DATA ANALYSIS FOR SCIENTISTS AND ENGINEERS

STUART L. MEYER

DATA ANALYSIS FOR SCIENTISTS AND ENGINEERS

STUART L. MEYER
Northwestern University

"Now this is the peculiarity of scientific method, that when once it has become a habit of mind, that mind converts all facts whatsoever into science. The field of science is unlimited; its material is endless, every group of natural phenomena, every phase of social life, every stage of past or present development is material for science. The unity of all science consists alone in its method, not in its material. The man who classifies facts of any kind whatever, who sees their mutual relation and describes their consequences,

is applying the scientific method and is a man of science. The facts may belong to the past history of mankind, to the social statistics of our great cities, to the atmosphere of the most distant stars, to the digestive organs of a worm, or to the life of a scarcely visible bacillus. It is not the facts themselves which form science, but the methods by which they are dealt with."

Karl Pearson, The Grammar of Science

2211/4

Copyright © 1975, by John Wiley & Sons, Inc.

All rights reserved. Published simultaneously in Canada.

No part of this book may be reproduced by any means, nor transmitted, nor translated into a machine language without the written permission of the publisher.

Library of Congress Cataloging in Publication Data

Meyer, Stuart L 1937-

Data analysis for scientists and engineers.

Bibliography: p.

1. Mathematical statistics. 2. Probabilities.

I. Title.

QA276.M437 519.2 74-8873

ISBN 0-471-59995-6

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

PREFACE

This book evolved from a personal need: the need to have in one place, with a consistent style and notation, practically all that an experimental scientist needs to know to deal with data and wants to know to satisfy his or her intellectual curiosity.

For many years there has really been no discipline in which to teach data analysis for experimental scientists. The usual medium in science departments for imparting knowledge in this area has been the teaching laboratory. I believe that an appreciation of the means of extracting and evaluating information from experimental data is one of the basic goals of any laboratory course. Moreover, this is a skill and appreciation that should be developed as early as possible in a student's career, regardless of whether he or she intends to be an experimental or theoretical scientist. Therefore, although this book can be used in departments that have formal courses on the subject, I have assumed that the student's first acquaintance with data analysis will come through the science laboratory and that mature knowledge will come largely from self-study.

The early parts of the book are written to accompany a typical first-course science laboratory, and versions of Parts I and II have been used for several years at Northwestern University as a supplement to the beginning physics laboratory (and as a guide for the graduate teaching assistants). In addition, a version of Parts III and IV has been used in an integrated program of mathematics, physics, and chemistry for engineering students. Despite this history. the book is intended primarily for selfstudy and reference by the student, and much of the material goes beyond the usual content of a first course to provide the core of what is needed by a professional scientific investigator. Therefore, I have kept the discussion as complete and lucid as possible with many worked-out examples and cases that are of direct interest to the science student.

The wide availability of digital computer capability has made traditional, formerly cumbersome analysis methods more convenient and accurate and also has permitted the use of more sophisticated techniques that are not practical with slide rules, pencils, and paper alone. Some of these techniques are introduced here because they will become utilized more and more in the near future. I have not discussed programming or specific computer programs, since this material is readily available

elsewhere. Also, the use of individual programs is often determined by the availability of library routines in a particular computer center, and it was more important to present the methods underlying applicable library programs instead of the programs themselves. Finally, the advances in technology have made available to individuals computing power that required a large facility only a decade ago. All of the numerical discussions and worked-out examples included here may be followed by the reader without any computational assistance and may be duplicated with a pocket calculator of the "electronic slide rule" type.

The level of this book requires only the rudiments of calculus as a preliminary. Although the early discussions are on a level that is understandable to the beginning student, the subject is developed so that it is fairly complete and selfcontained, and it ends at a level of sophistication that is suitable for the professional scientist. This will enable the beginning student to "grow into" the book. The volume also may be used as a general reference and guide as the reader becomes more sophisticated in the design and analysis of experiments. Many discussions, formulas, tables, and graphs are included for convenience, completeness. and review. I hope that the book will find a useful place on the permanent bookshelf of the working scientist.

I wrote this work from the viewpoint of the practitioner of data analysis, that is, the scientist or engineer using the techniques, rather than from the viewpoint of the mathematician who develops new ones. Nevertheless, it is important for the practitioner to understand the bases of the techniques that he uses. For this reason, a fair amount of time is spent in developing the ideas of data analysis instead of merely presenting a series of recipes. Few problems encountered in the real world fit any one recipe exactly. It is important, therefore, to understand data-analysis concepts

and methods thoroughly, and to have an appreciation for their spheres of usefulness.

The presentation is designed to be selfcontained, eschewing the elegant obscurity of sophisticated methods of proof for the tedious clarity of more straightforward ones. All available sources have been utilized, and my major efforts are directed toward making the concepts palatable at the level of the reader and making them form a comprehensible, coherent, and useful whole. If I have erred, it has been on the side of too many explanation instead of too few, more steps in the mathematics rather than not enough steps; although this might please the experts less, it will help the students more. There is a famous explanation of why a classical work of J. Willard Gibbs was not widely known: "It is a little book which is little read because it is a little hard." I have tried to make this book easy to understand, even at the expense of greater than minimum length. However, there is sufficient depth in this single volume to reward careful and continued study.

Even the simplest problem often has subtleties that require more nuances of thought than the casual reader may consider at first glance. Some of the ramifications are not needed early in the book, and we sometimes return to the same problem again when it is appropriate to discuss other aspects of it. In addition, considerable material has been added because of my personal (possibly idiosyncratic) tastes. This material is usually set in special type or otherwise identified as not being absolutely essential to the main line of discussion.

I am pleased to acknowledge the support of the U.S. Army Research Office—Durham under Grant DA-ARO-D-31-124-71-G175 whose assistance facilitated the completion of the manuscript. I thank Publishers—Hall Syndicate and Cartoon Features for arranging permission to use cartoons and to Trendline Inc. for permis-

sion to use a graph. My sincere appreciation goes to Professors A. J. F. Siegert, Meyer Dwass, Robert Eisberg, and Hugh Young for reading parts of the manuscript and for helpful suggestions and to Mr.

King L. Leung for able assistance with the calculation of the tables and graphs.

Stuart L. Meyer

Evanston, Illinois

CONTENTS

PART !

Introduction :	to	Scientific	Measurement
----------------	----	------------	-------------

1.	The Meaning of Measurement	3
	A Definition of Measurement	3
	Dimensional Analysis	5
	Testing Hypotheses	6
2.	The Conduct of an Experimental Investigation	7
	Design	7
	Crucial Times During an Investigation	8
3.	The Scientific Report	9
	Functions of the Scientific Report	9
	Components of the Scientific Report	10
4.	Procedure in a Laboratory and the Laboratory Notebook	12
	The Laboratory Notebook	12
5.	Experimental Errors	14
	Random Errors	14
	Systematic Errors	15
	Blunders	16
	Analysis of Errors	16
6.	Rejection of Data: Chauvenet's Criterion and Its Dangers	17
7.	The Philosophy of Sampling and the Definition of Statistical	
	Concepts	19
	Population Parameters	19
	Variation and Distributions	20
	Functions of Statistics	21
	Definitions of Basic Statistical Concepts	21
8.	Discussion of the Analysis of Samples	30
9.	Discussion of Discrete and Continuous Frequency Distributions and	
	Histograms	32

	Normalized Frequency Distribution	32
	Normalized Frequency Histogram	33
	Definitions	35
	Skewness	37
	Sheppard's Correction for Grouping Data	37
10		39
	General Case of Error Propagation	39
	Independent Errors	40
	Graphical Description of Error Propagation	41
	Minimum Variance (Least-Squared Error)	42
	Nonindependent or Correlated Errors	43
	Covariances of Calculated Quantities	45
	Generalization of (10.3)	45
	Error Propagation with Complex Variables	47
	RT II	
Introdu	ction to Graphical Techniques and Curve Fitting	
11.	Display Graphs	51
	Horizontal Bar Chart	51
	Pie Chart Or Area Diagram	51
	Volumetric or Solid Diagram	52
12.	Correlation Graphs	53
	Silhouette Chart	53
	Horizontal Bar Chart	54
	Vertical Bar Chart	54
	Line Chart	54
	Search for Correlations	55
	Correlation Coefficient	62
13.		63
	Use of Perspective	63
	Projections	63
	Contour Plots	64
14.	Straight-Line Graphs and Fitting	71
	Straight Line	71
	Calculation of the Least-Squares Straight Line	74
	Fitting Straight-Line Data When Both Variables Have Uncertainties	75
15.	Reduction to Straight-Line Graphs	76
	Log Plots	76
	Semilog Plots	79
	General Use of Logarithmic Scales	87
16.	Calculating Charts	90
	Fixed Scales	90
	Sliding Scales	90
	Nomograms	91

PART III Probability

17.	The Meaning of Probability	101
	Random Phenomena and Random Variables	101
	Probability Distributions and Their Description	102
	Chebychev's Inequality	105
	Derivation of Chebychev's Inequality	106
	Symmetrical and Asymmetrical Distributions	106
	Different Kinds of Probability	107
18.	Some Arithmetic on Combinations and Permutations	111
	Arrangements: Permutations and Variations	111
	Combinations	112
	The Binomial Theorem	112
	The Laplace Triangle	113
	Remarks on the Factorial Function	115
	Some Necessary Specifications in Combinatorial Analysis	116
	The Multinomial Theorem	118
19.	Event Calculus—The Logic of Probability	121
	Definitions	121
	Conditional Probabilities: Dependence and Independence	125
	Expectation Values—Recursion Relations	136
20.	Joint Probability Distributions and Functions of Random Variables	139
	Joint and Marginal Probability Distributions	139
	Expectation Values	140
	Independence	141
	Covariance	142
	Variance	144
	Calculus of Probability Density Functions (Univariate)	147
	Calculus of Probability Density Functions (Multivariate)	148
21.	Geometrical Probability, Random Numbers, and Monte Carlo	
	Experiments	153
	Buffon's Needle	153
	Bertrand's Paradox	156
	Randomness and Random Numbers Drawn from the Uniform	
	Distribution	157
	Simulation of Probability Problems: Monte Carlo Experiments	158
	Operations with Random Numbers	162
	Sums of Random Numbers	162
	Random Numbers Drawn from an Arbitrary Distribution	167
	Correlations	169
PART IV		
Some Pr	obability Distributions and Applications	
22.	The Binomial Distribution	181
	Definitions	181
	Reproductive Property of the Binomial Distribution	183
	Probability of a Range of Values	193

	Symmetry and Asymmetry Expostation Value of the Disposit Distribution	184
	Expectation Value of the Binomial Distribution Variance of the Binomial Distribution	185
		186
	The Expectation Value for the Number of Trials Required	
	for a Specified Number of Successes The Mode of the Binomial Distribution	186
	Rare Events	187
	Inverse Probability	189
	Law of Large Numbers	189
	The Frequency Definition of Probability	190
	The Law of Large Numbers and the Sample Mean	191
23		192
	Definition of the Probability	193
	Expectation Value and Variance	193
	Binomial Approximation to the Hypergeometric Distribution	194
	Inverse Probability	199
24	•	200
	Exact Model	202
	Poisson Approximation to the Binomial Distribution	202
	Expectation Value for the Poisson Distribution	207
	Variance for the Poisson Distribution	212
	Poisson Approximation to the Hypergeometric Distribution	212
	Reproductive Property of the Poisson Distribution	212
	Radioactive Decay and the Exponential Decay Distribution	213
	The Binomial Distribution of Poisson (BDOP)	213
	Interval Distribution	214
	Inverse Probability	216
	Cumulative Poisson—Distribution Function	216
25.		219 223
	Derivation of the Gaussian Distribution from Certain	223
	Assumptions	223
	Relation of the Mean Deviation to the Standard Deviation	223
	Derivation of Gaussian Distribution from the Binomial Distribution	226
	Derivation of Gaussian Distribution from the Poisson Distribution	227
	Inverse Probability	228
	Some Properties of the Normal Distribution	229
	Normal Deviate Test for the Difference of Two Sample Means	235
	Normal Approximation to the Binomial Distribution	237
	The Central Limit Theorem (Normal Convergence Theorem)	244
26.	The Chi-Square Distribution	254
	Chi-Square and Minimization	254
	Probability Density Functions for n Independent Degrees	234
•	of Freedom	259
	Mean, Mode, and Variance of the Chi-Square Distribution	259 261
	Computations with the Chi-Square Distribution	263
	Approximation to the Chi-Square Distribution	263 264
	The Sample Variance	26 4 269
27.	Student's t Distribution	269 274
	Definition of t and its p.d.f.	274 274
	Cauchy Distribution	27 4 275
	Applications of Student's t Distribution	273 279

28.	Miscellaneous Other Probability Distributions and Examples	283
	The Negative Binomial Distribution	283
	The Multinomial Distribution	284
	The Exponential Distribution	284
	The Weibull Distribution	284
	The Log-Normal Distribution	285
	The F-distribution	285
	Folded Distributions	286
	Folded Normal Distribution	287
	Truncated Distributions	287
	Truncated Normal Distribution	287
	The Bivariate Normal Distribution	288
	Multivariate Normal Distribution	290
PART V		
Statistic	al Inference	
29.	Estimation	293
	Confidence Intervals	294
	Estimation of a Population Mean for a Large, Homogeneous	
	Population	295
	Estimation of Population Mean for a Finite Population	296
	Stratified Sampling: Estimation of a Population Mean where the	
	Population is Large and Partitioned into Strata	297
	Estimation of a Probability (Binomial)	307
	Estimation of a Population Proportion	309
30.	Estimation and the Method of Maximum Likelihood	311
	Likelihood Estimators	311
	General Properties of Estimators	317
	Nonanalytical Solution of the Likelihood Equation	326
	Asymptotic Properties of the Likelihood Function	329
	Finite Data	330
	Error Expected Prior to a Measurement	331
	Inefficient Statistics	332
	Graphical Methods: the Score Function	333
31.	Hypothesis Testing and Significance	340
	Kinds of Hypotheses	340
	Consistency and Proof	340
	Two Kinds of Error and the Cost of Being Wrong	341
	Concepts in Hypothesis Testing	342
	The Neyman-Pearson Theorem	350
	The Likelihood Ratio	352
	The Generalized Likelihood Ratio	352
•	Large-Sample Properties of the Likelihood Ratio	354
	The Generalized χ^2 Test for Goodness-of-Fit	356
	Use of the χ^2 Test for Goodness-of-Fit	352
32.	Chi-Square Minimization Methods	351
	Review of χ^2	359
	One-Parameter χ^2 : $\mathbf{c} = c_1$	361
	Multiparameter χ^2 : $\mathbf{c} = (c_1, \ldots, c_r)$	364

33.	Least-Squares Methods; Curve Fitting	387
	General Formulation	387
	Linear Case	388
	Goodness-of-Fit	397
	Linear Least Squares with Linear Constraints	397
	Nonlinear Least Squares	399
APPENDIC	ers	
Α.		
A.	Review of Notation and Some Elementary Mathematics	401
ъ	Maxima and Minima of Functions	405
В.	Matrices, Determinants, and Linear Equations	407
I.	Units and Standards of Weights and Measures	419
II.	Dimensional Analysis	431
m.	Some Comments on the Factorial, Gamma, and Error Functions	434
	Stirling's Formula	436
	Gamma and Beta Functions	437
IV.	Eight Hundred Uniformly Distributed Random Numbers and Eight	
	Hundred Random Normal Deviates	439
v.	Tables of the Negative Exponential e^{-x}	449
VI.	Tables of the Gaussian (Normal) Distribution	457
VII.	Tables and Graphs of the Chi-Square Distribution	465
VIII.	Tables of the Student's t Distribution	483
Guide	for Further Reading and Bibliography	
Index		449
		50 5

PART I

Introduction to Scientific Measurement

THE MEANING OF MEASUREMENT

The distinction is sometimes made between the "exact" sciences and the other sciences. In the first category are usually put the physical sciences such as physics and chemistry; in the second category are, broadly speaking, biology, psychology, etc. This terminology is unfortunate since it seems to imply that physical science makes statements that are true whereas the others do not. In fact, all scientists deal with the truth. The distinction is that the exact sciences can more easily measure or at least assign a value to the amount of truth in a scientific statement. It is preferable to call the physical sciences "quantitative" disciplines, since one can discuss in numerical fashion the

amount of truth in any given statement of physical fact.

The alert student will note at this point that we have not yet defined truth. We must ask what it means to say that a measurement is "true" and what we mean when we say that a given statement about the physical world is "true." We make measurements in the physical sciences, and we perform experiments to test hypotheses about the physical world. There is no clear distinction between experiment and measurements, and the former of necessity involve the latter; that is, an experiment inescapably requires the measurement of something.

A Definition of Measurement

For the purposes of this discussion we shall consider that a measurement is the quantitative determination of the value of some fixed physical constant that is characteristic of a physical object or system or of a parameter that is needed for the description of a reproducible physical situation. Note carefully the adjectives fixed and reproducible. Both carry the necessary idea that the measurement can

be repeated either tangibly or conceptually. The important point is that an *independent* determination of the value of the measured quantity can be made.

SIGNIFICANCE

Examples of quantities subject to measurement are legion: the velocity of light in vacuum; the mass of a proton; the

length of an inch scale in centimeters. When the measurement is made, we assign a value to the result. If one looks in a handbook that is modern, one finds the following values: the velocity of light in vacuum is 2.997925×10^{10} cm/sec; the mass of the proton in MeV/c² (millions of electron volts divided by the square of the velocity of light) is 938.256 ± 0.005 ; and the length of an inch in centimeters is 2.54 exactly.

What do these numbers mean? It is intuitively easy to understand that one makes a measurement and gets a result. We have three results, however, and they appear to be in three different forms. The first number consists of seven digits with a decimal point as well as an exponent. By writing down seven digits, we are expressing a measure of the reliability of this number. We tacitly mean that the next to last digit is truly meaningful and that the last number is our best guess. We say that the number has seven significant figures. In this case the velocity of light is most likely to be halfway between the numbers 2,99792 and 2,99793. The use of the exponent is a standard way of separating the number of digits needed to specify the magnitude of a number from the number of digits needed to convey its significance.

The second number represents another way of conveying the significance of a numerical quantity. The mass of the proton is believed likely to be between the values 938.251 and 938.261 MeV. We shall discuss what "likely" means at a later time. At that point we shall be able to discuss whether two numbers that represent the same quantity are *consistent* with each other.

The last is the strangest one of all: 2.54 exactly. For one of the few times to be encountered, one's first impression is correct in this instance. This is a unique quantity known as a defined constant. This is the only kind of quantity that is exact. The metric and English systems of units arose independently, and for many years the conversion between them was a measured

quantity like all the (undefined) quantities we shall encounter. If you find an old mathematics or physics book, you may even find the conversion constant written as 2.54001. (The U.S. Coast and Geodetic Survey still uses 2.54001.) Recently, however, it was decided to fix the inch as the distance that is equal to 2.54 of the units known as the centimeter. This was defined in terms of 1/100 of the distance between two ruled lines inscribed on a platinumiridium bar kept under standard conditions in Sevres, France. Since 1960, the standard centimeter has been defined by international agreement in terms of the wavelength of the orange spectral line of the light emitted by the pure isotope krypton-86. The official centimeter is now defined to be 16,507.6373 wavelengths.

1

DIMENSIONS

The basic dimensions that we deal in are length (L), time (T), and mass (M). All else may be expressed in terms of these using various physical relations, since the two sides of any equation must have the same dimensions.

Thus, force F is defined in our basic set of dimensions by the relation between the acceleration produced on a mass and the force acting on it:

$$F = ma$$

We shall denote the equality of dimensions by $\stackrel{D}{=}$. Thus

$$F \stackrel{D}{=} MLT^{-2}$$

represents the dimensions of force.

The gravitational force equation tells us that the gravitational force between two masses M_1 and M_2 in isolation is proportional to the product of the masses and to the inverse of the square of the distance between them:

$$F = \frac{GM_1M_2}{r^2}$$

where G, the gravitational constant, has

dimensions

$$G \stackrel{\underline{D}}{=} M^{-2}L^{+2}F = M^{-2}L^{+2}MLT^{-2}$$
$$\stackrel{\underline{D}}{=} L^{3}M^{-1}T^{-2}$$

To determine the dimensions of any quantity we need only recall the equations relating the quantity of interest to quantities whose dimensions we know and treat the dimensions as ordinary algebraic symbols.

The arguments (x) of various functions such as $\exp(x)$ and $\sin(x)$ must be dimensionless.

UNITS

It is desirable to write all equations so that they are independent of the system of units. Since our systems of units are arbitrary, it would be absurd to do otherwise. It should be obvious that the left side of any equation must have the same units as the right side. This provides a convenient check on any equations we write down (a necessary but not sufficient condition for the correctness of the equation).

Except for dimensionless constants, all quantities used must be regarded in some system of units, for example, centimeter-gram-second (CGS) system, meter-kilogram-second (MKS) system, foot-pound-second (English) system, etc. As with dimensions, the units of the left-hand side of an equation must be the same as the right-hand side. The units should be continually checked through any calculation since errors arising from discrepancies in units are most common! All units used must be rationalized to be consistent,

since combinations of mixed units are myriad and hence inconvenient.

For example, an English moat (it must be English) is to be filled from a reservoir. How many acre-feet of water must be drawn from the reservoir to fill the moat to a depth of 2.00 fathoms if the moat is 0.500 furlongs in length and 900 bar-leycorns wide?

Volume V = 900 barleycorn-furlongfathoms

We may always multiply anything by unity. We recognize that

1 barleycorn =
$$\frac{1}{3}$$
 inch

$$1 \text{ fathom} = 6 \text{ feet}$$

1 furlong =
$$\frac{1}{8}$$
 mile

$$1 \text{ acre} = 43,560 \text{ square feet}$$

Therefore

$$V = 900 \text{ barleycorn} \frac{1}{3} \frac{\text{inch}}{\text{barleycorn}} \times \frac{1}{12} \frac{\text{foot}}{\text{inch}}$$

$$\times$$
 furlong $\frac{1}{8} \frac{\text{mile}}{\text{furlong}} 5280 \frac{\text{feet}}{\text{mile}}$

$$\times$$
 fathoms \cdot 6 $\frac{\text{feet}}{\text{fathom}}$

$$= (900)(1/3)(1/12)(1/8)(5280)(6)$$
 foot³

$$= 99,000 \text{ ft}^3 = 99,000 \text{ ft}^2 \frac{1 \text{ acre}}{43560 \text{ ft}^2}$$

$$= 2.27 \ 27(27) \ \text{acre-ft}$$

The advantages of the metric system should be obvious!

Units and standards of both the metric and the U.S. Customary Systems are discussed in detail in Appendix I.

Dimensional Analysis

Given a physical situation describable by physical variables x_1, x_2, \ldots , we can sometimes deduce from dimensional analysis certain limitations on the form of any possible relationship among the variables. Dimensional analysis is not capable of completely determining the unknown

functional relationship, but it can delimit the possibilities and, in some simple cases, it can give the complete relationship to within a constant of proportionality. Appendix II contains a discussion of this subject.