

MSiA 420, HW #1
due Monday 1/27/20, 11:59 pm

As with all HW (unless otherwise noted), upload your solutions for this assignment on Canvas, as a Word or pdf file, by the due date/time. For all problems for which you use R, include your R script in an appendix to your homework (clearly label which parts of the script correspond to which homework problems).

- 1) In class, we showed that the MLE of the mean of a random sample $\{y_1, y_2, \dots, y_n\}$ from an $N(\mu, \sigma^2)$ population is exactly the sample average (i.e., $\hat{\mu} = \bar{y}$). Show that the MLE for the standard deviation is:

$$\hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2}$$

Hint: Find the partial derivative of the likelihood function with respect to σ , then set this equal to zero and solve for σ . The result will be a function of the unknown μ , but you can plug in the MLE of μ from class. Hence, we are really finding the *joint* MLEs of μ and σ .

- 2) (Problem 13.10 from KNN). In a study of enzyme kinetics, a postulated model relating the velocity of reaction (Y) to the concentration (X) is of the form

$$Y_i = \frac{\gamma_0 X_i}{\gamma_1 + X_i} + \varepsilon_i$$

The velocity at 18 different concentrations were recorded as part of a study, the data for which are listed the Prob 2 worksheet of HW1_Data.xls.

- (a) When fitting nonlinear regression models, it is often important to have reasonably good initial guesses for the parameters. Towards this end, notice that without the error term the model is $Y'_i = \beta_0 + \beta_1 X'_i$, where $Y'_i = 1/Y_i$, $\beta_0 = 1/\gamma_0$, $\beta_1 = \gamma_1/\gamma_0$, and $X'_i = 1/X_i$. In light of this, fit a linear regression model to the transformed data with Y'_i the response and X'_i the predictor to obtain initial guesses of the form $\hat{\gamma}_0 = 1/\hat{\beta}_0$ and $\hat{\gamma}_1 = \hat{\beta}_1/\hat{\beta}_0$.
- (b) Using the initial guesses from part (a), find the nonlinear least squares estimates of γ_1 and γ_0 . Fit the model twice, using the two different R functions `nlm()` and `nls()`.
- 3) Refer to the same data from Problem (2).
- (a) Calculate the observed Fisher information matrix and the covariance matrix of the estimated parameter vector $\hat{\gamma} = [\hat{\gamma}_0, \hat{\gamma}_1]^T$ using the Hessian produced by `nlm()`. Based on this, calculate the standard errors of the estimated parameters.

- (b) Calculate the covariance matrix of $\hat{\gamma}$ using the `vcov()` function applied to the output of `nls()`, and based on this calculate the standard errors of the estimated parameters. Do the results agree with Part (a)?
 - (c) Using the results of Part (a), calculate two-sided 95% CIs on the parameters γ_0 and γ_1 . Compare this with the results of the `confint.default()` function applied to the output of `nls()`.
- 4) This is a repeat of Problem (3), but using bootstrapping to calculate the standard errors and confidence intervals. You can use the `boot()` command in R (requires the `boot` package to be loaded with the `library(boot)` command). Use at least 20,000 bootstrap replicates.
- (a) Calculate and plot bootstrapped histograms of $\hat{\gamma}_0$ and $\hat{\gamma}_1$, and calculate the corresponding bootstrapped standard errors.
 - (b) Calculate “crude” two-sided 95% CIs on γ_0 and γ_1 using the normal approximation to their bootstrapped distributions.
 - (c) Calculate the reflected two-sided 95% CIs on γ_0 and γ_1 (this corresponds to the `type = “basic”` option of the `boot.ci()` function).
 - (d) Do the CIs in part (c) agree with those in part (b)? Relate this to the histograms you see in part (a).
- 5) Use bootstrapping to calculate a two-sided 95% prediction interval on a “future” response Y^* at $X^* = 27$. Compare this to a two-sided 95% confidence interval on the predictable part $g(\mathbf{x}^*, \theta)$ of Y^* at $X^* = 27$. Which interval do you think better represents an interval that you would expect to contain the future response with roughly 95% chance? Explain
- 6) Use the AIC criterion to compare the model that you fitted in Problem (2b) with the alternative model $Y_i = \beta_0 + \beta_1 \sqrt{X_i} + \varepsilon_i$. Which model does AIC suggest is the better model?
- 7) Use n-fold cross-validation to compare the model that you fitted in Problem (2b) with the alternative model $Y_i = \beta_0 + \beta_1 \sqrt{X_i} + \varepsilon_i$. Which model does n-fold cross-validation suggest is the better model?
- 8) For the two models that you compared in Problems 6 and 7, construct plots of the residuals versus X . Based on the residual plots, does one model appear more appropriate than the other, and does this agree with your conclusions from Problems 6 and 7?