Homework 5

Aiden Kenny
STAT GR5205: Linear Regression Models
Columbia University

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Question 1

Collaborators: None

(a) Let Y be the number of nurses in the hospital and let X be the available faculty and services. The left and middle panels of Figure 1 show the histograms of Y and X, respectively. We see that Y is skewed right, while X appears to be normally-distributed. In addition, the scatterplot of Y vs. X, which is in the third panel of Figure 1, shows that there is a nonlinear relationship between Y and X. All of these indicate that Y is suitable for a data transformation. Specifically, we would like to perform a power transformation on Y.

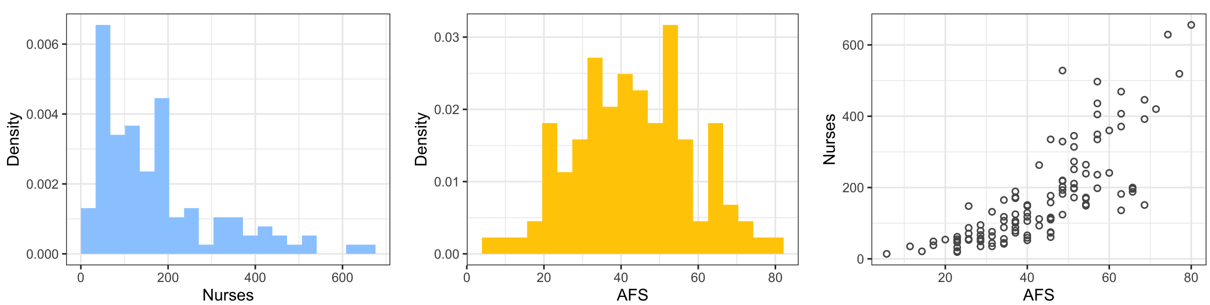

Figure 1: Histograms of Y and X and a scatterplot of Y vs. X.

(b) The power transformation function, and its inverse, are defined as

$$g_\lambda(Y) = \begin{cases} \dfrac{Y^\lambda - 1}{\lambda} & \text{if } \lambda \neq 0 \\ \log Y & \text{if } \lambda = 0. \end{cases} \quad \text{and} \quad g_\lambda^{-1}(Y) = \begin{cases} (1 + \lambda Y)^{1/\lambda} & \text{if } \lambda \neq 0 \\ \exp(Y) & \text{if } \lambda = 0. \end{cases}$$

Suppose we have our response vector $\mathbf{y}$ and our observed data $\mathbf{X}$. We are interested in fitting the model $\mathbf{g}_\lambda(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where $\mathbf{g}_\lambda(\mathbf{y})$ is the transformed response vector (i.e. the ith element is given by $g_\lambda(y_i)$), $\mathbb{E}[\boldsymbol{\epsilon}] = \mathbf{0}$, and $\text{Var}[\boldsymbol{\epsilon}] = \sigma^2\mathbf{I}$. For notational ease, we will denote $\mathbf{g}_\lambda(\mathbf{y})$ as $\mathbf{g}_\lambda$. If we make the further assumption that $\boldsymbol{\epsilon}$ is normally distributed, i.e. $\boldsymbol{\epsilon} \sim \text{N}(\mathbf{0}, \sigma^2\mathbf{I})$, then our response vector is also normally distributed, where $\mathbf{g}_\lambda \sim \text{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$. It's density function (and thus it's likelihood function) is given by

$$\begin{aligned} f(\mathbf{g}_\lambda \,|\, \boldsymbol{\beta}, \sigma^2, \lambda) &= \frac{1}{\sqrt{\det(2\pi\sigma^2\mathbf{I})}} \cdot \exp\left(-\frac{(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})^T \left(\sigma^2\mathbf{I}\right)^{-1} (\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})}{2} \right) \\ &= \frac{1}{(2\pi\sigma^2)^{n/2}} \cdot \exp\left(-\frac{(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})}{2\sigma^2} \right). \end{aligned}$$

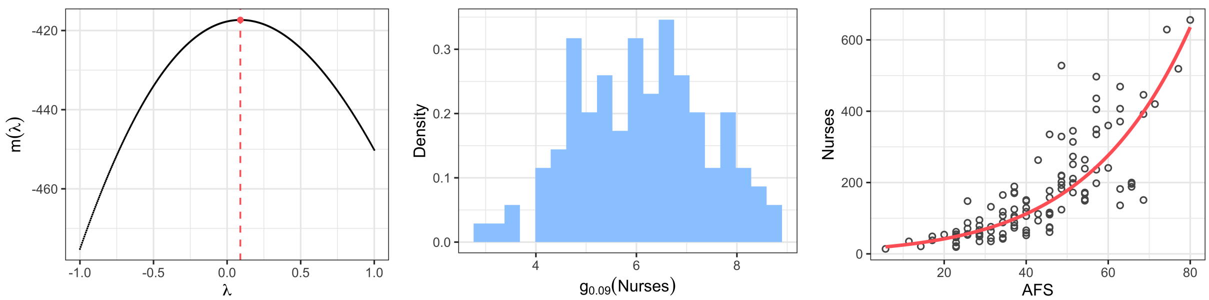

Figure 2: Relevant plots for the Box-Cox transformation of Y.

Since $\mathbf{y}$ is a transformation of $\mathbf{g}_\lambda$, we can derive the density for $\mathbf{y}$ as well. Notationally, this result may be somewhat confusing; even though we are finding the density for $\mathbf{y}$, we will still express the density (partly) in terms of $\mathbf{g}_\lambda$. It is important to remember that $\mathbf{g}_\lambda$ is a function of $\mathbf{y}$. Because the ith element of $\mathbf{g}_\lambda$ only depends on the ith element of $\mathbf{y}$, the Jacobian will be a diagonal matrix, and so

$$\mathbf{J} = \frac{\partial \mathbf{g}_\lambda}{\partial \mathbf{y}} = \operatorname{diag}\left(\frac{\partial g_\lambda(y_1)}{\partial y_1}, \ldots, \frac{\partial g_\lambda(y_n)}{\partial y_n}\right) = \operatorname{diag}\big(y_1^{\lambda-1}, \ldots, y_n^{\lambda-1}\big),$$

and so the density (and thus the likelihood) of $\mathbf{y}$ is given by

$$g(\mathbf{y} \,|\, \boldsymbol{\beta}, \sigma^2, \lambda) = f\big(\mathbf{g}_\lambda(\mathbf{y})\big) \cdot \big|\det(\mathbf{J})\big| = \frac{1}{(2\pi\sigma^2)^{n/2}} \cdot \exp\left(-\frac{(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})}{2\sigma^2}\right) \cdot \prod_{i=1}^n y_i^{\lambda-1}.$$

The log-likelihood $\ell(\mathbf{y}) = \log g(\mathbf{y})$ is given by

$$\ell(\mathbf{y} \,|\, \boldsymbol{\beta}, \sigma^2, \lambda) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{g}_\lambda - \mathbf{X}\boldsymbol{\beta})}{2\sigma^2} + (\lambda - 1)\sum_{i=1}^n \log(y_i).$$

As is standard with maximum likelihood estimation, we now differentiate ℓ with respect to the unknown parameters, set the derivatives to zero, and solve to get the maximum value of ℓ. For now, we are going to leave λ fixed and differentiate with respect to $\boldsymbol{\beta}$ and σ^2. Doing this for both gives us $\hat{\boldsymbol{\beta}}_{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{g}_\lambda$ and $\hat{\sigma}^2_{\text{MLE}} = \mathbf{g}_\lambda^T(\mathbf{I} - \mathbf{H})\mathbf{g}_\lambda$, where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is the hat matrix. It is worth noting that both $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ and $\hat{\sigma}^2_{\text{MLE}}$ are functions of λ. Plugging these values back into ℓ will maximize it with respect to $\boldsymbol{\beta}$ and σ^2, which means we will only have to maximize it with respect to λ. With some simplification, our new loss function is

$$m(\lambda) \coloneqq \ell(\mathbf{y} \,|\, \hat{\boldsymbol{\beta}}_{\text{MLE}}, \hat{\sigma}^2_{\text{MLE}}, \lambda) = -\frac{n}{2}\log\left(\frac{2\pi e}{n}\right) - \frac{n}{2}\log\left(\mathbf{g}_\lambda^T(\mathbf{I} - \mathbf{H})\mathbf{g}_\lambda\right) + (\lambda - 1)\sum_{i=1}^n \log(y_i).$$

Ideally, we would differentiate m with respect to λ, set $\partial m / \partial \lambda = 0$, and solve for λ. I was unable to derive a closed form solution for the result, but it is still possible to use graphical techniques or numerical methods to find the optimal value of λ.

We recall that both $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ and $\hat{\sigma}^2_{\text{MLE}}$ are functions of λ, so we cannot know their value until $\hat{\lambda}_{\text{MLE}}$ has been determined. Because of this, as we just showed, the likelihood function can be expressed as a function $m(\lambda)$ that only depends on λ, which can be maximized to find $\hat{\lambda}_{\text{MLE}}$. Once we find $\hat{\lambda}_{\text{MLE}}$, we can use this value to determine $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ and $\hat{\sigma}^2_{\text{MLE}}$.

The left panel of Figure 2 shows a plot of $m(\lambda)$ against λ for values $\lambda \in [-1, 1]$. The log-likelihood is maximized when $\hat{\lambda}_{\text{MLE}} = 0.09$. The middle panel shows the histogram of $g_{0.09}(Y)$, the transformed version of Y, and we can see with this value of λ that $\mathbf{g}_\lambda$ is normally distributed. We can now