Solution 1: Entropy

A fair die is rolled at the same time as a fair coin is tossed. Let A be the number on the upper surface of the die and let B describe the outcome of the coin toss, where

$$B = \begin{cases} 1, & \text{head}\,, \\ 0, & \text{tail}\,. \end{cases}$$

Two random variables X and Y are given by $X = A + B$ and $Y = A - B$, respectively.

(a) Calculate the entropies $H(X)$ and $H(Y)$, the conditional entropies $H(Y|X)$ and $H(X|Y)$, the joint entropy $H(X,Y)$ and the mutual information $I(X;Y)$.

Solution:

Let a, b, x, and y denote the realisations of the random variables A, B, X, and Y, respectively. Each event (a,b) is associated with exactly one event (x,y) and the probability for such an event is given by

$$p_{AB}(a,b) = p_{XY}(x,y) = \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{12}$$

Consequently, we obtain for the joint entropy

$$\begin{aligned} H(X,Y) &= -\sum_{x,y} p_{X,Y}(x,y) \log_2 p_{XY}(x,y) = -12 \cdot \frac{1}{12} \log_2 \frac{1}{12} \\ &= \log_2 12 \\ &= 2 + \log_2 3 \end{aligned}$$

Below we list the possible values of the random variables X and Y, the associated events (a,b), and the probability masses $p_X(x)$ and $p_Y(y)$.

x	events (a,b)	$p_X(x)$
1	$(1,0)$	1/12
2	$(2,0),(1,1)$	1/6
3	$(3,0),(2,1)$	1/6
4	$(4,0),(3,1)$	1/6
5	$(5,0),(4,1)$	1/6
6	$(6,0),(5,1)$	1/6
7	$(6,1)$	1/12

y	events (a,b)	$p_Y(y)$
0	$(1,1)$	1/12
1	$(1,0),(2,1)$	1/6
2	$(2,0),(3,1)$	1/6
3	$(3,0),(4,1)$	1/6
4	$(4,0),(5,1)$	1/6
5	$(5,0),(6,1)$	1/6
6	$(6,0)$	1/12

The random variable $X = A + B$ can take the values 1 to 7. The probability masses $p_X(x)$ for the values 1 and 7 are equal to 1/12, since they correspond to exactly one event. The probability masses for the values 2 to 6 are equal to 1/6, since each of these values corresponds to two events (a,b). An analogue result is obtained for the random variable $Y = A - B$.

The marginal entropies are given by

$$\begin{aligned} H(X) &= -\sum_{x} p_X(x) \log_2 p_X(x) \\ &= -2 \cdot \frac{1}{12} \log_2 \frac{1}{12} - 5 \cdot \frac{1}{6} \log_2 \frac{1}{6} \\ &= \frac{1}{6} \cdot (\log_2 4 + \log_2 3) + \frac{5}{6} \cdot (\log_2 2 + \log_2 3) \\ &= \frac{7}{6} + \log_2 3 \end{aligned}$$

and for Y

$$\begin{aligned}
H(Y) &= -\sum_y p_Y(y)\log_2 p_Y(y)\\
&= -2\cdot\frac{1}{12}\log_2\frac{1}{12} - 5\cdot\frac{1}{6}\log_2\frac{1}{6}\\
&= \frac{1}{6}\cdot(\log_2 4+\log_2 3) + \frac{5}{6}\cdot(\log_2 2+\log_2 3)\\
&= \frac{7}{6}+\log_2 3
\end{aligned}$$

We can determine the conditional entropies using

$$H(X|Y) = H(X,Y) - H(Y) = 2+\log_2 3 - \frac{7}{6} - \log_2 3 = \frac{5}{6}$$

$$H(Y|X) = H(X,Y) - H(X) = 2+\log_2 3 - \frac{7}{6} - \log_2 3 = \frac{5}{6}$$

The mutual information $I(X;Y)$ can be determined acording to

$$I(X;Y) = H(X) - H(X|Y) = \frac{7}{6}+\log_2 3 - \frac{5}{6} = \frac{1}{3}+\log_2 3$$

or

$$I(X;Y) = H(Y) - H(Y|X) = \frac{7}{6}+\log_2 3 - \frac{5}{6} = \frac{1}{3}+\log_2 3$$

(b) Show that, for independent discrete random variables X and Y,

$$I(X;X+Y) - I(Y;X+Y) = H(X) - H(Y)$$

Solution:

Using the definition of mutual information for discrete random variables, $I(X;Y) = H(Y) - H(Y|X)$, we can write

$$\begin{aligned}
I(X;X+Y) - I(Y;X+Y) &= H(X+Y) - H(X+Y|X) - H(X+Y) + H(X+Y|Y)\\
&= H(X|Y) - H(Y|X)\\
&= H(X) - H(Y)\,.
\end{aligned}$$

The first step follows from the fact that modifying the mean of a pmf doesn't change the entropy. For the second step, we used the fact that the conditional entropy $H(X|Y)$ is equal to the marginal entropy $H(X)$ for independent random variables X and Y.

Solution 2: Kullback-Leibler Divergence

(a) Let f be the pmf of the $Bin(n,p)$ distribution and q the density of the $\mathcal{N}(\mu,\sigma^2)$.

(i)

$$D_{KL}(f||q) = \mathbb{E}_f[\log\frac{f(X)}{q(X,\theta)}] = \mathbb{E}_f[\log f(X)] - \mathbb{E}_f[\log q(X|\theta)]$$

(ii) For the gradients, we must derive the partial derivatives of the second part of the KLD. The involved log-density is

$$\log q(X|\theta) = const. - 0.5\log\sigma^2 - \frac{1}{2\sigma^2}(X-\mu)^2.$$

$$\partial D_{KL}(f||q)/\partial\mu = \partial - \mathbb{E}_f\log[q(X|\theta)] = \mathbb{E}_f\frac{1}{\sigma^2}(X-\mu) \qquad (1)$$

$$\partial D_{KL}(f||q)/\partial\sigma^2 = \partial - \mathbb{E}_f \log[q(X|\theta)] = \mathbb{E}_f[\frac{1}{2\sigma^2} + \frac{-1}{2\sigma^4}(X-\mu)^2] \qquad (2)$$

(iii) Yes, there is. We can first set (1) to zero and get: $\mu = \mathbb{E}_f(X) \Leftrightarrow \mu = np$. We then use this solution for the second equation (2), which we also set to zero first:

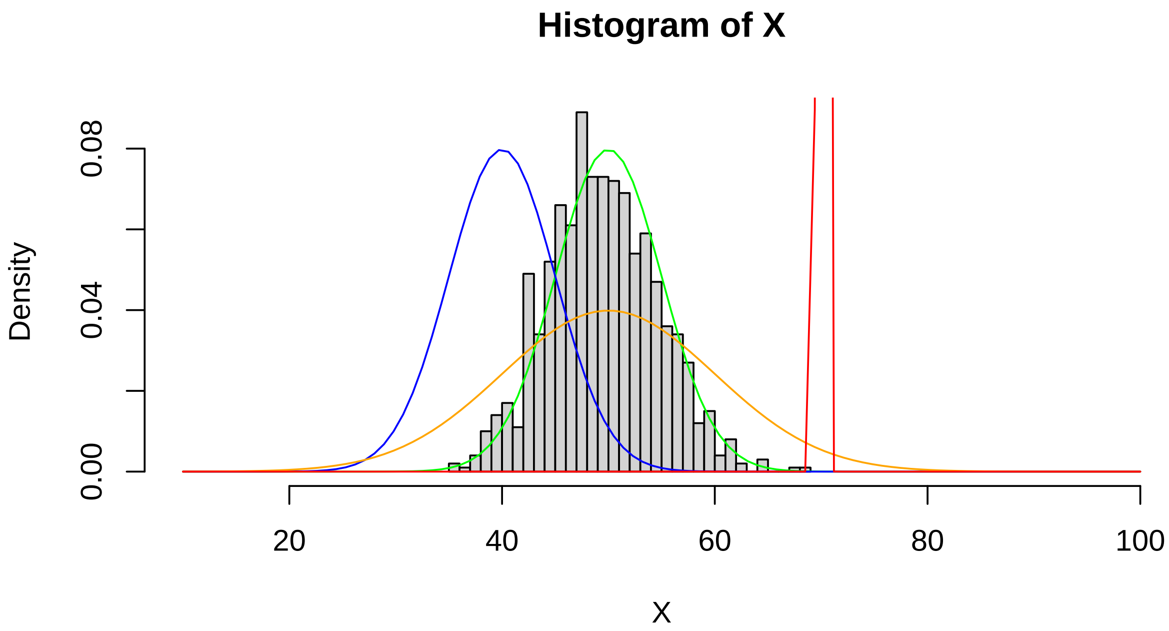
$$(2) = 0 \Leftrightarrow \sigma^2 = \mathbb{E}_f[(X-\mu)^2] = \mathrm{Var}_f(X) + (\mathbb{E}_f[X-\mu])^2 = np(1-p) + (\mathbb{E}_f[X-\mu])^2.$$

Using $\mu = np$, the second term vanishes and we get the optimal $\sigma^2 = np(1-p) = \mathrm{Var}_f(X)$. Note that we would have to prove that the second derivative is < 0 to be sure that we found a minimum!

(iv) We could, alternatively, use the gradients and do gradient descent to find the optimal $\boldsymbol{\theta}$.

(b)

```
nr_points = 1000
p = 0.5
n = 100
# create data
X <- rbinom(nr_points, prob = p, size = n)

# define different Normal density functions
normal_optimal <- function(x) dnorm(x, mean = n*p, sd = sqrt(n*p*(1-p)))
normal_shift <- function(x) dnorm(x, mean = n*p - 10, sd = sqrt(n*p*(1-p)))
normal_scale_increase <- function(x) dnorm(x, mean = n*p, sd = sqrt(n*p*(1-p))*2)
normal_right_scale_decrease <- function(x) dnorm(x, mean = n*p + 20, sd = p*(1-p))

hist(X, breaks = 25, xlim = c(10, 100), freq = FALSE)
curve(normal_optimal, from = 10, to = 100, add = TRUE, col = "green")
curve(normal_shift, from = 10, to = 100, add = TRUE, col = "blue")
curve(normal_scale_increase, from = 10, to = 100, add = TRUE, col = "orange")
curve(normal_right_scale_decrease, from = 10, to = 100, add = TRUE, col = "red")
```



For these distributions, we get the following KL divergence values (up to an additive constant):

$$D_{KL}(f||q) = const. + 0.5\log\sigma^2 + \frac{1}{2\sigma^2}(\mathrm{Var}_f(X) + (np-\mu)^2))$$

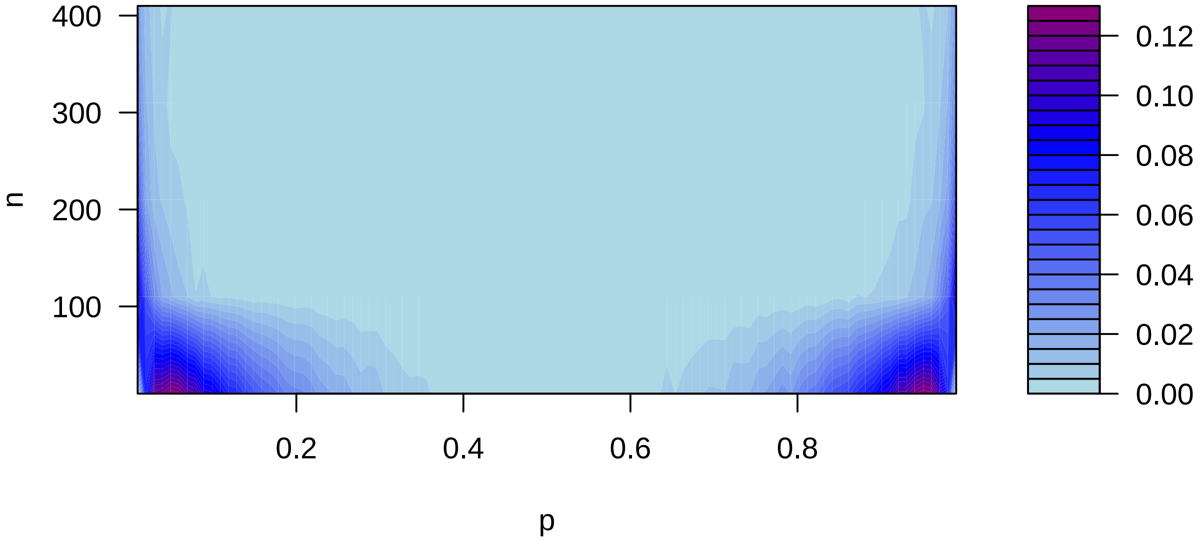
```
kld_value <- function(mu,sigma2)
{
  0.5*log(sigma2) +
    0.5 * (sigma2)^(-1) * (n*p*(1-p) + (n*p - mu)^2)
}
(optimal_green <- kld_value(n*p,n*p*(1-p)))

## [1] 2.109438

(shift_blue <- kld_value(n*p-10,n*p*(1-p)))

## [1] 4.109438

(scale_increase_orange <- kld_value(n*p,n*p*(1-p)*4))

## [1] 2.427585

(right_scale_decrease_red <- kld_value(n*p+20, (p*(1-p))^2))

## [1] 3398.614
```

(c) Since we are now required to calculate the exact KLD values, we would also have to calculate $\mathbb{E}_f(\log f(X))$, which is somewhat more difficult. If you search the internet for a solution (→ "entropy of a binomial distribution"), you will find an approximate solution using the de-Moivre-Laplace theorem. Alternatively, we could make use of the central limit theorem, but then we would just approximate f with a normal distribution with $\mu = np$ and $\sigma^2 = np(1-p)$, which would give us a constant KLD of zero (the very same happens if you use the first approximation using the de-Moivre-Laplace-theorem). We here instead will approximate the expectation using a large sample from the true underlying distribution:

$$D_{KL}(f||q) \approx \frac{1}{B}\sum_{b=1}^{B}[\log f(X) - \log q(X|\mu = np, \sigma^2 = np(1-p))]$$

```
p_seq <- seq(0.01, 0.99, l = 100)
n_seq <- seq(10, 500, by = 100)
B <- 10000

kld_value_approx <- function(n,p){

  # sample a large number of data points from true distribution
  x <- rbinom(B, prob = p, size = n)

  # approximate the mean; threshold values to 0 if < 0 due
  # to the approximation
  pmax(
    mean(
      dbinom(x, prob = p, size = n, log = TRUE) -
        dnorm(x, mean = n*p, sd = sqrt(n*p*(1-p)), log = TRUE),
      na.rm = TRUE
    ),
    0)

}

kld_val <- sapply(n_seq, function(this_n)
  sapply(p_seq, function(this_p) kld_value_approx(this_n, this_p)))
```

```
cols = rev(colorRampPalette(c('darkred','red','blue','lightblue'))(50))

filled.contour(x = p_seq, y = n_seq, z = kld_val,
               xlab = "p", ylab = "n",
               col = cols
               )
```



(d) Based on the previous result, one can see that the KLD is very close to zero but has larger values for very small or very large values of p and / in combination with a small number of experiments n. These are exactly the cases where the normal approximation of a binomial distribution does not work so well.