



Lista 3, Verossimilhança (parte II)

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```
# packages =====  
library(bbmle)  
library(ggplot2)  
library(gridExtra)  
library(fishualize)  
library(mvtnorm)
```

Contents

Exercise 1: dist. Gaussiana com dados censurados/intervalares	3
(a) Escrever a função de verossimilhança.	3
(b) Obter as estimativas de máxima verossimilhança.	3
(c) Obter as verossimilhanças perfilhadas.	4
(d) Obter os erro-padrão das estimativas.	5
(e) Obter a aproximação quadrática da verossimilhança.	5
(f) Obter intervalos de confiança (verossimilhança e Wald) para os parâmetros.	8
Exercise 2: dist. Gaussiana bivariada	9
(a) Matriz de informação de Fisher	10
(b) Obtenha a verossimilhança conjunta de (σ^2, ρ) e compare I_{22} com I_{22}^{-1}	12
(c) Investigue como a aproximação quadrática se comporta. Tente transformações de ρ e σ^2 para obter uma função de verossimilhança mais regular	15
(d) Compare a verossimilhança de ρ baseada na transformação z de Fisher com a verossimilhança perfilhada	19
Exercise 3: regressão Gaussiana	22
(a) Encontre a função de verossimilhança	22
(b) Encontre as estimativas de máxima verossimilhança.	23
(c) Obtenha a verossimilhança conjunta para os parâmetros β_0 e β_1	23
Considerando σ fixo com valor igual à sua estimativa	23
Obtendo a verossimilhança perfilhada em relação a σ	25
(d) Obtenha a verossimilhança perfilhada para β_0 e β_1 individualmente	26
Exercise 4: regressão Gaussiana censurada	27
(a) Encontre a função de verossimilhança	28
(b) Encontre as estimativas de máxima verossimilhança.	28
(c) Obtenha a verossimilhança conjunta para os parâmetros β_0 e β_1	29
Considerando σ fixo com valor igual à sua estimativa	29
Obtendo a verossimilhança perfilhada em relação a σ	30
(d) Obtenha a verossimilhança perfilhada para β_0 e β_1 individualmente	32

Exercise 1: dist. Gaussiana com dados censurados/intervalares

Foram tomadas as seguintes observações independentes de uma v.a. $X \sim \text{Normal}(\mu, \sigma^2)$.

- 56.4, 54.2, 65.3, 49.2, 50.1, 56.9, 58.9, 62.5, 70, 61.
- Sabe-se que outras 5 observações são menores que 50.
- Sabe-se que outras 3 observações são maiores que 65.

(a) Escrever a função de verossimilhança.

The likelihood can be expressed as

$$\begin{aligned} L(\theta) &= \left(\prod_{i=1}^{10} f(x_i) \right) \times (F(50))^5 \times (1 - F(65))^3 \\ &= \left(\prod_{i=1}^{10} \phi \left(\frac{y_i - \mu}{\sigma} \right) \right) \times \left(\Phi \left(\frac{50 - \mu}{\sigma} \right) \right)^5 \times \left(1 - \Phi \left(\frac{65 - \mu}{\sigma} \right) \right)^3 \\ l(\theta) &= \sum_{i=1}^{10} \log \phi \left(\frac{y_i - \mu}{\sigma} \right) + 5 \log \Phi \left(\frac{50 - \mu}{\sigma} \right) + 3 \log \left(1 - \Phi \left(\frac{65 - \mu}{\sigma} \right) \right). \end{aligned}$$

<r code>

```
data_1 <- c(56.4, 54.2, 65.3, 49.2, 50.1, 56.9, 58.9, 62.5, 70, 61)
intervAussian_lkl <- function(mu, sigma) {
  component_1 <- sum(dnorm(data_1, mean = mu, sd = sigma, log = TRUE))
  component_2 <- 5 * log(pnorm(50, mean = mu, sd = sigma))
  component_3 <- 3 * log(1 - pnorm(65, mean = mu, sd = sigma))
  lkl <- component_1 + component_2 + component_3
  return(-lkl) ## minus, since the optim routine performs a minimization
}
```

(b) Obter as estimativas de máxima verossimilhança.

<r code>

```
model_fit <- mle2(intervAussian_lkl,
  start = list("mu" = mean(data_1), "sigma" = sd(data_1)))
(par_est <- model_fit@coef)
```

```
mu    sigma
56.33051 11.13274
```

FYI: In the ten points sample we have $\bar{x} = 58.45$ and $s^2 = 6.527$.

(c) Obter as verossimilhanças perfilhadas.

To obtain the likelihood profile for μ we need to create a grid of μ 's and for each value of this grid find the value, $\hat{\sigma}_\mu$, that maximizes the profile likelihood. We do this for μ and σ , the results can be seen in Figure 1.

<r code>

```
intervAussian_profile <- function(grid, fun, par_est, xlab, main) {
  ggplot() +
    geom_line(aes(x = grid, y = sapply(grid, fun)), size = 1.5) +
    geom_vline(xintercept = par_est, linetype = "dashed") +
    labs(x = xlab, y = NULL, title = main) +
    theme_minimal()
}
grid.arrange(
  intervAussian_profile(
    grid = seq(32, 77, .5),
    fun = function(i) {
      logLik(mle2(intervAussian_lkl,
                  start = list("sigma" = sd(data_1)),
                  data = list("mu" = i)))
    }, par_est = par_est[1], xlab = expression(mu),
    main = expression(
      "logLik for the optimal" ~ sigma ~ "given a fixed" ~ mu)),
  intervAussian_profile(
    grid = seq(5, 50, .5),
    fun = function(i) {
      logLik(mle2(intervAussian_lkl,
                  start = list("mu" = mean(data_1)),
                  data = list("sigma" = i)))
    }, par_est = par_est[2], xlab = expression(sigma),
    main = expression(
      "logLik for the optimal" ~ mu ~ "given a fixed" ~ sigma)),
  ncol = 2)
```

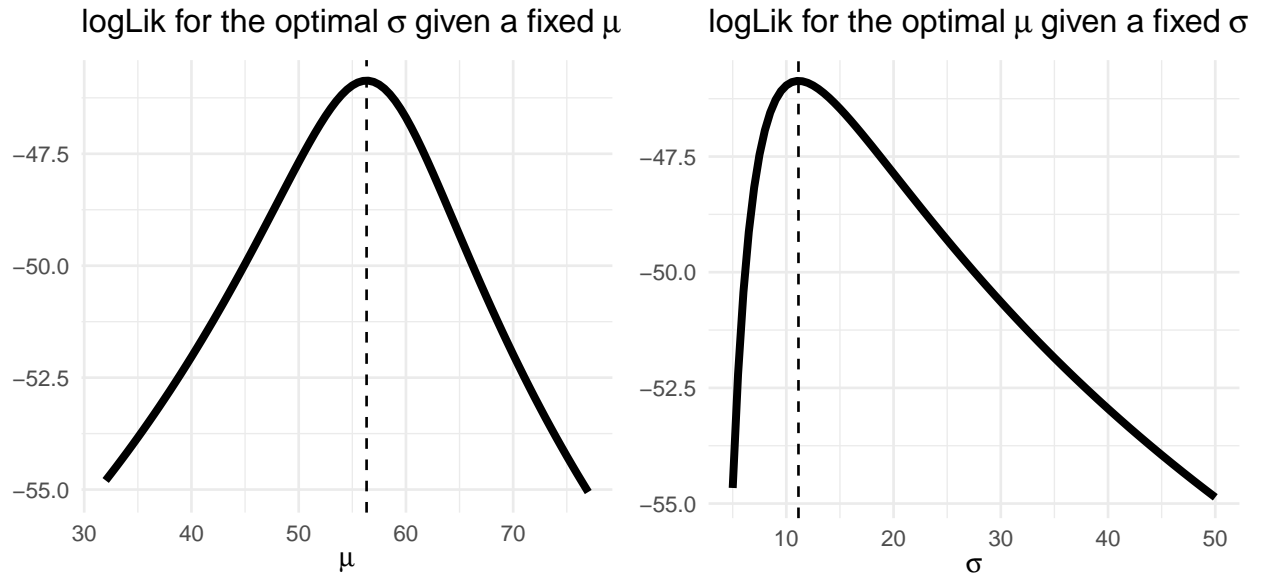


Figure 1: Profile log-likelihoods for μ and σ in a Gaussian sample made of interval/censored data. In dashed, the respective MLE's.

(d) Obter os erro-padrão das estimativas.

```
sqrt(diag(model_fit@vcov))
```

<r code>

```
mu    sigma
2.794350 2.791622
```

(e) Obter a aproximação quadrática da verossimilhança.

```
intervAussian_deviance <- function(mu_grid, sigma_grid) {
  lkl_grid <- intervAussian_lkl(mu_grid, sigma_grid)
  lkl_est <- intervAussian_lkl(par_est[1], par_est[2])
  return(2 * (lkl_grid - lkl_est))
}
intervAussian_deviance <- Vectorize(intervAussian_deviance,
                                   c("mu_grid", "sigma_grid"))
intervAussian_taylor <- function(mu, sigma) {
  par_grid <- c(mu, sigma)
```

<r code>

```

half <- (par_grid - model_fit@coef)
Ie <- solve(model_fit@vcov)
taylor <- logLik(model_fit) - .5 * half %*% Ie %*% half
return(taylor)
}
taylor_deviance <- function(mu_grid, sigma_grid) {
  taylor_grid <- intervAussian_taylor(mu_grid, sigma_grid)
  taylor_est <- intervAussian_taylor(par_est[1], par_est[2])
  return(-2 * (taylor_grid - taylor_est))
}
taylor_deviance <- Vectorize(taylor_deviance, c("mu_grid", "sigma_grid"))
mu_grid <- seq(40, 70, length.out = 50)
sigma_grid <- seq(0, 30, length.out = 50)
deviance_grid <- outer(mu_grid, sigma_grid, FUN = intervAussian_deviance)
taylor_grid <- outer(mu_grid, sigma_grid, FUN = taylor_deviance)

rownames(deviance_grid) <- rownames(taylor_grid) <- mu_grid
colnames(deviance_grid) <- colnames(taylor_grid) <- sigma_grid

deviance_grid <- reshape2::melt(deviance_grid)
taylor_grid <- reshape2::melt(taylor_grid)
contour_levels <- c(.99, .95, .9, .8, .7, .5, .3, .1, .05, .01)
ggplot() +
  theme_minimal() +
  stat_contour(data = deviance_grid,
              aes(Var1, Var2, z = value, fill = ..level..),
              geom = "polygon",
              breaks = qchisq(contour_levels, df = 2), alpha = .5) +
  stat_contour(data = taylor_grid,
              aes(Var1, Var2, z = value, fill = ..level..),
              geom = "polygon",
              breaks = qchisq(contour_levels, df = 2), alpha = .25) +
  guides(fill = "none") +
  scale_fill_fish(option = "Trimma_lantana", direction = -1) +
  labs(x = expression(mu), y = expression(sigma),
       title = "Deviance contours", subtitle = "MLE's, in white.") +
  geom_vline(xintercept = par_est[1], col = "white") +
  geom_hline(yintercept = par_est[2], col = "white")

```

Deviance contours
MLE's, in white.

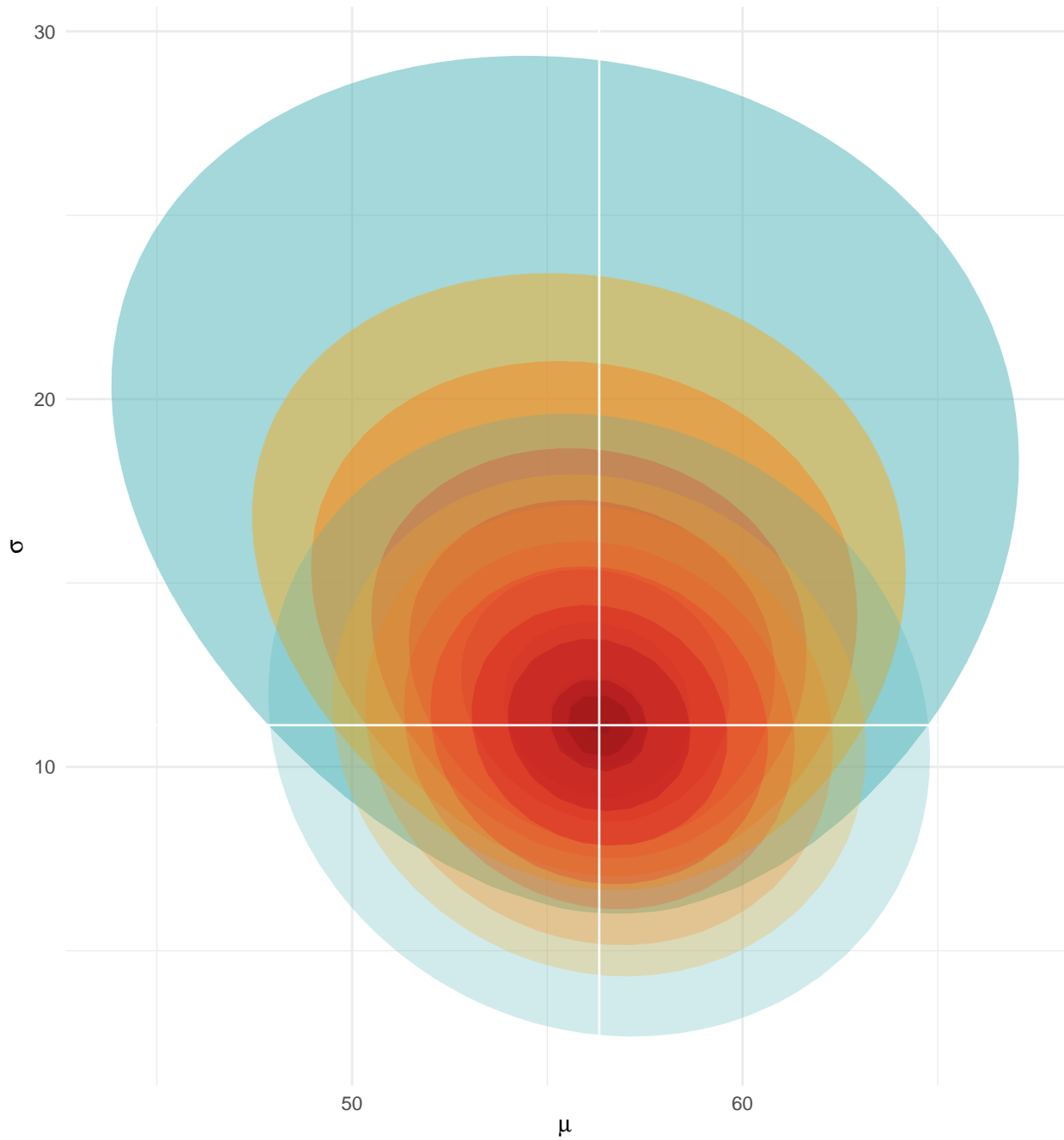


Figure 2: Deviances for the censored/interval Gaussian data. The bigger deviance is the true one, based in the log-likelihood. The smaller one, well-behaved, is based in the quadratic approximation (2nd order Taylor approximation) of the log-likelihood.

(f) Obter intervalos de confiança (verossimilhança e Wald) para os parâmetros.

In Figure 3 we see that the regions obtained from the two approaches are quite similar.

<r code>

```
mu_grid <- seq(55, 57.5, length.out = 50)
sigma_grid <- seq(10, 12.5, length.out = 50)

deviance_grid <- outer(mu_grid, sigma_grid, FUN = intervAussian_deviance)
taylor_grid <- outer(mu_grid, sigma_grid, FUN = taylor_deviance)

rownames(deviance_grid) <- rownames(taylor_grid) <- mu_grid
colnames(deviance_grid) <- colnames(taylor_grid) <- sigma_grid

deviance_grid <- reshape2::melt(deviance_grid)
taylor_grid <- reshape2::melt(taylor_grid)

contour_levels <- c(.95, .05, .01)
ggplot() +
  theme_minimal() +
  stat_contour(data = deviance_grid,
              aes(Var1, Var2, z = value, fill = ..level..),
              geom = "polygon",
              breaks = qchisq(contour_levels, df = 2),
              alpha = .5) +
  stat_contour(data = taylor_grid,
              aes(Var1, Var2, z = value, fill = ..level..),
              geom = "polygon",
              breaks = qchisq(contour_levels, df = 2),
              alpha = .25) +
  guides(fill = "none") +
  scale_fill_fish(option = "Cirrhilabrus_solorensis") +
  labs(x = expression(mu), y = expression(sigma),
       title = "99 and 95% deviance contours",
       subtitle = "MLE's, in white.") +
  geom_vline(xintercept = par_est[1], col = "white") +
  geom_hline(yintercept = par_est[2], col = "white")
```


99 and 95% deviance contours
MLE's, in white.

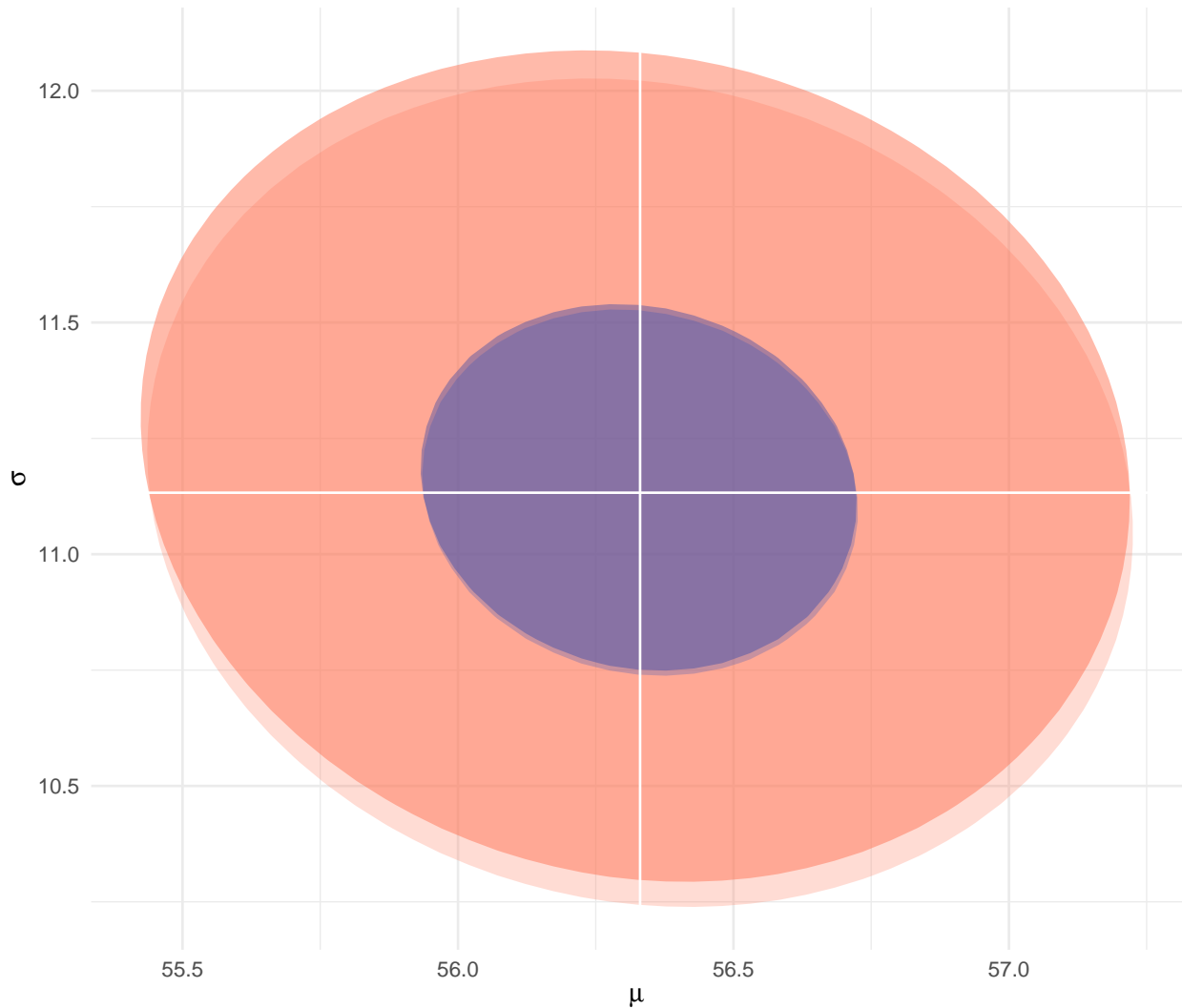


Figure 3: 99 and 95% confidence regions based on cut in the deviances. The stronger one is the likelihood-based, the other is the quadratic approximation (a.k.a., Wald based-interval).

Exercise 2: dist. Gaussiana bivariada

Seja $(x_i, y_i), \dots, (x_n, y_n)$ uma amostra aleatória de uma distribuição normal bivariada com média zero e matriz de covariância:

$$\Sigma = \sigma^2 \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}.$$

(a) Mostrar que a matriz de informação de Fisher é dada por

$$\begin{bmatrix} \frac{n}{\sigma^4} & -\frac{n\rho}{\sigma^2(1-\rho^2)} \\ -\frac{n\rho}{\sigma^2(1-\rho^2)} & \frac{n(1+\rho^2)}{1-\rho^2} \end{bmatrix}.$$

$$- \ln L(\sigma^2) = - \ln \sigma^2 - \frac{n}{2} \ln(1-R^2) - \frac{\sum x^2}{2(1-R^2)\sigma^2} + \frac{2R\sum xy}{2(1-R^2)\sigma^2} - \frac{\sum y^2}{2(1-R^2)\sigma^2}$$

$$l'(\sigma^2) = -\frac{n}{\sigma^2} + \frac{\sum x^2 - 2R\sum xy + \sum y^2}{2(1-R^2)\sigma^4}$$

$$l''(\sigma^2) = \frac{n}{\sigma^4} - \frac{\sum x^2 - 2R\sum xy + \sum y^2}{(1-R^2)\sigma^6}$$

$$E[-H] = \frac{1}{(1-R^2)\sigma^6} E[\sum x^2 - 2R\sum xy + \sum y^2] - \frac{n}{\sigma^4}$$

$$= \frac{1}{(1-R^2)\sigma^6} \left[n(W[X] + IE^2[X]) - 2RnIE[XY] + n(W[Y] + IE^2[Y]) \right] - \frac{n}{\sigma^4}$$

Figure 4: Verossimilhança, já em log, apenas com os componentes relevantes. Derivadas em relação a σ^2 e início do cálculo de seu componente na Informação de Fisher.

$$E[-H] = \frac{1}{(1-R^2)\sigma^2} [n\sigma^2 - 2RnIE[XY] + n\sigma^2] - \frac{n}{\sigma^4}$$

$$= \frac{2n(\sigma^2 - RIE[XY])}{(1-R^2)\sigma^6} - \frac{n}{\sigma^4} = \frac{2n(\sigma^2 - R(R\sigma^2))}{(1-R^2)\sigma^6} - \frac{n}{\sigma^4}$$

$$= \frac{2n\sigma^2(1-R^2)}{(1-R^2)\sigma^6} - \frac{n}{\sigma^4} = \frac{2n}{\sigma^4} - \frac{n}{\sigma^4} = \left[\frac{n}{\sigma^4} \right]$$

Figure 5: Componente 11 da Informação de Fisher de ordem 2x2.

$$\begin{aligned}
\frac{\partial^2 \ell}{\partial \sigma^2 \partial R} &= \frac{\partial}{\partial R} \left[\frac{\sum X^2}{2(1-R^2)\sigma^4} - \frac{2R\sum XY}{2(1-R^2)\sigma^4} + \frac{\sum Y^2}{2(1-R^2)\sigma^4} \right] \\
&= -\frac{\sum X^2 (1-R^2)^{-2} (-2R)}{2\sigma^4} - \frac{\sum XY (1-R^2)\sigma^4 - R\sum XY (-2R)\sigma^4}{[(1-R^2)\sigma^4]^2} - \frac{\sum Y^2 (1-R^2)^{-2} (-2R)}{2\sigma^4} \\
&= \frac{2R\sum X^2}{2(1-R^2)^2\sigma^4} - \frac{\sum XY (1-R^2)\sigma^4}{(1-R^2)^2\sigma^8} - \frac{2R^2\sigma^4\sum XY}{\sigma^8(1-R^2)^2} + \frac{2R\sum Y^2}{2(1-R^2)^2\sigma^4} \\
&= \frac{R\sum X^2}{(1-R^2)^2\sigma^4} - \frac{\sum XY}{(1-R^2)\sigma^4} - \frac{2R^2\sum XY}{(1-R^2)^2\sigma^4} + \frac{R\sum Y^2}{(1-R^2)^2\sigma^4} \\
&= \frac{R\sum X^2 - (1-R^2)\sum XY - 2R^2\sum XY + R\sum Y^2}{(1-R^2)^2\sigma^4} = \frac{R\sum X^2 - \sum XY - R^2\sum XY + R\sum Y^2}{(1-R^2)^2\sigma^4} \\
\text{IE}[-H] &= \frac{1}{(1-R^2)^2\sigma^4} \left[n\text{IE}[XY] + R^2 n\text{IE}[XY] - nR \left[\cancel{W[X]} + \text{IE}^2[X] \right] - nR \left[\cancel{W[Y]} + \text{IE}^2[Y] \right] \right] \\
&= \frac{1}{(1-R^2)^2\sigma^4} \left[\cancel{nr\sigma^2} + R^2 nr\sigma^2 - nr\sigma^2 - \cancel{nr\sigma^2} \right] = \frac{nr\sigma^2(R^2-1)}{(1-R^2)^2\sigma^4} = -\frac{(1-R^2)nr}{(1-R^2)^2\sigma^2} = \boxed{-\frac{nr}{(1-R^2)\sigma^2}}
\end{aligned}$$

Figure 6: Componente off-diagonal da Informação de Fisher de ordem 2x2.

$$\begin{aligned}
\dot{\ell}(R) &= -\frac{n}{2} \frac{1}{(1-R^2)} (-2R) - \frac{\sum X^2 (-1)(1-R^2)^{-2} (-2R)}{2\sigma^2} - \frac{\sum Y^2 (-1)(1-R^2)^{-2} (-2R)}{2\sigma^2} \\
&\quad + \frac{\sum XY (1-R^2)\sigma^2 - R\sum XY (-2R)\sigma^2}{(1-R^2)^2\sigma^4} \\
&= \frac{nr}{(1-R^2)} - \frac{R\sum X^2}{(1-R^2)^2\sigma^2} - \frac{R\sum Y^2}{(1-R^2)^2\sigma^2} + \frac{\sum XY\sigma^2(1-R^2) + 2R^2\sum XY\sigma^2}{(1-R^2)^2\sigma^4} \\
&= \frac{nr}{1-R^2} - \frac{R(\sum X^2 + \sum Y^2)}{(1-R^2)^2\sigma^2} + \frac{\sum XY\sigma^2 - \sum XY\sigma^2 R^2 + \sum XY\sigma^2 2R^2}{(1-R^2)^2\sigma^4} \\
\ddot{\ell}(R) &= \frac{n(1-R^2) - nr(-2R)}{(1-R^2)^2} - \frac{(\sum X^2 + \sum Y^2)(1-R^2)^2\sigma^2 - R(\sum X^2 + \sum Y^2)2\sigma^2(1-R^2)(-2R)}{(1-R^2)^4\sigma^4} \\
&\quad - \frac{2\sum XY\sigma^2 (-2R)}{(1-R^2)^3\sigma^4} + \frac{2R\sum XY\sigma^2(1-R^2)^2\sigma^4 - \sum XY\sigma^2 R^2 2(1-R^2)(-2R)\sigma^4}{(1-R^2)^4\sigma^8} \\
&= \frac{n - nr + 2nr}{(1-R^2)^2} - \frac{(\sum X^2 + \sum Y^2)\sigma^2(1-R^2)^2 + 4R^2\sigma^2(1-R^2)(\sum X^2 + \sum Y^2)}{(1-R^2)^4\sigma^4} \\
&\quad + \frac{4R\sum XY}{(1-R^2)^3\sigma^4} + \frac{2R\sigma^6\sum XY(1-R^2)^2 + 4R^3\sigma^6\sum XY(1-R^2)}{(1-R^2)^4\sigma^8} \\
&= \frac{n(1+R^2)}{(1-R^2)^2} - \frac{\sum X^2 + \sum Y^2}{(1-R^2)^2\sigma^2} - \frac{4R^2(\sum X^2 + \sum Y^2) + 4R\sum XY}{(1-R^2)^3\sigma^2} + \frac{2R\sum XY}{(1-R^2)^2\sigma^2} + \frac{4R^3\sum XY}{(1-R^2)^3\sigma^2}
\end{aligned}$$

Figure 7: Derivadas em relação a ρ .

$$\begin{aligned}
 E[-I''(R)] &= -\frac{n(1+R^2)}{(1-R^2)^2} + \frac{1}{(1-R^2)^2\sigma^2} [n(W[X] + E^2[X]) + n(W[Y] + E^2[Y])] + \frac{4R^2}{(1-R^2)^3\sigma^2} [n(W[X] + E^2[X]) + n(W[Y] + E^2[Y])] - \frac{4RnE[XY]}{(1-R^2)^3\sigma^2} \\
 &= -\frac{n(1+R^2)}{(1-R^2)^2} + \frac{1}{(1-R^2)^2\sigma^2} [n\sigma^2 + n\sigma^2] + \frac{4R^2}{(1-R^2)^3\sigma^2} [n\sigma^2 + n\sigma^2] - \frac{4RnR\sigma^2}{(1-R^2)^3\sigma^2} - \frac{2RnR\sigma^2}{(1-R^2)^3\sigma^2} - \frac{4R^3nR\sigma^2}{(1-R^2)^3\sigma^2} = \frac{-n-nR^2}{(1-R^2)^2} + \frac{2n\sigma^2}{(1-R^2)^2\sigma^2} + \frac{8nR^2}{(1-R^2)^3\sigma^2} - \frac{4nR^2\sigma^2}{(1-R^2)^3\sigma^2} \\
 &\quad - \frac{2nR^2\sigma^2}{(1-R^2)^2\sigma^2} - \frac{4nR^4}{(1-R^2)^3\sigma^2}
 \end{aligned}$$

Figure 8: Início do cálculo do componente 22, em relação a ρ , da Informação de Fisher de ordem 2x2.

$$\begin{aligned}
 &= \frac{-n-nR^2}{(1-R^2)^2} + \frac{2n-2nR^2}{(1-R^2)^2} + \frac{8nR^2-4nR^2-4nR^4}{(1-R^2)^3} \\
 &= \frac{n-3nR^2}{(1-R^2)^2} + \frac{4nR^2-4nR^4}{(1-R^2)^3} \\
 &= \frac{n-3nR^2}{(1-R^2)^2} + \frac{4nR^2(1-R^2)}{(1-R^2)^3} \\
 &= \frac{n-3nR^2+4nR^2}{(1-R^2)^2} = \frac{n(1+R^2)}{(1-R^2)^2}
 \end{aligned}$$

FISHER INFORMATION MATRIX

$$\begin{bmatrix} \frac{n}{\sigma^4} & -\frac{nR}{(1-R^2)\sigma^2} \\ -\frac{nR}{(1-R^2)\sigma^2} & \frac{n(1+R^2)}{(1-R^2)^2} \end{bmatrix}$$

Figure 9: Componente 22 e matriz, completa, de Informação de Fisher.

(b) Considere os dados a seguir assumindo que a média é conhecida no valor observado de forma que os valores podem ser centrados. Obtenha a verossimilhança conjunta de (σ^2, ρ) . Compare I_{22} com I_{22}^{-1} e comente os resultados.

```

data_2 <- data.frame(x = c(109, 96, 109, 114, 85, 113, 107, 101,
                        88, 96, 116, 96, 100, 117, 104, 81),
                   y = c(116, 95, 113, 109, 91, 115, 100, 95,
                        77, 79, 122, 94, 88, 119, 115, 90))

```

<r code>

```

bigaussian <- function(sigma2, rho, z = FALSE,
                      logsigma2 = FALSE, logisticrho = FALSE) {
  if (z) rho <- (exp(2 * rho) - 1)/(1 + exp(2 * rho))
  if (logsigma2) sigma2 <- exp(sigma2)
  if (logisticrho) rho <- qlogis(rho)
  lkl <- sum(dmvnorm(data_2,
                    mean = apply(data_2, 2, mean),
                    sigma = sigma2 * matrix(c(1, rho, rho, 1), 2),
                    log = TRUE))
  return(-lkl)
}
model_fit <- mle2(bigaussian, start = list("sigma2" = 150, "rho" = .5))
(par_est <- model_fit@coef)

```

<r code>

```

      sigma2      rho
150.008070  0.792046

```

```

bigaussian_deviance <- function(sigma2_grid, rho_grid, z = FALSE,
                               logsigma2 = FALSE, logisticrho = FALSE) {
  lkl_grid <- bigaussian(sigma2_grid, rho_grid, z, logsigma2, logisticrho)
  lkl_est <- bigaussian(par_est[1], par_est[2], z, logsigma2, logisticrho)
  return(2 * (lkl_grid - lkl_est))
}
bigaussian_deviance <- Vectorize(bigaussian_deviance,
                                c("sigma2_grid", "rho_grid"))

```

```

sigma2_grid <- seq(70, 535, length.out = 50)
rho_grid <- seq(.25, .95, length.out = 50)

```

```

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance)
rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid

```

```

deviance_grid <- reshape2::melt(deviance_grid)

contour_levels <- c(.99, .95, .9, .8, .7, .5, .3, .1, .05, .01)
ggplot() +
  theme_minimal() +
  stat_contour(data = deviance_grid,
              aes(Var1, Var2, z = value, fill = ..level..),
              geom = "polygon",
              breaks = qchisq(contour_levels, df = 2)) +
  guides(fill = "none") +
  scale_fill_fish(option = "Trimma_lantana", direction = -1) +
  labs(x = expression(sigma^2), y = expression(rho),
       title = "Deviance contour", subtitle = "MLE's, in white.") +
  geom_vline(xintercept = par_est[1], col = "white") +
  geom_hline(yintercept = par_est[2], col = "white")

```

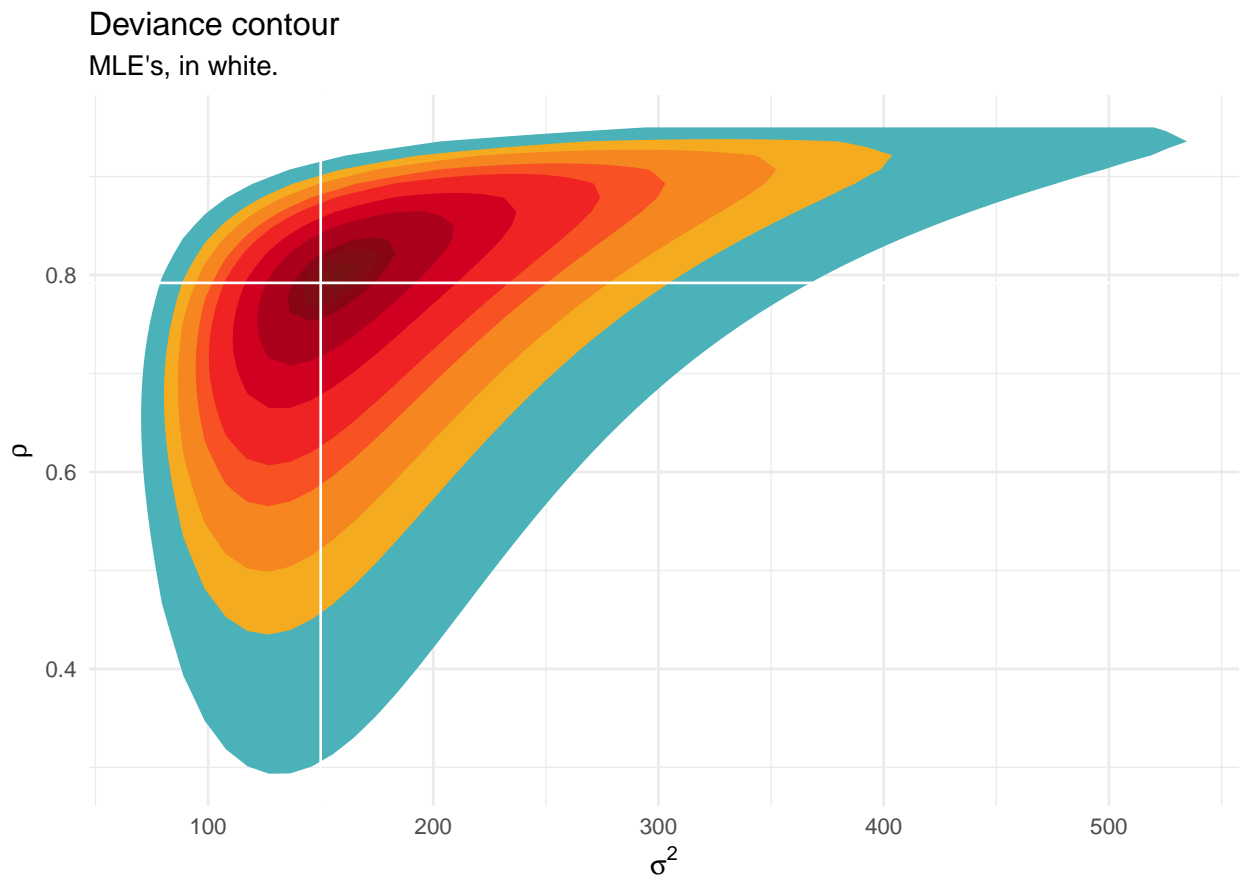


Figure 10: Deviance contour of a bivariate Gaussian of zero mean.

(c) Investigue como a aproximação quadrática se comporta neste problema. Tente transformações de ρ e σ^2 para obter uma função de verossimilhança mais regular.

<r code>

```
bigaussian_taylor <- function(sigma2, rho) {
  par_grid <- c(sigma2, rho)
  half <- (par_grid - par_est)
  Ie <- solve(model_fit@vcov)
  taylor <- logLik(model_fit) - .5 * half %*% Ie %*% half
  return(taylor)
}
taylor_deviance <- function(sigma2_grid, rho_grid) {
  taylor_grid <- bigaussian_taylor(sigma2_grid, rho_grid)
  taylor_est <- bigaussian_taylor(par_est[1], par_est[2])
  return(-2 * (taylor_grid - taylor_est))
}
taylor_deviance <- Vectorize(taylor_deviance, c("sigma2_grid", "rho_grid"))
sigma2_grid <- seq(10, 290, length.out = 50)
rho_grid <- seq(.5, 1.1, length.out = 50)
taylor_grid <- outer(sigma2_grid, rho_grid, FUN = taylor_deviance)
rownames(taylor_grid) <- sigma2_grid
colnames(taylor_grid) <- rho_grid
taylor_grid <- reshape2::melt(taylor_grid)
grid.arrange(
  ggplot() +
  theme_minimal() +
  stat_contour(data = taylor_grid, geom = "polygon",
              aes(Var1, Var2, z = value, fill = ..level..),
              breaks = qchisq(contour_levels, df = 2)) +
  guides(fill = "none") +
  scale_fill_fish(option = "Trimma_lantana", direction = -1) +
  labs(x = expression(sigma^2), y = expression(rho),
       title = "Deviance of the quadratic approx.",
       subtitle = "MLE's, in white.", tag = "A") +
  geom_vline(xintercept = par_est[1], col = "white") +
  geom_hline(yintercept = par_est[2], col = "white"),
  ggplot() +
```

```

theme_minimal() +
stat_contour(data = deviance_grid, geom = "polygon",
            aes(Var1, Var2, z = value, fill = ..level..),
            breaks = qchisq(contour_levels, df = 2), alpha = .5) +
stat_contour(data = taylor_grid, geom = "polygon",
            aes(Var1, Var2, z = value, fill = ..level..),
            breaks = qchisq(contour_levels, df = 2), alpha = .75) +
guides(fill = "none") +
scale_fill_fish(option = "Trimma_lantana", direction = -1) +
labs(x = expression(sigma^2), y = expression(rho),
     title = "Deviance contours",
     subtitle = "MLE's, in white.", tag = "B") +
geom_vline(xintercept = par_est[1], col = "white") +
geom_hline(yintercept = par_est[2], col = "white"), ncol = 2)

```

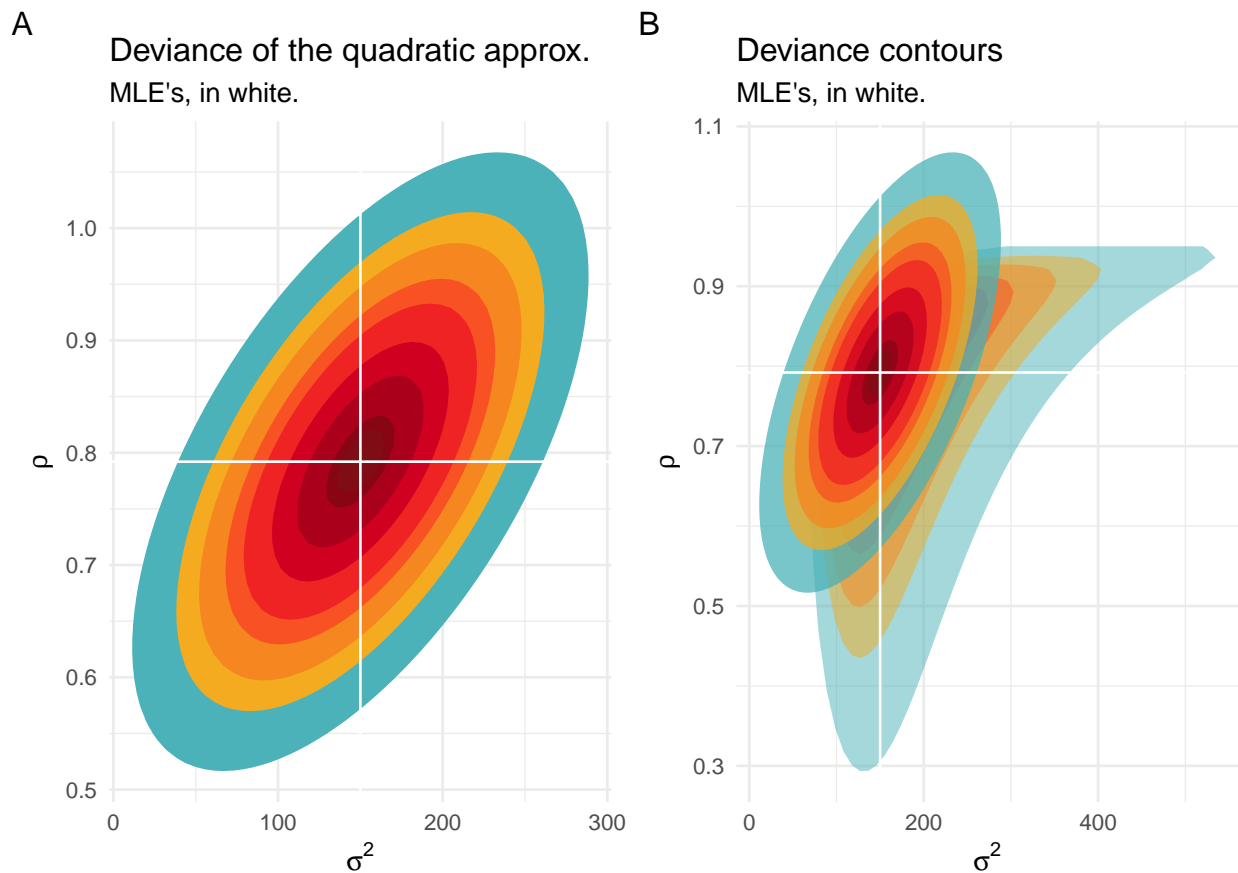


Figure 11: A: Deviance contour of the quadratic approximation for a bivariate Gaussian with zero mean; B: Quadratic approx. added into the original likelihood-based deviance contour.

<r code>

```
bigaussian_trans <- function(dataset, xlab, ylab, tag, par_est) {
  ggplot() +
    theme_minimal() +
    stat_contour(data = dataset,
                 aes(Var1, Var2, z = value, fill = ..level..),
                 geom = "polygon",
                 breaks = qchisq(contour_levels, df = 2)) +
    guides(fill = "none") +
    scale_fill_fish(option = "Trimma_lantana", direction = -1) +
    labs(x = xlab, y = ylab, tag = tag) +
    geom_vline(xintercept = par_est[1], col = "white") +
    geom_hline(yintercept = par_est[2], col = "white")
}

## transforming only sigma2 =====
par_est <- mle2(bigaussian,
               start = list("sigma2" = log(150), "rho" = .5),
               data = list(logsigma2 = TRUE))@coef

sigma2_grid <- seq(log(70), log(535), length.out = 50)
rho_grid <- seq(.25, .95, length.out = 50)

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance,
                      logsigma = TRUE)

rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid

deviance_grid <- reshape2::melt(deviance_grid)

p1 <- bigaussian_trans(dataset = deviance_grid,
                      xlab = expression(log(sigma^2)),
                      ylab = expression(rho),
                      tag = "A", par_est = par_est)

## transforming only rho =====
par_est <- mle2(bigaussian,
               start = list("sigma2" = 150, "rho" = plogis(.5)),
               data = list(logisticrho = TRUE))@coef
```

```

sigma2_grid <- seq(70, 535, length.out = 50)
rho_grid <- seq(plogis(.25), plogis(.95), length.out = 50)

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance,
                       logisticrho = TRUE)

rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid

deviance_grid <- reshape2::melt(deviance_grid)

p2 <- bigaussian_trans(dataset = deviance_grid,
                      xlab = expression(sigma^2),
                      ylab = expression(logistic(rho)),
                      tag = "B", par_est = par_est)
## transforming both parameters =====
par_est <- mle2(bigaussian,
               start = list("sigma2" = log(150), "rho" = plogis(.5)),
               data = list(logsigma2 = TRUE, logisticrho = TRUE))@coef

sigma2_grid <- seq(log(70), log(535), length.out = 50)
rho_grid <- seq(plogis(.25), plogis(.95), length.out = 50)

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance,
                       logsigma2 = TRUE, logisticrho = TRUE)

rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid

deviance_grid <- reshape2::melt(deviance_grid)

p3 <- bigaussian_trans(dataset = deviance_grid,
                      xlab = expression(log(sigma^2)),
                      ylab = expression(logistic(rho)),
                      tag = "C", par_est = par_est)
## plotting everything =====
grid.arrange(p1, p2, p3, ncol = 3)

```

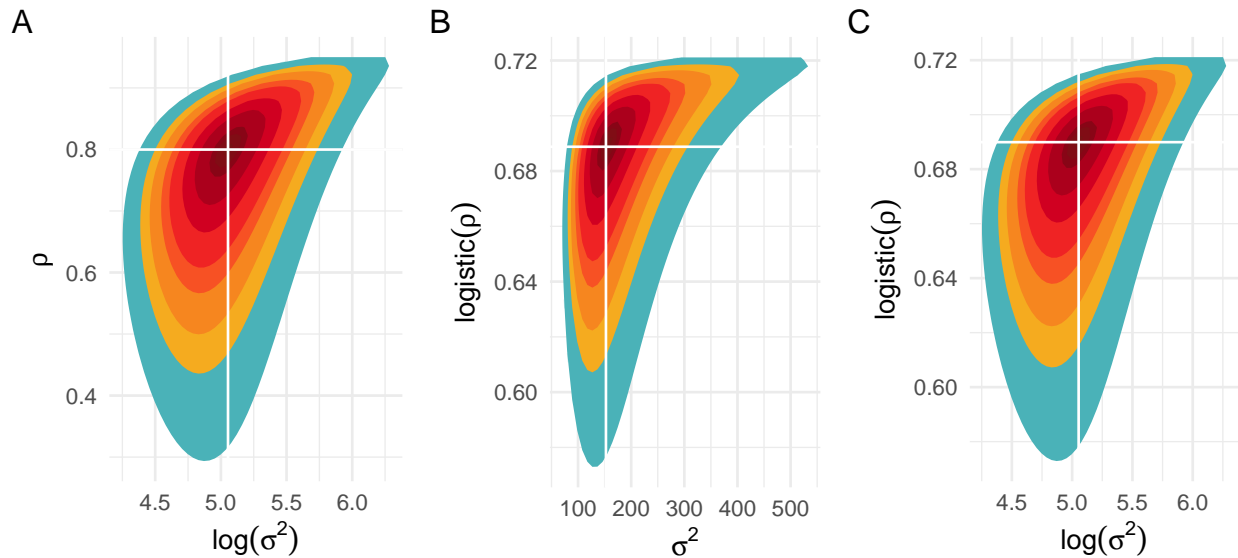


Figure 12: Deviance contours for different parameter transformations. Since here the parameter ρ is positive, we applied the logistic function. In white, the MLE's.

(d) A chamada transformação z de Fisher da correlação amostral é dada por

$$z = \frac{1}{2} \log \frac{1 + \hat{\rho}}{1 - \hat{\rho}}.$$

Compare a verossimilhança de ρ baseada na transformação z de Fisher com a verossimilhança perfilhada.

```

## original scale =====<
model_fit <- mle2(bigaussian, start = list("sigma2" = 150, "rho" = .5))
par_est <- model_fit@coef

sigma2_grid <- seq(70, 535, length.out = 50)
rho_grid <- seq(.25, 1, length.out = 50)

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance)
rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid
deviance_grid <- reshape2::melt(deviance_grid)

```

<r code>

```

p1 <- bigaussian_trans(dataset = deviance_grid,
                      xlab = expression(sigma^2),
                      ylab = expression(rho),
                      par_est = par_est, tag = "A.1") +
  labs(title = "Original Deviance contour")

data_profile <- as.data.frame(profile(model_fit, which = "rho"))

my_profile <- function(dataset, xlab, main, tag) {
  dataset <- subset(dataset, abs(z) < 3)
  ggplot(dataset, aes(x = focal, y = abs(z))) +
    geom_line(size = 1) + geom_point(size = 2) + theme_minimal() +
    labs(x = xlab, title = main, tag = tag)
}

p3 <- my_profile(data_profile, xlab = expression(rho), tag = "A.2",
                main = expression(rho ~ "likelihood profile"))
## fisher z-transformation =====
model_fit <- mle2(bigaussian,
                 start = list("sigma2" = 150,
                              "rho" = .5 * (log(1 + .5) - log(1 - .5))),
                 data = list(z = TRUE))
par_est <- model_fit@coef

ztrans <- function(rho) .5 * (log(1 + rho) - log(1 - rho))
rho_grid <- sapply(seq(-1, 1, length.out = 50), function(i) ztrans(i))

deviance_grid <- outer(sigma2_grid, rho_grid, FUN = bigaussian_deviance,
                      z = TRUE)
rownames(deviance_grid) <- sigma2_grid
colnames(deviance_grid) <- rho_grid
deviance_grid <- reshape2::melt(deviance_grid)

p2 <- bigaussian_trans(dataset = deviance_grid,
                      xlab = expression(sigma^2),
                      ylab = expression(z(rho)), par_est = par_est,
                      tag = "B.1") +
  labs(title = expression("with Fisher z-transformation in" ~ rho))

```

```

data_profile <- as.data.frame(profile(model_fit, which = "rho"))

p4 <- my_profile(data_profile, xlab = expression(z(rho)), tag = "B.2",
                 main = expression(z(rho) ~ "likelihood profile"))
## plotting =====
grid.arrange(p1, p2, p3, p4, nrow = 2, ncol = 2)

```

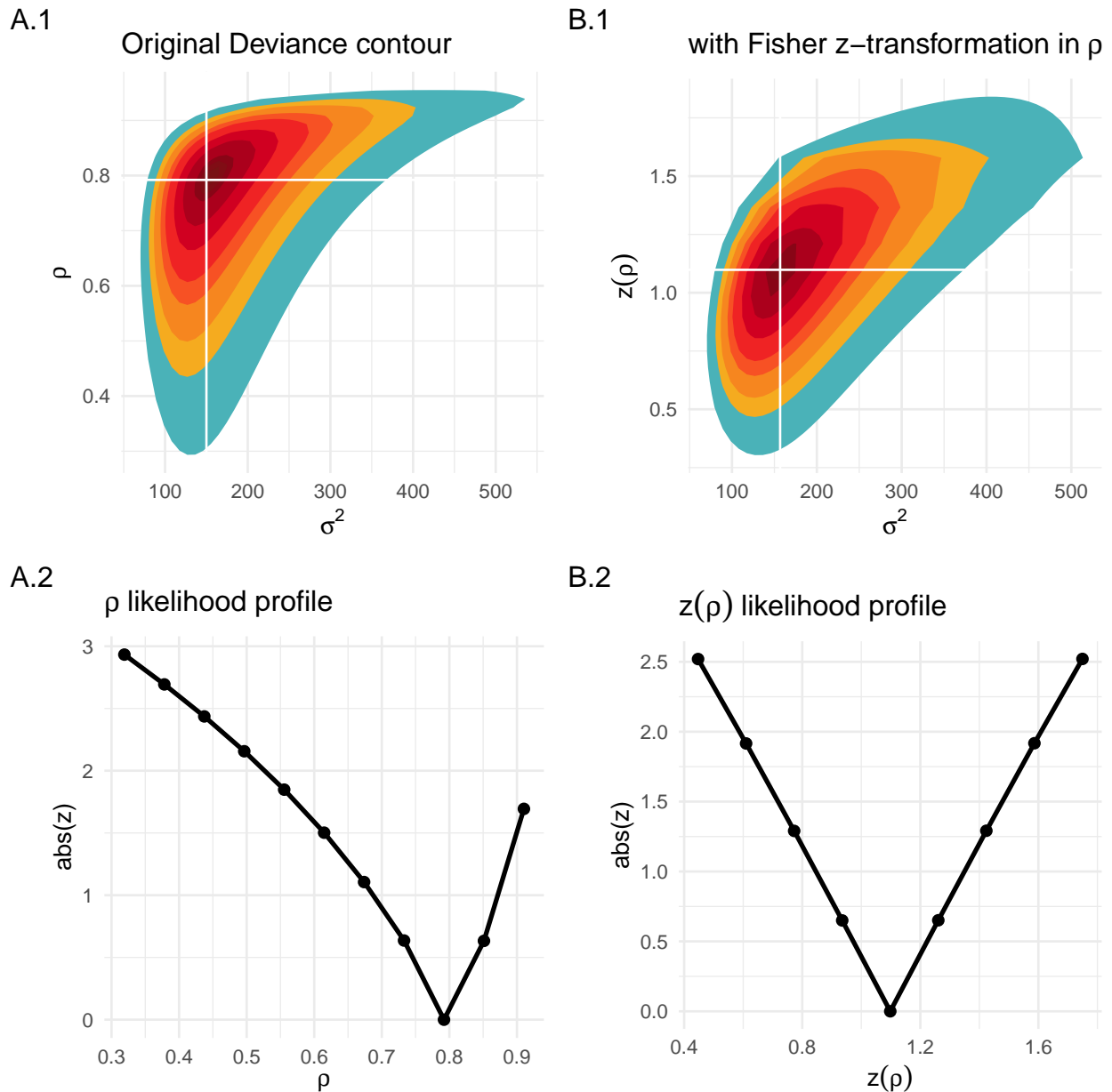


Figure 13: A: original likelihood. A.1 is the deviance contour, A.2 is the likelihood profile for ρ ; B: applying the Fisher z-transformation in ρ . B.1 is the resulting deviance contour, B.2 is the likelihood profile for $z(\rho)$.

Exercise 3: regressão Gaussiana

Considere os dados da tabela a seguir (adaptados/modificados de Montgomery & Runger, 1994) aos quais deseja-se ajustar um modelo de regressão linear simples relacionando a variável resposta Y (pureza em %) a uma variável explicativa X (nível de hidrocarbonetos).

X	0.99	1.02	1.15	1.29	1.46	1.36	0.87	1.23	1.55	1.40
Y	99.01	89.05	91.43	93.74	96.73	94.45	87.59	91.77	99.42	93.65
X	1.19	1.15	0.98	1.01	1.11	1.20	1.26	1.32	1.43	0.95
Y	93.54	92.52	90.56	89.54	89.85	90.39	93.25	93.41	94.98	87.33

<r code>

```
data_3 <- data.frame(  
  x = c(.99, 1.02, 1.15, 1.29, 1.46, 1.36, .87, 1.23, 1.55, 1.4,  
        1.19, 1.15, .98, 1.01, 1.11, 1.2, 1.26, 1.32, 1.43, .95),  
  y = c(99.01, 89.05, 91.43, 93.74, 96.73, 94.45, 87.59, 91.77, 99.42,  
        93.65, 93.54, 92.52, 90.56, 89.54, 89.85, 90.39, 93.25, 93.41,  
        94.98, 87.33))
```

(a) Encontre a função de verossimilhança.

Assuming a Normal distribution for $Y|X$, we have the following log-likelihood, in matrixial form

$$\begin{aligned}l(\theta; Y) &= -\frac{n}{2} \log 2\pi - n \log \sigma - \frac{1}{2\sigma^2} \|Y - X\beta\|^2 \\ &= \text{constant} - n \log \sigma - \frac{1}{2\sigma^2} \|Y - X\beta\|^2,\end{aligned}$$

were $\theta = [\beta_0 \ \beta_1 \ \sigma]^\top$, $\beta = [\beta_0 \ \beta_1]^\top$, and $\mu_i = \beta_0 + \beta_1 x_i$.

<r code>

```
gaussian3_reg <- function(b0, b1, sigma) {  
  mu <- b0 + b1 * data_3$x  
  lkl <- sum(dnorm(data_3$y, mean = mu, sd = sigma, log = TRUE))  
  return(-lkl)  
}
```

(b) Encontre as estimativas de máxima verossimilhança.

```
model_fit <- mle2(gaussian3_reg,                                     <r code>
                  start = list(b0 = min(data_3$y), b1 = 1.5,
                               sigma = sd(data_3$y)))
(par_est <- model_fit@coef)

      b0      b1      sigma
77.988429 12.225489  2.343799
```

Just checking...

```
lm(y ~ x, data_3)$coef # beta_0 and beta_1                                     <r code>

(Intercept)          x
  77.98996    12.22453

par_est[[3]]**2 # sigma^2

[1] 5.493392

(summary(lm(y ~ x, data_3))$sigma**2) * (nrow(data_3) - 2) / nrow(data_3)

[1] 5.493386
```

Checked, ✓.

(c) Obtenha a verossimilhança conjunta para os parâmetros β_0 e β_1 :

Considerando σ fixo com valor igual à sua estimativa,

```
gaussian3_deviance <- function(b0_grid, b1_grid, theta_est) {          <r code>
  b0_est <- theta_est[[1]]
  b1_est <- theta_est[[2]]
  sigma_est <- theta_est[[3]]
  lk1_grid <- gaussian3_reg(b0_grid, b1_grid, sigma_est)
  lk1_est <- gaussian3_reg(b0_est, b1_est, sigma_est)
```

```

    return(2 * (lkl_grid - lkl_est))
  }
  gaussian3_deviance <- Vectorize(gaussian3_deviance,
                                c("b0_grid", "b1_grid"))
  b0_grid <- seq(67, 89, length.out = 50)
  b1_grid <- seq(3, 21, length.out = 50)
  deviance_grid <- outer(b0_grid, b1_grid, FUN = gaussian3_deviance,
                        theta_est = par_est)
  rownames(deviance_grid) <- b0_grid
  colnames(deviance_grid) <- b1_grid
  deviance_grid <- reshape2::melt(deviance_grid)
  bigaussian_trans(deviance_grid,
                  xlab = expression(beta[0]), ylab = expression(beta[1]),
                  tag = NULL, par_est = par_est) +
  labs(title = "Deviance contour", subtitle = "MLE's, in white.")

```

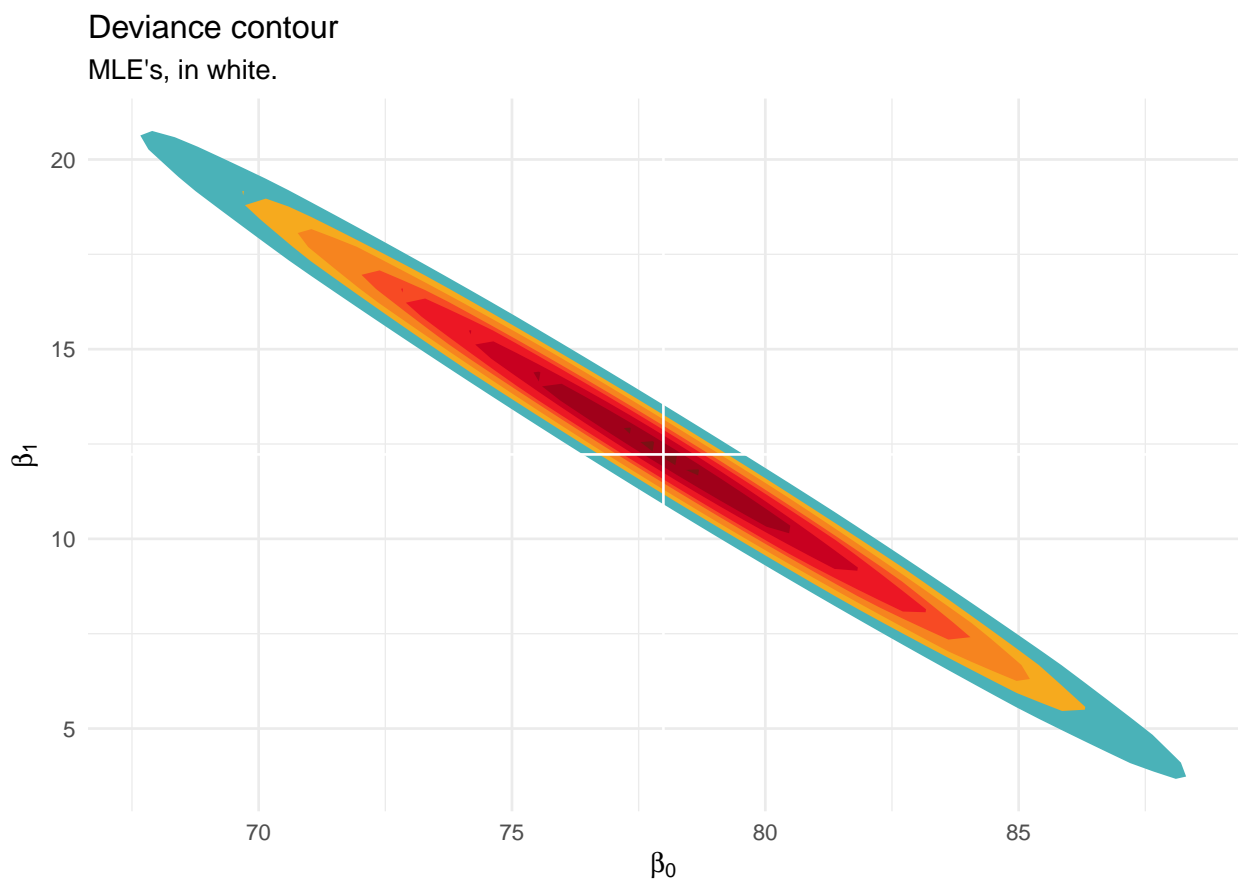


Figure 14: Deviance contour for the β 's of a simple Gaussian linear regression with the standard deviation fixed in it's MLE.

Obtendo a verossimilhança perfilhada em relação a σ .

```
sigma_grid <- seq(1, 15, length.out = 50)
beta_perf <- matrix(0, nrow = length(sigma_grid), ncol = 3)
for (i in seq(sigma_grid)) {
  beta_perf[i, ] <- unlist(
    mle2(gaussian3_reg, start = list(b0 = min(data_3$y), b1 = 1.5),
      data = list(sigma = sigma_grid[i]))@details[1:2])
}
ggplot() + theme_minimal() +
  geom_line(aes(x = sigma_grid, y = -beta_perf[ , 3]), size = 1.5) +
  geom_vline(xintercept = par_est[3], linetype = "dashed") +
  labs(x = expression(sigma), y = NULL,
    title = expression(sigma ~ "profile likelihood"),
    subtitle = "MLE, in dashed.")
```

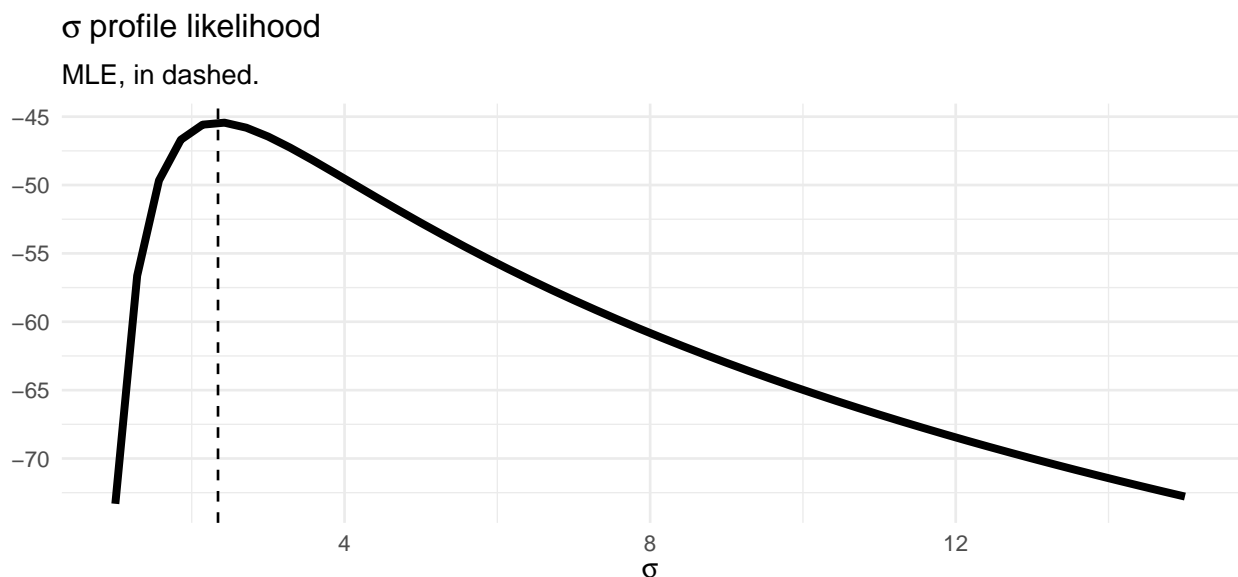


Figure 15: σ profile likelihood in a simple Gaussian linear regression. In dashed, the MLE.

And how the β 's fluctuates across the grid of σ ?

```
summary(beta_perf[ , 1]) # beta_0
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
77.99	77.99	78.02	78.04	78.07	78.20

```
summary(beta_perf[ , 2]) # beta_1
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
12.05	12.15	12.20	12.19	12.22	12.23

Very few, as expected. Since the estimation of β doesn't depend on σ .

(d) Obtenha a verossimilhança perfilhada para os parâmetros β_0 e β_1 individualmente.

```
coef_profile <- function(grid, coef = c("b0", "b1")) {                                     <r code>
  n <- length(grid)
  prof <- numeric(n)
  for (i in seq(n)) {
    prof[i] <-
      switch(coef,
              "b0" = mle2(gaussian3_reg,
                          start = list(b1 = 1.5),
                          data = list(b0 = grid[i],
                                      sigma = par_est[[3]])
                          )@details$value,
              "b1" = mle2(gaussian3_reg,
                          start = list(b0 = min(data_3$y)),
                          data = list(b1 = grid[i],
                                      sigma = par_est[[3]])
                          )@details$value)
  }
  return(-prof)
}
## beta_0 =====
b0_grid <- seq(56, 100, length.out = 50)
p1 <- ggplot() + theme_minimal() +
  geom_line(aes(x = b0_grid, y = coef_profile(b0_grid, "b0")),
            size = 1.5) +
  geom_vline(xintercept = par_est[1], linetype = "dashed") +
  labs(x = expression(beta[0]), y = NULL,
       title = expression(beta[0] ~ "profile likelihood"),
```

```

      subtitle = "MLE, in dashed.", tag = "A")
## beta_1 =====
b1_grid <- seq(-6, 30, length.out = 50)
p2 <- ggplot() + theme_minimal() +
  geom_line(aes(x = b1_grid, y = coef_profile(b1_grid, "b1")),
            size = 1.5) +
  geom_vline(xintercept = par_est[2], linetype = "dashed") +
  labs(x = expression(beta[1]), y = NULL,
       title = expression(beta[1] ~ "profile likelihood"),
       subtitle = "MLE, in dashed.", tag = "B")
## plotting =====
grid.arrange(p1, p2, ncol = 2)

```

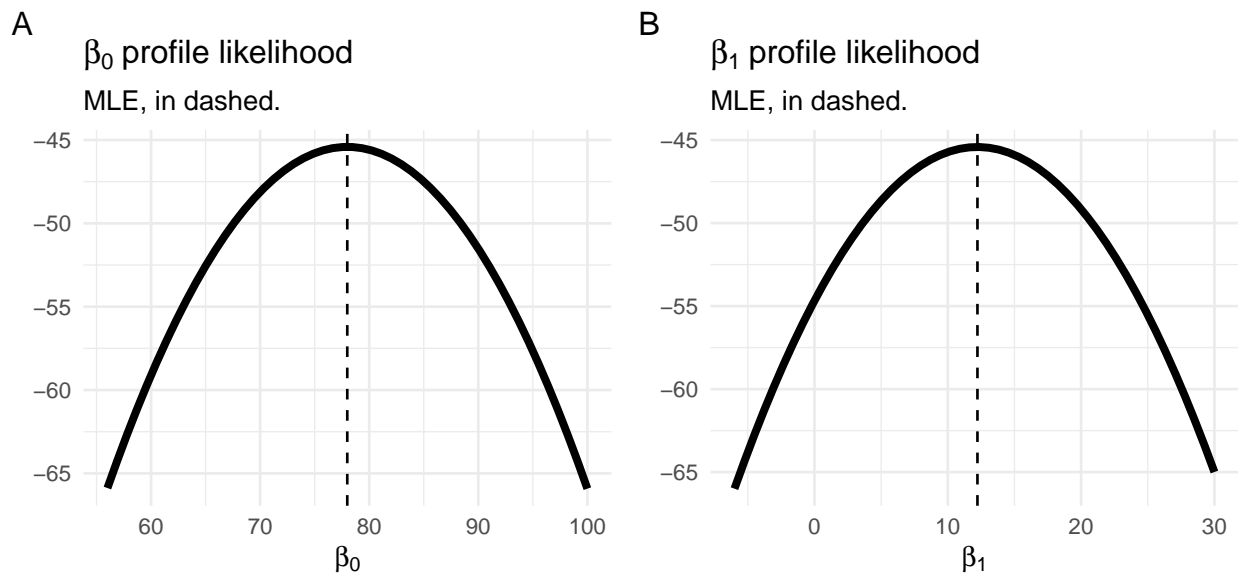


Figure 16: Profile likelihoods for β_0 and β_1 in a simple Gaussian linear regression. In dashed, the MLE's.

Exercise 4: regressão Gaussiana censurada

Repita o exercício anterior porém considerando os dados modificados como indicado na tabela a seguir.

X	0.99	1.02	1.15	1.29	1.46	1.36	0.87	1.23	1.55	1.40
Y	99.01	≤ 90	91.43	[91, 95]	96.73	94.45	87.59	91.77	[96, 100]	93.65
X	1.19	1.15	0.98	1.01	1.11	1.20	1.26	1.32	1.43	0.95
Y	≥ 92.5	92.52	90.56	89.54	89.85	[89, 93]	93.25	93.41	≥ 93	87.33

(a) Encontre a função de verossimilhança.

<r code>

```
data_4 <- data.frame(
  x = c(.99, 1.15, 1.46, 1.36, .87, 1.23, 1.4,
        1.15, .98, 1.01, 1.11, 1.26, 1.32, .95),
  y = c(99.01, 91.43, 96.73, 94.45, 87.59, 91.77, 93.65,
        92.52, 90.56, 89.54, 89.85, 93.25, 93.41, 87.33))

gaussian4_reg <- function(b0, b1, sigma) {
  mu <- b0 + b1 * data_4$x
  lkl_exact <- sum(dnorm(data_4$y, mean = mu, sd = sigma, log = TRUE))
  ##-----
  lkl_1 <- log(pnorm(90, mean = b0 + b1 * 1.02, sd = sigma))
  ##-----
  lkl_2 <- log(pnorm(95, mean = b0 + b1 * 1.29, sd = sigma) -
              pnorm(91, mean = b0 + b1 * 1.29, sd = sigma))
  ##-----
  lkl_3 <- log(pnorm(100, mean = b0 + b1 * 1.55, sd = sigma) -
              pnorm(96, mean = b0 + b1 * 1.55, sd = sigma))
  ##-----
  lkl_4 <- log(1 - pnorm(92.5, mean = b0 + b1 * 1.19, sd = sigma))
  ##-----
  lkl_5 <- log(pnorm(93, mean = b0 + b1 * 1.20, sd = sigma) -
              pnorm(89, mean = b0 + b1 * 1.20, sd = sigma))
  ##-----
  lkl_6 <- log(1 - pnorm(93, mean = b0 + b1 * 1.43, sd = sigma))
  return(-(lkl_exact + lkl_1 + lkl_2 + lkl_3 + lkl_4 + lkl_5 + lkl_6))
}
```

(b) Encontre as estimativas de máxima verossimilhança.

```
model_fit <- mle2(gaussian4_reg,
                 start = list(b0 = min(data_4$y), b1 = 1.5,
                              sigma = sd(data_4$y)))
```

<r code>

```
(par_est <- model_fit@coef)
```

```
      b0      b1      sigma
78.410145 11.869453 2.432607
```

Considering only the exact observations, we get these β 's

<r code>

```
lm(y ~ x, data_4)
```

Call:

```
lm(formula = y ~ x, data = data_4)
```

Coefficients:

```
(Intercept)          x
      80.58         10.04
```

(c) Obtenha a verossimilhança conjunta para os parâmetros β_0 e β_1 :

Considerando σ fixo com valor igual à sua estimativa,

```
gaussian4_deviance <- function(b0_grid, b1_grid, theta_est) {
  b0_est <- theta_est[[1]]
  b1_est <- theta_est[[2]]
  sigma_est <- theta_est[[3]]
  lkl_grid <- gaussian4_reg(b0_grid, b1_grid, sigma_est)
  lkl_est <- gaussian4_reg(b0_est, b1_est, sigma_est)
  return(2 * (lkl_grid - lkl_est))
}
gaussian4_deviance <- Vectorize(gaussian4_deviance,
                               c("b0_grid", "b1_grid"))
b0_grid <- seq(67, 90, length.out = 50)
b1_grid <- seq(2, 22, length.out = 50)
```

<r code>

```

deviance_grid <- outer(b0_grid, b1_grid, FUN = gaussian4_deviance,
                      theta_est = par_est)
rownames(deviance_grid) <- b0_grid
colnames(deviance_grid) <- b1_grid
deviance_grid <- reshape2::melt(deviance_grid)
bigaussian_trans(deviance_grid,
                 xlab = expression(beta[0]), ylab = expression(beta[1]),
                 tag = NULL, par_est = par_est) +
labs(title = "Deviance contour", subtitle = "MLE's, in white.")

```

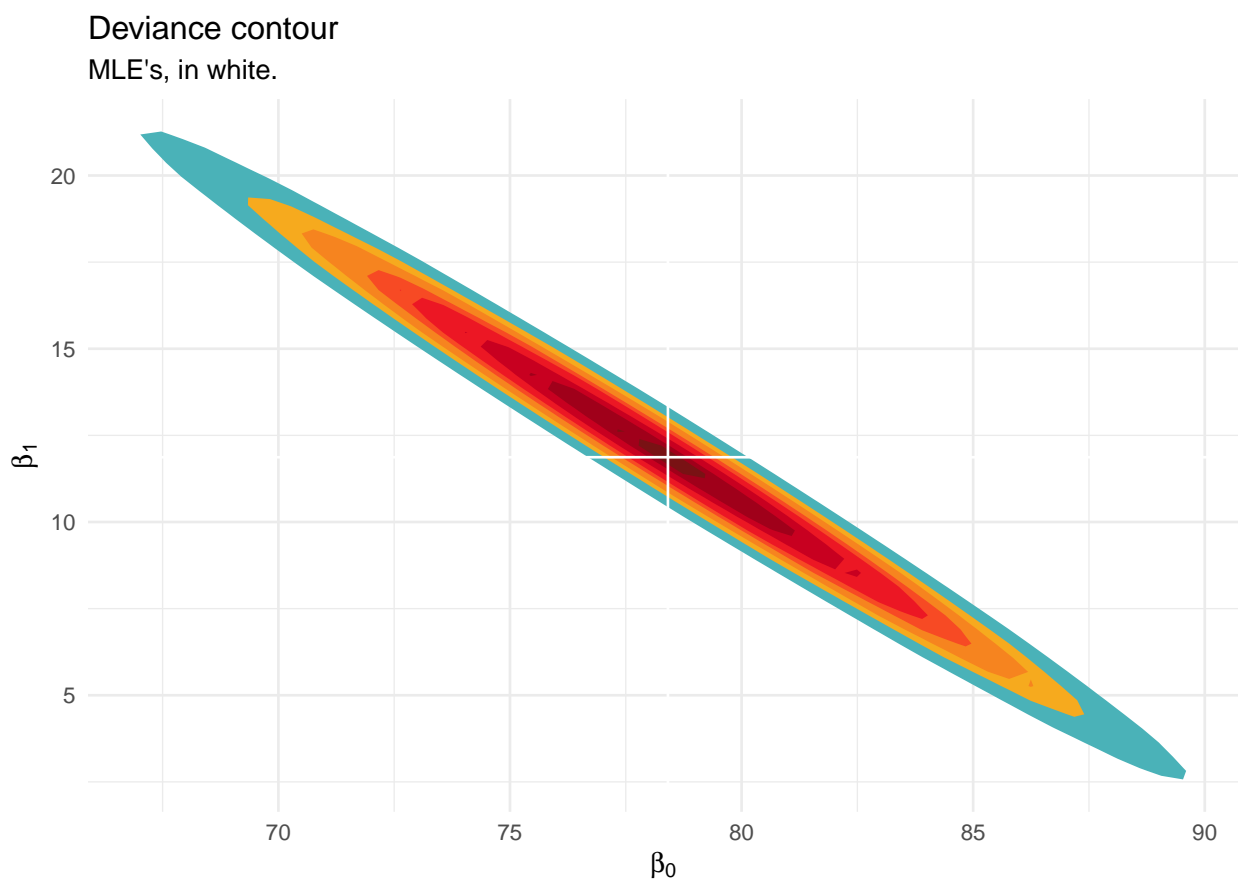


Figure 17: Deviance contour for the β 's of a Gaussian linear regression with some censored observations and with the standard deviation fixed in it's MLE.

Obtendo a verossimilhança perfilhada em relação a σ .

<r code>

```
sigma_grid <- seq(1, 17.5, length.out = 50)
beta_perf <- matrix(0, nrow = length(sigma_grid), ncol = 3)
for (i in seq(sigma_grid)) {
  beta_perf[i, ] <- unlist(
    mle2(gaussian4_reg, start = list(b0 = min(data_4$y), b1 = 1.5),
      data = list(sigma = sigma_grid[i]))@details[1:2])
}
ggplot() + theme_minimal() +
  geom_line(aes(x = sigma_grid, y = -beta_perf[ , 3]), size = 1.5) +
  geom_vline(xintercept = par_est[3], linetype = "dashed") +
  labs(x = expression(sigma), y = NULL,
    title = expression(sigma ~ "profile likelihood"),
    subtitle = "MLE, in dashed.")
```

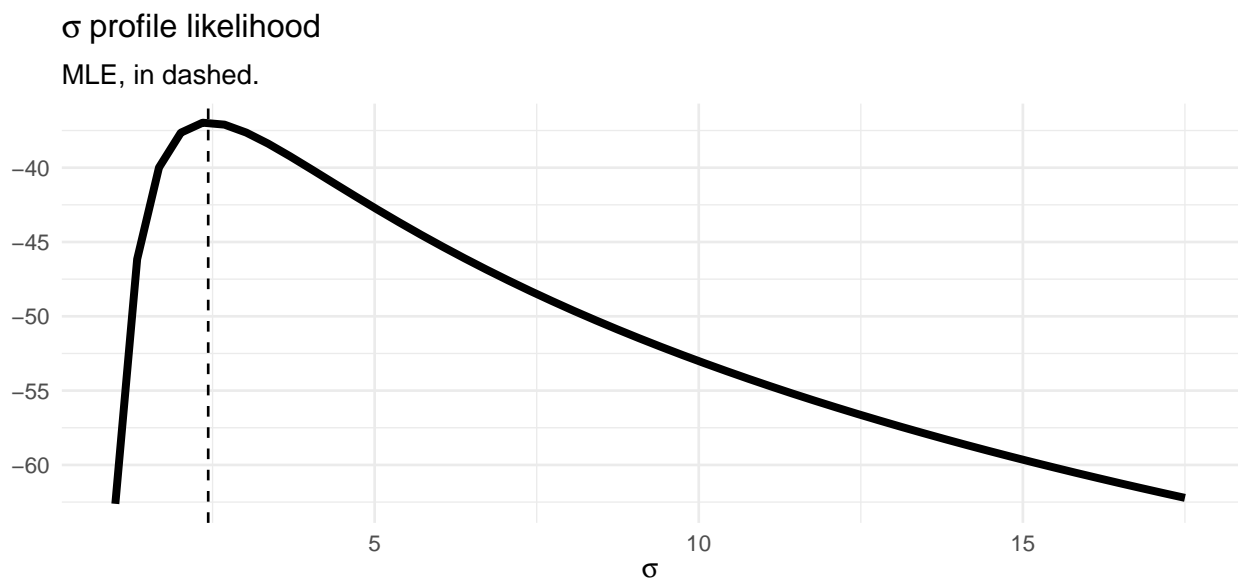


Figure 18: σ profile likelihood in a Gaussian linear regression with some censored observations. In dashed, the MLE.

And how the β 's fluctuates across the grid of σ ?

<r code>

```
summary(beta_perf[ , 1]) # beta_0
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
70.40	72.35	74.70	74.68	76.84	79.54

```
summary(beta_perf[ , 2]) # beta_1
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
10.90	13.27	15.21	15.23	17.31	19.09

Very few, as expected. Since the estimation of β doesn't depend on σ .

(d) Obtenha a verossimilhança perfilhada para os parâmetros β_0 e β_1 individualmente.

```
coef_profile <- function(grid, coef = c("b0", "b1")) { <r code>
  n <- length(grid)
  prof <- numeric(n)
  for (i in seq(n)) {
    prof[i] <-
      switch(coef,
             "b0" = mle2(gaussian4_reg,
                        start = list(b1 = 5),
                        data = list(b0 = grid[i],
                                    sigma = par_est[[3]])
                        )@details$value,
             "b1" = mle2(gaussian4_reg,
                        start = list(b0 = min(data_4$y)),
                        data = list(b1 = grid[i],
                                    sigma = par_est[[3]])
                        )@details$value)
  }
  return(-prof)
}

## beta_0 =====
b0_grid <- seq(68.1, 89, length.out = 50)
p1 <- ggplot() + theme_minimal() +
  geom_line(aes(x = b0_grid, y = coef_profile(b0_grid, "b0")),
           size = 1.5) +
  geom_vline(xintercept = par_est[1], linetype = "dashed") +
  labs(x = expression(beta[0]), y = NULL,
       title = expression(beta[0] ~ "profile likelihood"),
```



```

      subtitle = "MLE, in dashed.", tag = "A")
#####
## beta_1 =====
b1_grid <- seq(-7, 31, length.out = 50)
p2 <- ggplot() + theme_minimal() +
  geom_line(aes(x = b1_grid, y = coef_profile(b1_grid, "b1")),
            size = 1.5) +
  geom_vline(xintercept = par_est[2], linetype = "dashed") +
  labs(x = expression(beta[1]), y = NULL,
       title = expression(beta[1] ~ "profile likelihood"),
       subtitle = "MLE, in dashed.", tag = "B")
#####
## plotting =====
grid.arrange(p1, p2, ncol = 2)

```

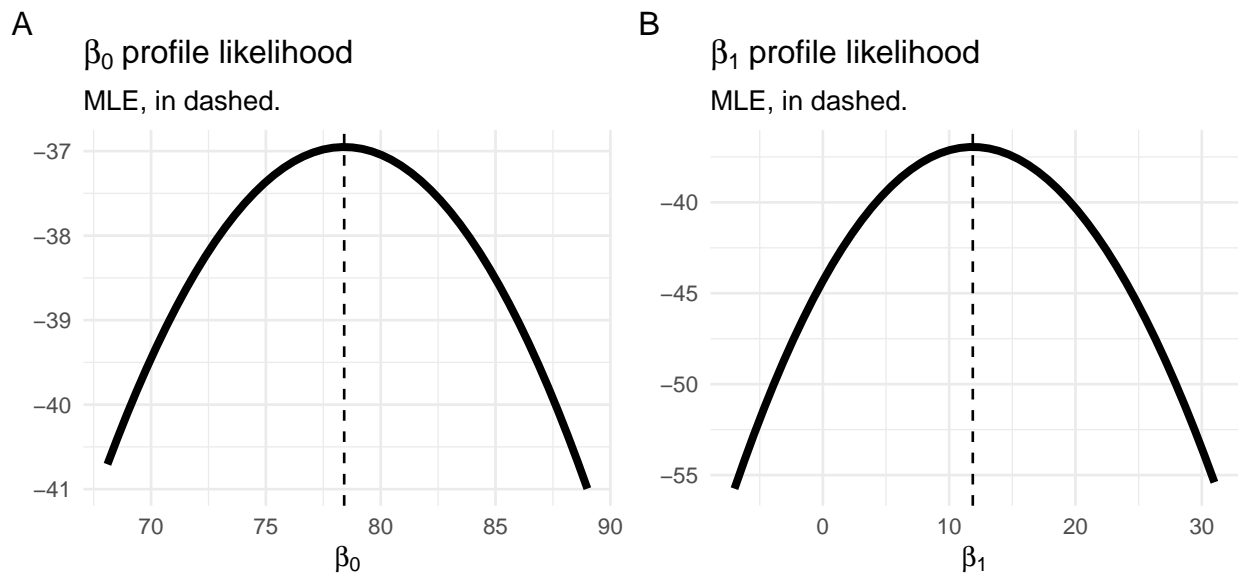


Figure 19: Profile likelihoods for β_0 and β_1 in a Gaussian linear regression with some censored observations. In dashed, the MLE's.

Last modification on ...

[1] "2019-10-25 20:35:51 -03"