the distribution Q relative to a distribution P is defined as:

$H(P, Q) = -E_{x\sim p}[log_b(Q(x))]$

For discrete distributions with $P(x)$ and $Q(x)$ as PMFs:

$H(P, Q) = -\sum_{x\in X} P(x)log_b(Q(x))$

And for continous distributions with $p(x)$ and $q(x)$ as PDFs:

$H(P, Q) = -\int_{x\in X} p(x)log_b(q(x))dx$

Is basically the expectation of logarithm of probability of Q with probabilites of P. It measures the difference between two probability distributions, therefore it can be used as loss function. (which we'll discuss later)

Example

In this example, we're gonna calculate the relative entropy of two probability distributions. First we do it without using the library methods.

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In [14]:
```
import math

def cross_entropy(p, q):
    res = 0
    for x in range(len(p)):
        res -= p[x] * math.log(q[x])
    return res

actual_values = [0, 1, 0]
predicted_values = [0.05, 0.85, 0.10]

print(cross_entropy(actual_values, predicted_values))
```

```
0.16251892949777494
```

Now we use `tensorflow` to calculate the cross entropy loss.

In [15]:
```
import tensorflow as tf

loss = tf.keras.losses.CategoricalCrossentropy()
loss = loss(actual_values, predicted_values)
print(loss.numpy)
```

```
2024-04-13 04:36:29.132037: I tensorflow/core/platform/cpu_feature_guard.cc:182] This TensorFlow binary is optimized to u
se available CPU instructions in performance-critical operations.
To enable the following instructions: SSE3 SSE4.1 SSE4.2, in other operations, rebuild TensorFlow with the appropriate c
ompiler flags.
<bound method _EagerTensorBase.numpy of <tf.Tensor: shape=(), dtype=float32, numpy=0.1625189>>
2024-04-13 04:36:32.683175: I tensorflow/core/common_runtime/process_util.cc:146] Creating new thread pool with default i
nter op setting: 2. Tune using inter_op_parallelism_threads for best performance.
```

For another prediction in which our model acts terrible, the loss would be much higher:

In [16]:
```
actual_values = [0, 1, 0]
predicted_values = [0.85, 0.05, 0.10]

print(cross_entropy(actual_values, predicted_values))
```

```
2.995732273553991
```

The relation between cross - entropy, KL divergnce and entropy

The cross - entropy, KL divergence and entropy all link up in this famous formula:

$$H(P,Q) = H(P) + D_{KL}(P \mid\mid Q)$$

Proof

For discrete distributions:

$$H(P,Q) = -\sum_{x \in X} P(x) log_b(Q(x))$$

$$H(P) = -\sum_{x \in X} P(x) log_b(P(x))$$

$$D_{KL}(P \mid\mid Q) = \sum_{x \in X} P(x)[log_b(P(x)) - log_b(Q(x))] = \sum_{x \in X} P(x) log_b(P(x)) - \sum_{x \in X} P(x) log_b(Q(x))$$

$$H(P) + D_{KL}(P \mid\mid Q) = -\sum_{x \in X} P(x) log_b(P(x)) + \sum_{x \in X} P(x) log_b(P(x)) - \sum_{x \in X} P(x) log_b(Q(x)) = -\sum_{x \in X} P(x) log_b(Q(x)) = H(P,Q)$$

And for continous distributions:

$$H(P,Q) = -\int_{x \in X} p(x) log_b(q(x)) dx$$

$$H(P) = -\int_{x \in X} p(x) log_b(p(x)) dx$$

$$D_{KL}(P \mid\mid Q) = \int_{x \in X} p(x)[log_b(p(x)) - log_b(q(x))] dx = \int_{x \in X} p(x) log_b(p(x)) dx - \int_{x \in X} p(x) log_b(q(x)) dx$$

$$H(P) + D_{KL}(P \mid\mid Q) = -\int_{x \in X} p(x) log_b(p(x)) dx + \int_{x \in X} p(x) log_b(p(x)) dx - \int_{x \in X} p(x) log_b(q(x)) dx = -\int_{x \in X} p(x) log_b(q(x)) dx = H(P,Q)$$

Example

Let's see if this equation works in practice as well.

In [17]:
```
def entropy(p):
    res = 0
    for x in range(len(p)):
        res -= p[x] * math.log(p[x])
    return res
```

Processing math: 96%

```
p = np.random.randint(1, 11, size=(20))
q = np.random.randint(1, 11, size=(20))

p = p / np.sum(p)
q = q / np.sum(q)

print("H(P)", entropy(p))
print("H(P, Q)", cross_entropy(p, q))
print("D_KL(P || Q)", relative_entropy(p, q))

print("H(P) + D_KL(P || Q) = ", entropy(p) + relative_entropy(p, q))
```

```
H(P) 2.8525747156989896
H(P, Q) 3.184719427881523
D_KL(P || Q) 0.33214471218253266
H(P) + D_KL(P || Q) =  3.184719427881522
```

Applications in machine learning

Because cross - entropy and relative entropy are both a way to measure how close two distributions are, they give us the idea of using them as a loss function (in neural networks etc).

Consider a neural network that solves a multi-class classification task. Each sample has a known class label with a probability of 1, and a probability of 0 for all other labels. A model can estimate the probability of an example belonging to each class label. Cross-entropy can then be used to calculate the difference between the two probability distributions. We can use the result as a error function and use various algorithms to minimize the loss functions (such as gradient descent). Using the cross-entropy error function instead of the sum-of-squares for a classification problem leads to faster training.

Let's name the known probability distribution of each class label for an example in the dataset P, and the probability distribution of each class label that is predicted by our model, Q. Our goal is to minimize $H(P, Q)$.

Minimizing the KL divergence and the cross entropy for a classification task are identical. which means Minimizing this KL divergence corresponds exactly to minimizing the cross-entropy between the distributions. Let's see why:

$$D_{KL}(P\ ||\ Q) = \sum_{x \in X} P(x) log_b(\frac{P(x)}{Q(x)}) = \sum_{x \in X} P(x) log_b(P(x)) - \sum_{x \in X} P(x) log_b(Q(x))$$

$$\frac{\partial D_{KL}(P\ ||\ Q)}{\partial \theta} = \frac{\partial \sum_{x \in X} P(x) log_b(P(x))}{\partial \theta} - \frac{\partial \sum_{x \in X} P(x) log_b(Q(x))}{\partial \theta}$$

We know that $P(x)$ is not a function of θ, so the first term would be 0:

$$\frac{\partial D_{KL}(P\ ||\ Q)}{\partial \theta} = - \frac{\partial \sum_{x \in X} P(x) log_b(Q(x))}{\partial \theta}$$

Which is equal to $\frac{\partial H(P, Q)}{\partial \theta}$.

So argmin.

If our problem is a binary classifaction, the formula would look like this:

H(P, Q) = -[P(0) \times log(Q(0)) + P(1) \times log(Q(1))]

Example

In this example, I'm gonna use mnist dataset for handwritten digits and train a model for classify handwritten digits.

Note: because the code would take between 10-20 minutes to run, I've already ran the code and got the results.

Here's the code:

```
import keras
from keras.datasets import mnist
from keras.models import Sequential
from keras.layers import Dense, Dropout, Flatten
from keras.layers import Conv2D, MaxPooling2D
from keras import backend as K

# the data, split between train and test sets
(x_train, y_train), (x_test, y_test) = mnist.load_data()

print(x_train.shape, y_train.shape)

x_train = x_train.reshape(x_train.shape[0], 28, 28, 1)
x_test = x_test.reshape(x_test.shape[0], 28, 28, 1)

num_classes = 10
input_shape = (28, 28, 1)
# convert class vectors to binary class matrices
```

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```
y_train = keras.utils.to_categorical(y_train, num_classes)
y_test = keras.utils.to_categorical(y_test, num_classes)
x_train = x_train.astype('float32')
x_test = x_test.astype('float32')
x_train /= 255
x_test /= 255
print('x_train shape:', x_train.shape)
print(x_train.shape[0], 'train samples')
print(x_test.shape[0], 'test samples')

batch_size = 128
epochs = 10
model = Sequential()
model.add(Conv2D(32, kernel_size=(3, 3),activation='relu',input_shape=input_shape))
model.add(Conv2D(64, (3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Dropout(0.25))
model.add(Flatten())
model.add(Dense(256, activation='relu'))
model.add(Dropout(0.5))
model.add(Dense(num_classes, activation='softmax'))
model.compile(loss=keras.losses.categorical_crossentropy,optimizer=keras.optimizers.Adadelta(),metrics=
['accuracy'])

hist = model.fit(x_train, y_train,batch_size=batch_size,epochs=epochs,verbose=1,validation_data=(x_test,
y_test))
print("The model has successfully trained")
model.save('mnist.h5')
print("Saving the model as mnist.h5")

score = model.evaluate(x_test, y_test, verbose=0)
print('Test loss:', score[0])
print('Test accuracy:', score[1])
```

The convolutional layers is not our concern here, the important part is that we're using `softmax` as activation functions and cross - entropy loss.

Here is the results:

```
(60000, 28, 28) (60000,)
x_train shape: (60000, 28, 28, 1)
60000 train samples
10000 test samples
Epoch 1/10
469/469 [==============================] - 169s 359ms/step - loss: 2.2857 - accuracy: 0.1480 -
val_loss: 2.2619 - val_accuracy: 0.3198
Epoch 2/10
469/469 [==============================] - 157s 335ms/step - loss: 2.2484 - accuracy: 0.2405 -
val_loss: 2.2167 - val_accuracy: 0.4422
Epoch 3/10
469/469 [==============================] - 155s 331ms/step - loss: 2.2001 - accuracy: 0.3377 -
val_loss: 2.1570 - val_accuracy: 0.5635
Epoch 4/10
469/469 [==============================] - 158s 337ms/step - loss: 2.1348 - accuracy: 0.4193 -
val_loss: 2.0718 - val_accuracy: 0.6495
Epoch 5/10
469/469 [==============================] - 163s 348ms/step - loss: 2.0396 - accuracy: 0.4967 -
val_loss: 1.9481 - val_accuracy: 0.6884
Epoch 6/10
469/469 [==============================] - 155s 331ms/step - loss: 1.9039 - accuracy: 0.5561 -
val_loss: 1.7733 - val_accuracy: 0.7254
Epoch 7/10
469/469 [==============================] - 156s 332ms/step - loss: 1.7234 - accuracy: 0.6085 -
val_loss: 1.5466 - val_accuracy: 0.7653
Epoch 8/10
469/469 [==============================] - 159s 340ms/step - loss: 1.5103 - accuracy: 0.6462 -
val_loss: 1.2962 - val_accuracy: 0.7854
Epoch 9/10
469/469 [==============================] - 163s 348ms/step - loss: 1.3003 - accuracy: 0.6765 -
val_loss: 1.0697 - val_accuracy: 0.8022
Epoch 10/10
469/469 [==============================] - 157s 336ms/step - loss: 1.1288 - accuracy: 0.6977 -
val_loss: 0.8963 - val_accuracy: 0.8173
The model has successfully trained
Saving the model as mnist.h5
Test loss: 0.8962876200675964
Test accuracy: 0.817300021648407
```

Resources

- Deep Learning Project – Handwritten Digit Recognition using Python

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- A Gentle Introduction to Cross-Entropy for Machine Learning
- An Introduction to Cross-Entropy Loss Functions
- Cross - entropy wikipedia page
- KL divergence wikipedia page
- Divergence wikipedia page)

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