# **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, (2<sup>nd</sup> ed.). Springer-Verlag.
- [4] S. R., Searle (1971). Linear Models. New York: Wiley.

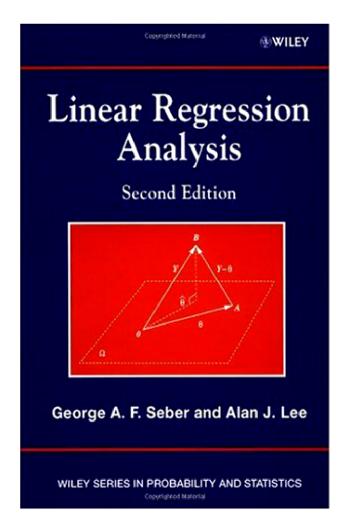
The PDF versions of references are available in the link <a href="http://rikhtehgaran.iut.ac.ir/">http://rikhtehgaran.iut.ac.ir/</a>

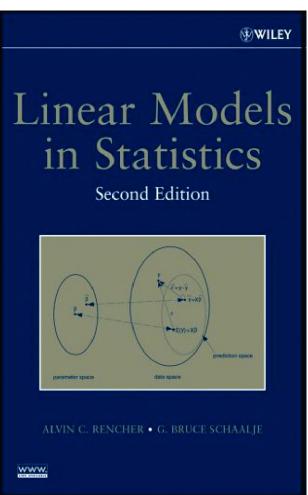
# **Prerequisites:**

- •. Linear Algebra
- Basic Statistical Inference.

## **Grading Policy:**

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











# Contents

# Ch. 2. Matrix Algebra. (Rencher and Schaalje)

Pı	eface	·	xv
1	Vect	ors of Random Variables	1
	1.1	Notation	1
	1.2	Statistical Models	2
	1.3	Linear Regression Models	4
	1.4	Expectation and Covariance Operators	5
		Exercises 1a	8
	1.5	Mean and Variance of Quadratic Forms	9
		Exercises 1b	12
	1.6	Moment Generating Functions and Independence	13
		Exercises 1c	15
	Misc	cellaneous Exercises 1	15
2	Mul	tivariate Normal Distribution	17
	2.1	Density Function	17
		Exercises 2a	19
	2.2	Moment Generating Functions	20
		Exercises 2b	23
	2.3	Statistical Independence	24

		Exercises 2c	26
	2.4	Distribution of Quadratic Forms	27
		Exercises 2d	31
	Misc	ellaneous Exercises 2	31
3	Linea	ar Regression: Estimation and Distribution Theory	35
	3.1	Least Squares Estimation	35
		Exercises 3a	41
	3.2	Properties of Least Squares Estimates	42
		Exercises 3b	44
	3.3	Unbiased Estimation of $\sigma^2$	44
		Exercises 3c	47
	3.4	Distribution Theory	47
		Exercises 3d	49
	3.5	Maximum Likelihood Estimation	49
	3.6	Orthogonal Columns in the Regression Matrix	51
		Exercises 3e	52
	3.7	Introducing Further Explanatory Variables	54
		3.7.1 General Theory	54
		3.7.2 One Extra Variable	57
		Exercises 3f	58
	3.8	Estimation with Linear Restrictions	59
		3.8.1 Method of Lagrange Multipliers	60
		3.8.2 Method of Orthogonal Projections	61
		Exercises 3g	62
	3.9	Design Matrix of Less Than Full Rank	62
		3.9.1 Least Squares Estimation	62
		Exercises 3h	64
		3.9.2 Estimable Functions	64
		Exercises 3i	65
		3.9.3 Introducing Further Explanatory Variables	65
		3.9.4 Introducing Linear Restrictions	65
		Exercises 3j	66
	3.10	Generalized Least Squares	66
		Exercises 3k	69
	3.11	Centering and Scaling the Explanatory Variables	69
		3.11.1 Centering	<b>7</b> 0
		3.11.2 Scaling	71

				CONTENTS	vii
		E	xercises 31		72
	$\frac{3.12}{3.12}$	Bayes	<del>ian Estimation</del>		73
		•	exercises 3m		76
	3.13	Robus	st Regression		77
	•	3.13.1	M-Estimates		78
		3.13.2	Estimates Based on Robust Location and	Scale	
			Measures		80
			Measuring Robustness		82
		3.13.4	Other Robust Estimates		88
		$\mathbf{E}$	xercises 3n		93
	Miso	cellaneo	ous Exercises 3		93
4	Hy	othesis	s Testing		97
	4.1	Introd	duction		97
	4.2	Likeli	hood Ratio Test		98
	4.3	$F ext{-}\mathrm{Tes}$	st.		99
		4.3.1	Motivation		99
		4.3.2	Derivation		99
		E	xercises 4a		102
		4.3.3	Some Examples		103
		4.3.4	The Straight Line		107
		$\mathbf{E}$	xercises 4b		109
	4.4	Multi	ple Correlation Coefficient		110
		E	xercises 4c		113
	4.5	Cano	nical Form for H		113
		E	exercises 4d		114
	4.6	Good	ness-of-Fit Test		115
	4.7	F-Tes	t and Projection Matrices		116
	Mis	cellaneo	ous Exercises 4		117
5	Con	fidence	Intervals and Regions		119
	5.1	$\mathbf{Simul}$	taneous Interval Estimation		119
		5.1.1	Simultaneous Inferences		119
		5.1.2	Comparison of Methods		124
		5.1.3	Confidence Regions		125
		5.1.4	Hypothesis Testing and Confidence Interva	ls	127
	5.2	Confi	dence Bands for the Regression Surface		129
		5.2.1	Confidence Intervals		129
		5.2.2	Confidence Bands		129

	5.3	Predi	ction Intervals and Bands for the Response	131
		5.3.1	Prediction Intervals	131
		5.3.2	Simultaneous Prediction Bands	133
	5.4	Enlar	ging the Regression Matrix	135
	Miso	cellanec	ous Exercises 5	136
6	$\operatorname{Stra}$	ight-Li	ne Regression	139
	6.1	The S	Straight Line	139
		6.1.1	Confidence Intervals for the Slope and Intercept	139
		6.1.2	Confidence Interval for the $x$ -Intercept	140
		6.1.3	Prediction Intervals and Bands ,	141
		6.1.4	Prediction Intervals for the Response	145
		6.1.5	Inverse Prediction (Calibration)	145
		E	Exercises 6a	148
	6.2	Straig	ght Line through the Origin	149
	6.3	Weigl	hted Least Squares for the Straight Line	150
		6.3.1	Known Weights	150
		6.3.2	Unknown Weights	151
		E	Exercises 6b	153
	6.4	Comp	paring Straight Lines	154
		6.4.1	General Model	154
		6.4.2	Use of Dummy Explanatory Variables	156
		E	Exercises 6c	157
	6.5	${f Two}$ -	Phase Linear Regression	159
	6.6	$_{ m Local}$	Linear Regression	162
	Mis	cellane	ous Exercises 6	163
7	Poly	<del>/nomia</del> l	<del>l Regression</del>	165
	7.1	Polyr	nomials in One Variable	165
		7.1.1	Problem of Ill-Conditioning	165
		7.1.2	Using Orthogonal Polynomials	166
		7.1.3	Controlled Calibration	172
	7.2	Piece	ewise Polynomial Fitting	172
		7.2.1	Unsatisfactory Fit	172
		7.2.2	Spline Functions	173
		7.2.3	Smoothing Splines	176
	7.3	Polyr	nomial Regression in Several Variables	180
		•	Response Surfaces	180

			CONT	ENTS	ix
		7.3.2	Multidimensional Smoothing		184
	Misc		ous Exercises 7		185
	14112(	cnaneo	ds Exercises /		100
8	Ana	lysis of	Variance		187
	8.1	Intro	duction		187
	8.2	One-V	Way Classification		188
		8.2.1	General Theory		188
		8.2.2	Confidence Intervals		192
		8.2.3	Underlying Assumptions		195
		E	Exercises 8a		196
	8.3	Two-	Way Classification (Unbalanced)		197
		8.3.1	Representation as a Regression Model		197
		8.3.2	Hypothesis Testing		197
		8.3.3	Procedures for Testing the Hypotheses		201
		8.3.4	Confidence Intervals		204
		E	Exercises 8b		205
	8.4	Two-	Way Classification (Balanced)		206
		E	Exercises 8c		209
	8.5	Two-	Way Classification (One Observation per Mean)		211
		8.5.1	Underlying Assumptions		212
	8.6	Highe	er-Way Classifications with Equal Numbers per Mea	n	216
		8.6.1	Definition of Interactions		216
		8.6.2	Hypothesis Testing		217
		8.6.3	Missing Observations		220
		E	Exercises 8d		221
	8.7	Desig	ens with Simple Block Structure		221
	8.8	Analy	ysis of Covariance		222
		E	Exercises 8e		224
	Misc	cellanec	ous Exercises 8		225
		;			
9	Dep	artures	from Underlying Assumptions		227
	9.1	Intro	duction		227
	9.2	Bias			228
		9.2.1	Bias Due to Underfitting		<b>22</b> 8
		9.2.2	Bias Due to Overfitting		230
		E	Exercises 9a		231
	9.3	Incor	rect Variance Matrix		231
		F	Exercises 9b		232

### x CONTENTS

	9.4	Effect	of Outliers	233
	9.5	Robus	tness of the $F$ -Test to Nonnormality	235
		9.5.1	Effect of the Regressor Variables	235
		9.5.2	Quadratically Balanced F-Tests	236
		E	xercises 9c	239
	9.6	Effect	of Random Explanatory Variables	240
		9.6.1	Random Explanatory Variables Measured without	
			Error	240
		9.6.2	Fixed Explanatory Variables Measured with Error	241
		9.6.3	Round-off Errors	245
		9.6.4	Some Working Rules	245
		9.6.5	Random Explanatory Variables Measured with Error	246
		9.6.6	Controlled Variables Model	248
	9.7	Colline	earity	249
		9.7.1	Effect on the Variances of the Estimated Coefficients	249
		9.7.2	Variance Inflation Factors	254
		9.7.3	Variances and Eigenvalues	255
		9.7.4	Perturbation Theory	255
		9.7.5	Collinearity and Prediction	261
		$\mathbf{E}_{2}$	xercises 9d	261
	Misc	ellaneo	us Exercises 9	262
10			from Assumptions: Diagnosis and Remedies	265
		Introd		265
	10.2		ials and Hat Matrix Diagonals	266
			xercises 10a	270
	10.3	Dealin	ng with Curvature	271
		10.3.1	Visualizing Regression Surfaces	271
		10.3.2	Transforming to Remove Curvature	275
		10.3.3	Adding and Deleting Variables	277
		E	xercises 10b	279
	10.4	Nonco	onstant Variance and Serial Correlation	281
		10.4.1	Detecting Nonconstant Variance	281
			•	
			Estimating Variance Functions	288
		10.4.2	Estimating Variance Functions Transforming to Equalize Variances	288 291
		10.4.2 10.4.3	_	
		10.4.2 10.4.3 10.4.4	Transforming to Equalize Variances	291
	10.5	10.4.2 10.4.3 10.4.4 E	Transforming to Equalize Variances Serial Correlation and the Durbin-Watson Test	291 292
	10.5	10.4.2 10.4.3 10.4.4 E	Transforming to Equalize Variances  Serial Correlation and the Durbin-Watson Test xercises 10c	291 292 294

		10.5.2	Transforming the Response	297
		10.5.3	Transforming Both Sides	299
		E	xercises 10d	300
	10.6	Detect	ting and Dealing with Outliers	301
		10.6.1	Types of Outliers	301
		10.6.2	Identifying High-Leverage Points	304
		10.6.3	Leave-One-Out Case Diagnostics	306
		10.6.4	Test for Outliers	<b>31</b> 0
		10.6.5	Other Methods	311
		$\mathbf{E}_{i}$	xercises 10e	314
	10.7	Diagn	osing Collinearity	315
		10.7.1	Drawbacks of Centering	316
		10.7.2	Detection of Points Influencing Collinearity	<b>31</b> 9
		10.7.3	Remedies for Collinearity	320
		E	xercises 10f	326
	Misc	ellaneo	us Exercises 10	327
11	Com	<del>putati</del> c	onal Algorithms for Fitting a Regression	<b>32</b> 9
	11.1	Introd	luction	<b>32</b> 9
		11.1.1	Basic Methods	<b>32</b> 9
	11.2	Direct	Solution of the Normal Equations	<b>33</b> 0
		11.2.1	Calculation of the Matrix $X'X$	330
		11.2.2	Solving the Normal Equations	331
		$\mathbf{E}$	xercises 11a	337
	11.3	QR D	ecomposition	338
		11.3.1	Calculation of Regression Quantities	340
		11.3.2	Algorithms for the QR and WU Decompositions	341
		$\mathbf{E}$	xercises 11b	352
	11.4	Singu	lar Value Decomposition	353
		11.4.1	Regression Calculations Using the SVD	353
		11.4.2	Computing the SVD	354
	11.5	Weigh	ited Least Squares	355
	11.6	Addin	g and Deleting Cases and Variables	356
		11.6.1	Updating Formulas	356
		11.6.2	Connection with the Sweep Operator	<b>3</b> 57
		11.6.3	Adding and Deleting Cases and Variables Using QR	360
	11.7		ring the Data	363
	11.8	Comp	paring Methods	365

	11.8.1 Resources	365
	11.8.2 Efficiency	366
	11.8.3 Accuracy	369
	11.8.4 Two Examples	372
	11.8.5 Summary	373
	Exercises 11c	374
	11.9 Rank-Deficient Case	376
	11.9.1 Modifying the QR Decomposition	376
	11.9.2 Solving the Least Squares Problem	378
	11.9.3 Calculating Rank in the Presence of Round-off Error	<b>37</b> 8
	11.9.4 Using the Singular Value Decomposition	379
	11.10 Computing the Hat Matrix Diagonals	379
	11.10.1 Using the Cholesky Factorization	380
	11.10.2 Using the Thin QR Decomposition	380
	11.11 Calculating Test Statistics	380
	11.12 Robust Regression Calculations	382
	11.12.1 Algorithms for $L_1$ Regression	382
	11.12.2 Algorithms for M- and GM-Estimation	384
	11.12.3 Elemental Regressions	385
	11.12.4 Algorithms for High-Breakdown Methods	385
	Exercises 11d	<b>3</b> 88
	Miscellaneous Exercises 11	<b>3</b> 89
12	Prediction and Model Selection	391
	12.1 Introduction	<b>3</b> 91
	12.2 Why Select?	393
	Exercises 12a	399
	12.3 Choosing the Best Subset	399
	12.3.1 Goodness-of-Fit Criteria	400
	12.3.2 Criteria Based on Prediction Error	401
	12.3.3 Estimating Distributional Discrepancies	407
	12.3.4 Approximating Posterior Probabilities	410
	Exercises 12b	413
	12.4 Stepwise Methods	413
	12.4.1 Forward Selection	414
	12.4.2 Backward Elimination	416
	12.4.3 Stepwise Regression	418
	Exercises 12c	<b>42</b> 0

		CONTENTS	xiii
12.5	Shrink	age Methods	420
	12.5.1	Stein Shrinkage	420
	12.5.2	Ridge Regression	423
	12.5.3	Garrote and Lasso Estimates	425
	$\mathbf{E}_{2}$	xercises 12d	427
12.6	Bayesi	ian Methods	<b>42</b> 8
	12.6.1	Predictive Densities	<b>42</b> 8
	12.6.2	Bayesian Prediction	431
	12.6.3	Bayesian Model Averaging	433
	E	xercises 12e	433
12.7	Effect	of Model Selection on Inference	434
	12.7.1	Conditional and Unconditional Distributions	434
	12.7.2	Bias	436
	12.7.3	Conditional Means and Variances	437
	12.7.4	Estimating Coefficients Using Conditional Likelihood	437
	12.7.5	Other Effects of Model Selection	438
	$\mathbf{E}_{i}$	xercises 12f	438
12.8	Comp	utational Considerations	439
	12.8.1	Methods for All Possible Subsets	439
	12.8.2	Generating the Best Regressions	442
	12.8.3	All Possible Regressions Using QR Decompositions	446
	${f E}$	xercises 12g	447
12.9	Comp	arison of Methods	447
	12.9.1	Identifying the Correct Subset	447
	12.9.2	Using Prediction Error as a Criterion	448
	${f E}$	xercises 12h	456
Misc	ellaneo	us Exercises 12	456
pend	ix A Sc	ome Matrix Algebra	457
A.1	$\operatorname{Trace}$	and Eigenvalues	457
A.2	Rank		458
A.3	Positi	ve-Semidefinite Matrices	460
A.4	Positi	ve-Definite Matrices	461
A.5	Perm	utation Matrices	464
A.6	Idemp	ootent Matrices	464
A.7	Eigen	value Applications	465
A.8	Vecto	r Differentiation	466
A.9	Patter	rned Matrices	466

### xiv CONTENTS

A.10	Generalized Inverse	469
A.11	Some Useful Results	471
A.12	Singular Value Decomposition	471
A.13	Some Miscellaneous Statistical Results	472
A.14	Fisher Scoring	473
Appendi	x B Orthogonal Projections	475
B.1	Orthogonal Decomposition of Vectors	475
B.2	Orthogonal Complements	477
B.3	Projections on Subspaces	477
Appendi	x C Tables	479
C.1	Percentage Points of the Bonferroni t-Statistic	480
C.2	Distribution of the Largest Absolute Value of $k$ Student $t$ Variables	482
C.3	Working-Hotelling Confidence Bands for Finite Intervals	489
Outline	Solutions to Selected Exercises	491
Reference	ees	531
Index		549

#### 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). Then we can combine the data into the single model

$$E(Y) = \mu_1 + (\mu_2 - \mu_1) x$$
  
=  $\beta_0 + \beta_1 x$ ,



where x=0 when Y is a  $U_1$  observation and x=1 when Y is a  $U_2$  observation. Here  $\mu_1=\beta_0$  and  $\mu_2=\beta_0+\beta_1$ , the difference being  $\beta_1$ . We can extend this idea to the case of comparing m means using m-1 dummy variables.

In a similar fashion we can combine two straight lines,

$$U_j = \alpha_j + \gamma_j x_1 \quad (j = 1, 2),$$



and 1 otherwise. The combined model is

$$E(Y) = \alpha_1 + \gamma_1 x_1 + (\alpha_2 - \alpha_1) x_2 + (\gamma_2 - \gamma_1) x_1 x_2$$
  
=  $\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$ .