Linear Models 1

Isfahan University of Technology Fall Semester, 2014

References:

- [1] G. A. F., <u>Seber</u> and A. J. <u>Lee</u> (2003). Linear Regression Analysis (2nd ed.). Hoboken, NJ: Wiley.
- [2] A. C. <u>Rencher</u> and G. B. <u>Schaalje</u> (2008). Linear Models in Statistics (2nd ed.). John Wiley & Sons, Inc.
 - [3] R. B., Bapat (2000), Linear Algebra and Linear Models, (2nd ed.). Springer-Verlag.
 - [4] S. R., Searle (1971). Linear Models. New York: Wiley.

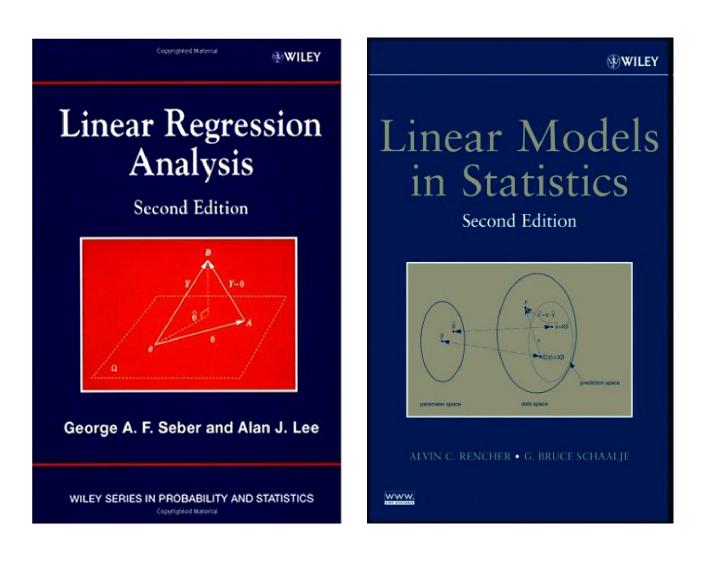
The PDF versions of references are available in the link http://rikhtehgaran.iut.ac.ir/

Prerequisites:

- •. Linear Algebra
- Basic Statistical Inference.

Grading Policy:

- Assignments & Quizes: 3-5 points.
- Midterm Exam: 5-7 points .
- Final Exam: 10 points.





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Why statistical models?

It is in human nature to try and understand the physical and natural phenomena that occur around us. When observations on a phenomenon can be quantified, such an attempt at understanding often takes the form of building a **mathematical model**, even if it is only a simplistic attempt to capture the essentials. Either because of our ignorance or in order to keep it simple, many relevant factors may be left out. Also models need to be validated through measurement, and such measurements often come with error. In order to account for the measurement or observational errors as well as the factors that may have been left out, one needs a *statistical* model which incorporates some amount of uncertainty.

Why a linear model?

Some of the reasons why we undertake a detailed study of the linear model are as follows.

(a) Because of its simplicity, the linear model is better understood and easier to interpret than most of the other competing models, and the methods of analysis and inference are better developed Therefore, if there is no particular reason to presuppose another model, the linear model may be used at least as a first step.

(b) The linear model formulation is useful even for certain nonlinear models which can be reduced to the linear form by means of a transformation.

(c) Results obtained for the linear model serve as a stepping stone for the analysis of a much wider class of related models such as mixed effects model, state-space and other time series models.

(d) Suppose that the response is modelled as a nonlinear function of the explanatory variables plus error. In many practical situations only a part of the domain of this function is of interest. For example, in a manufacturing process, one is interested in a narrow region centered around the operating point. If the above function is reasonably smooth in this region, a linear model serves as a good first order approximation to what is globally a nonlinear model.

Many statistical concepts can be viewed in the framework of linear models

suppose that we wish to compare the means of two populations, say, $\mu_i = E[U_i]$ (i = 1, 2).



In a similar fashion we can combine two straight lines,

