

### Solution 1: Kullback-Leibler Divergence and model misspecification

(a) The Kullback-Leibler Divergence is defined as:

$$\begin{aligned} D(g, f_\theta) &= \mathbb{E}_g \left[ \log \left( \frac{g(x)}{f_\theta(x)} \right) \right] \\ &= \underbrace{\mathbb{E}_g [\log(g(x))]}_{(a)} - \underbrace{\mathbb{E}_g [\log(f_\theta(x))]}_{(b)} \end{aligned} \quad (1)$$

As we are looking for the set of parameters  $\theta$  that minimizes  $D(g, f_\theta)$ , we know the following:

- (a) does not depend on  $\theta$ , and can be considered as a constant.
- To minimize  $D(g, f_\theta)$  is equivalent to maximize (b)

Using the definition of the normal distribution:

$$\begin{aligned} (b) &= \mathbb{E}_g [\log(f_\theta(x))] \\ &= \mathbb{E}_g \left[ \log \left( \frac{1}{\sqrt{\sigma^2 2\pi}} \right) - \frac{1}{2} \frac{(x - \mu)^2}{\sigma^2} \right] \\ &= \log \left( \frac{1}{\sqrt{\sigma^2 2\pi}} \right) - \mathbb{E}_g \left[ \frac{1}{2} \frac{(x - \mu)^2}{\sigma^2} \right] \\ &= -\log \sqrt{\sigma^2 2\pi} - \underbrace{\mathbb{E}_g \left[ \frac{1}{2} \frac{x^2 - 2x\mu + \mu^2}{\sigma^2} \right]}_{(c)} \end{aligned} \quad (2)$$

Solving the component (c) in the equation 2 we get:

$$\begin{aligned} (c) &= -\frac{1}{2\sigma^2} \underbrace{\mathbb{E}_g [x^2]}_{\text{Var}_g(x) + \mathbb{E}_g[x]^2} + \frac{2\mu}{2\sigma^2} \mathbb{E}_g[x] - \frac{\mu^2}{2\sigma^2} \\ &= -\frac{2\sigma_0^2 + \mu_0^2}{2\sigma^2} + \frac{\mu\mu_0}{\sigma^2} - \frac{\mu^2}{2\sigma^2} \end{aligned} \quad (3)$$

Using the results obtained in 2 and 3, we get the expression that we want to maximize:

$$(b) = -\log \sqrt{\sigma^2 2\pi} - \frac{2\sigma_0^2 + \mu_0^2}{2\sigma^2} + \frac{\mu\mu_0}{\sigma^2} - \frac{\mu^2}{2\sigma^2} \quad (4)$$

To maximize 4, we derive the expression with respect to each parameter. We also need to do a second derivative to be sure that the point is a maximum.

First, we derive with respect to the mean parameter  $\mu$ :

$$\frac{\partial(b)}{\partial\mu} = 0 - 0 + \frac{\mu_0}{\sigma^2} - \frac{\mu}{\sigma^2} \stackrel{!}{=} 0 \longrightarrow \mu_{opt} = \mu_0 \quad (5)$$

This value of  $\mu$  is a possible maximum, we check the second derivative:

$$\frac{\partial^2(b)}{\partial^2\mu} = -\frac{1}{\sigma^2} < 0 \quad (6)$$

As the second derivative is less than 0 at any point,  $\mu_{opt}$  maximizes (b) and minimizes the Kullback-Leibler divergence accordingly. We now derive with respect to the variance parameter  $\sigma^2$ :

$$\begin{aligned}
\frac{\partial(b)}{\partial\sigma^2} &= -\frac{1}{2\sigma^2} + \frac{2\sigma_0^2 + \mu_0^2}{2\sigma^4} - \frac{\mu\mu_0}{\sigma^4} + \frac{\mu^2}{2\sigma^4} \\
&= -\frac{1}{2\sigma^2} + \frac{2\sigma_0^2 + \mu_0^2 - 2\mu\mu_0 + \mu^2}{2\sigma^4} \\
&= -\frac{1}{2\sigma^2} + \frac{2\sigma_0^2 + (\mu - \mu_0)^2}{2\sigma^4} \stackrel{!}{=} 0 \longrightarrow \sigma_{opt}^2 = 2\sigma_0^2 + \underbrace{(\mu - \mu_0)^2}_{=0 \text{ if } \mu=\mu_{opt}}
\end{aligned} \tag{7}$$

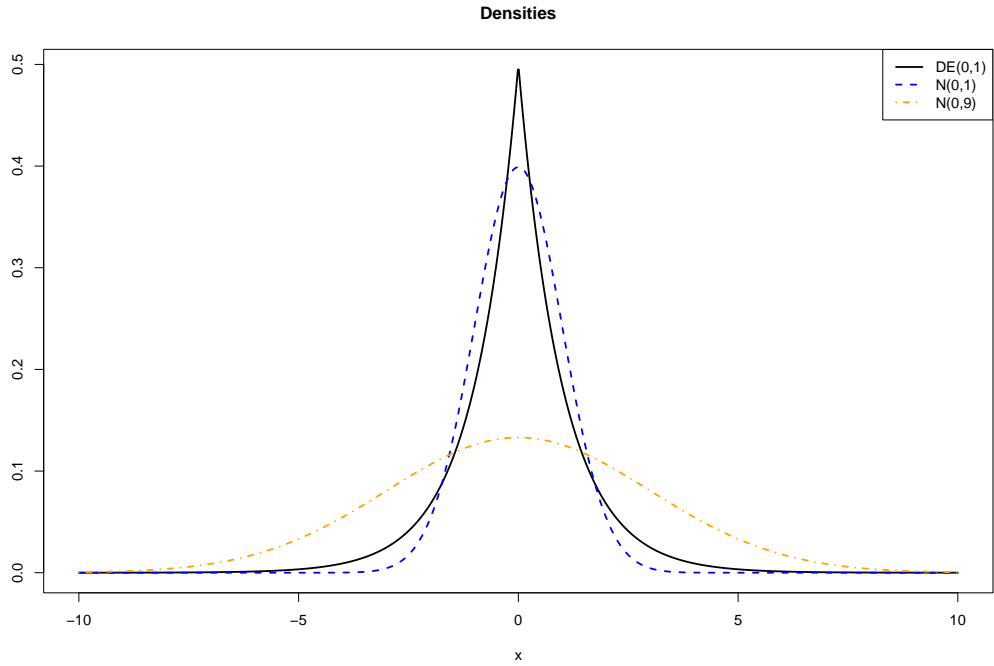
This value of  $\sigma^2$  is a possible maximum, we check the second derivative:

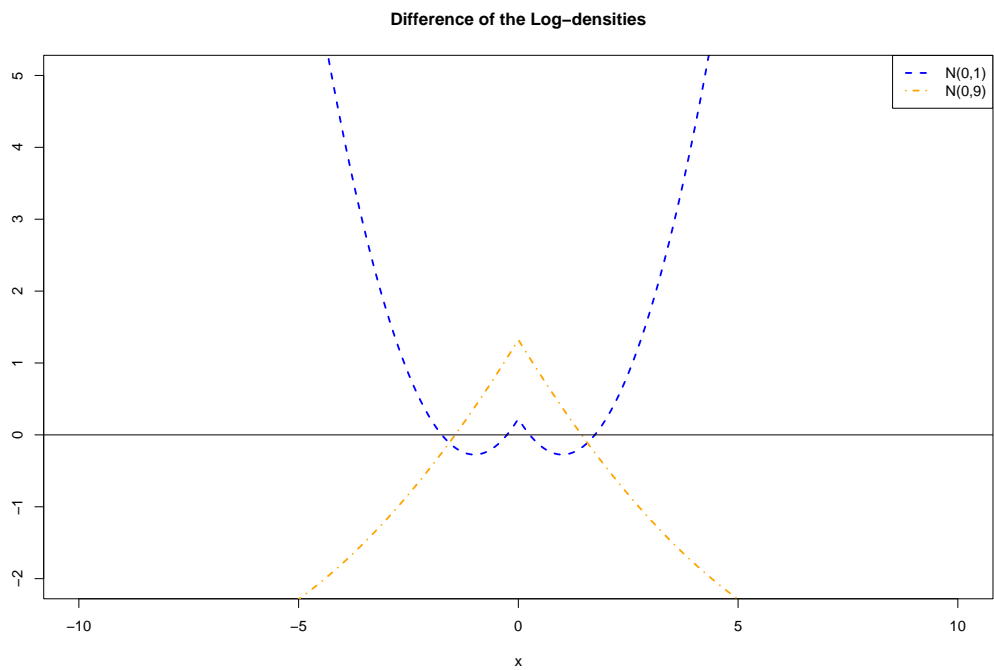
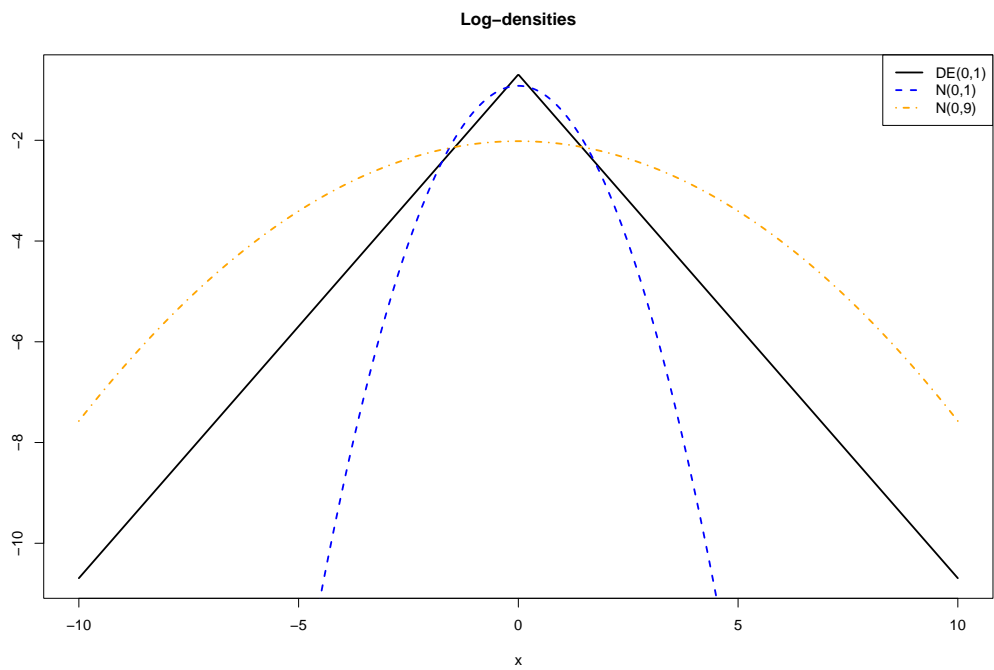
$$\begin{aligned}
\frac{\partial^2(b)}{\partial^2\sigma^2} &= \frac{1}{2\sigma^4} - \frac{(2\sigma_0^2 + (\mu - \mu_0)^2)}{\sigma^6} \\
\left. \frac{\partial^2(b)}{\partial^2\sigma^2} \right|_{\sigma^2=\sigma_{opt}^2} &= \frac{1}{2(2\sigma_0^2 + (\mu - \mu_0)^2)^2} - \frac{1}{(2\sigma_0^2 + (\mu - \mu_0)^2)^2} < 0
\end{aligned} \tag{8}$$

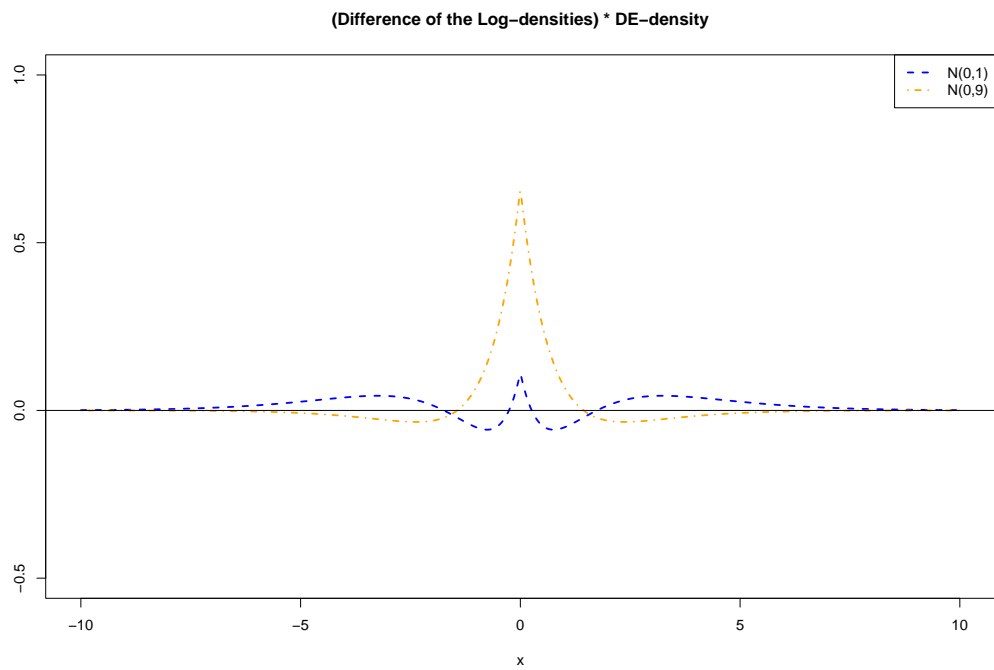
As the second derivative is less than 0 at the point we are looking,  $\sigma_{opt}^2$  maximizes (b) and thus minimizes the Kullback-Leibler Divergence.

The following graphs may be helpful to understand the problem:

- The KL-Divergence, step by step:

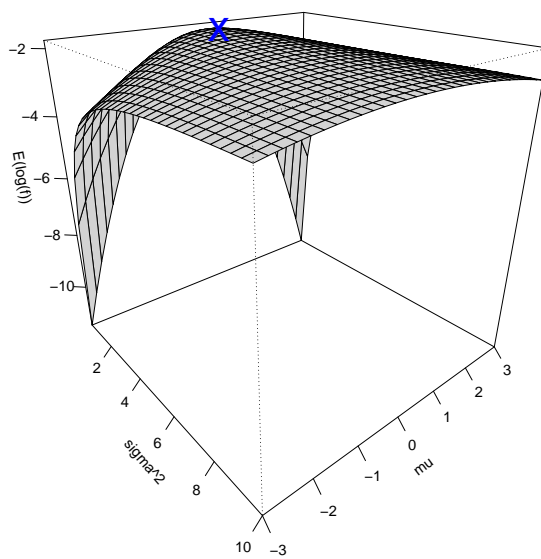


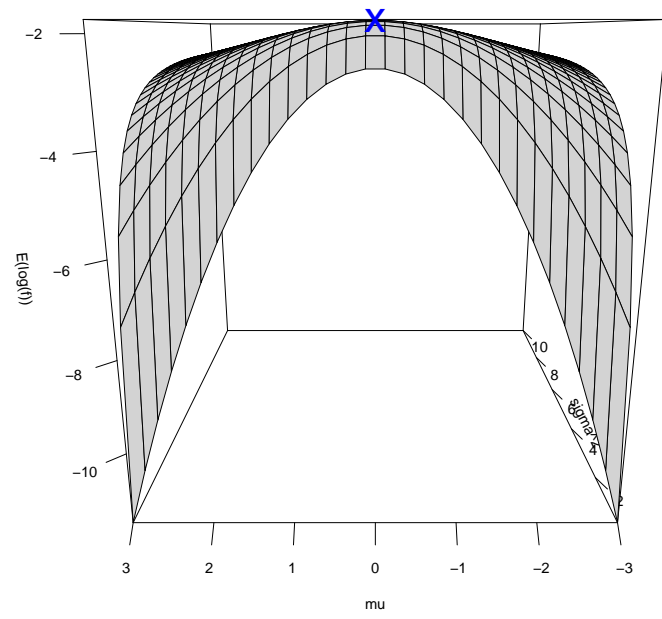
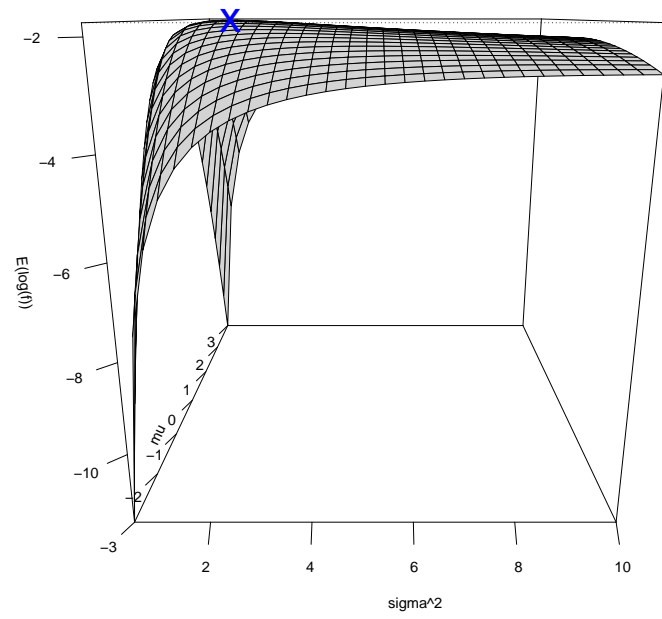




⇒ Now, the KLD is the integral of the function(s) in the last plot.

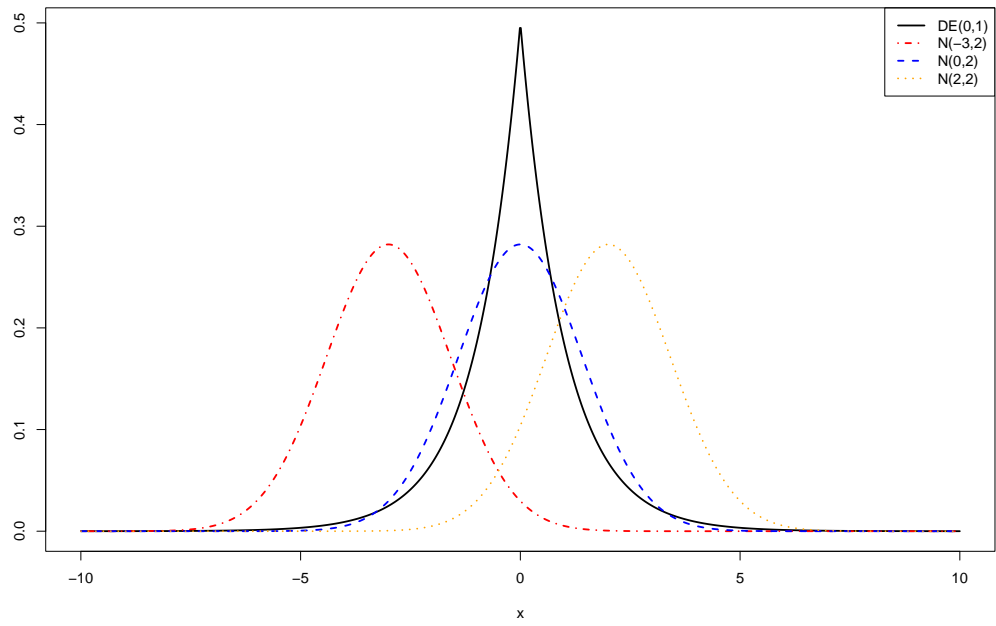
- 3D-Plot of the expression that we want to maximize ( for parameters  $\mu_0 = 0$  and  $\sigma_0 = 1$ ):





- Different configurations for the parameter  $\mu$  and the optimal configuration:

Same Variance



Original and misspecified density, with optimal parameters.

