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# **Growth Curve Models and Statistical Diagnostics**

Jianxin Pan and Kaitai Fang

(生长曲线模型及其统计诊断)



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*To the memory of my mother, to my father in his 70<sup>th</sup> year, and to my wife Haiyan and my son Kainan for their patience during the writing of this book.*

J.X. Pan

Jianxin Pan  
Centre for Medical Statistics  
Department of Mathematics  
Keele University  
Staffordshire, ST5 5BG  
United Kingdom

*To my wife Tingmei and my two daughters, Ying and Yan, for their constant support.*

K.T. Fang

Kaitai Fang  
Department of Mathematics  
Hong Kong Baptist University  
224 Waterloo Road, Kowloon  
Hong Kong



# Preface

A growth curve model (GCM) is a generalized multivariate analysis-of-variance model (GMANOVA), first summarized by Potthoff and Roy (1964) and studied subsequently by many authors including Rao (1965), Khatri (1966) and von Rosen (1989). The GCM is especially useful for investigating growth problems on short time series in areas such as economics, biology, medical research, and epidemiology. It is also a fundamental tool for analyzing longitudinal data especially with serial correlation (Jones, 1993) and repeated measures (Crowder and Hand, 1990). It is not uncommon, however, to find outliers and influential observations in growth data that significantly affect statistical inference in the GCM.

The purpose of this book is to introduce the theory of the GCM with particular emphasis on statistical diagnostics, which is mainly based on recent work on diagnostics made by the authors and their collaborators. This book is intended for researchers who are working in the area of theoretical studies related to the GCM as well as multivariate statistical diagnostics, and for applied statisticians working in application of the GCM to practical areas. Hence, on the one hand, we provide theoretical proofs for the most theorems in this book. On the other hand, applications of these techniques to practical data analysis are emphasized; for example, almost every approach discussed in this book is illustrated with practical examples. In addition, the computer programmes for calculating various measurements involved in this book have been written in S-PLUS and GENSTAT. We will put the computer programmes on our web site in due course. A link to the web site can be found in the list of author web pages at the Springer web page, [www.springer-ny.com](http://www.springer-ny.com).

The statistical diagnostics considered in this book focuses mainly on GCMs with two specific covariance structures, namely, *Rao's simple covariance structure* (SCS) and *unstructured covariance* (UC), since these two covariance structures are very common in practice and some other covariance structures are their special cases. For example, the *uniform covariance*

*structure* and *random-effects covariance structure* are two special cases of SCS. GCMs with other covariance structures can also be analyzed in a similar manner. The multivariate diagnostic techniques addressed in this book are classified into two categories: *global influence* (also known as *case-deletion* approach) and *local influence*; and each of these is used to diagnose the adequacy of GCMs within the likelihood and Bayesian frameworks as well.

Chapter 1 of this book gives a background of statistical diagnostics, a brief introduction to multiple outlier identification in multivariate data sets, a brief review of the GCM, and the related model selection criteria with respect to covariance structure. Also, the main approaches and results on statistical inferences and diagnostics in GCMs are presented in a summarized form in this chapter. In addition, preparatory materials related to matrix derivatives and matrix-variate distributions are provided for later use.

In Chapter 2, the fundamental concepts of GCMs are introduced and several most commonly encountered forms of the models are explained in terms of practical examples in biology, agriculture and medical sciences. The generalized least square estimate (GLSE) and admissibility of estimates on linear combinations of regression coefficients are discussed. We show that the GLSE of the regression coefficient is also the best linear unbiased estimate (BLUE) in the sense of matrix loss functions. We also study here the necessary and sufficient conditions of admissible estimates of linear combinations of the regression coefficients.

Maximum likelihood estimate (MLEs) of the regression coefficient and dispersion component in growth curve models are discussed in Chapter 3. We also study the expectation and variance-covariance matrix of the estimates. In general, the MLE of the regression coefficient is different from the GLSE given in Chapter 2. In fact, the latter is a linear function of the response variable while the former is not. There is indeed a special case, however, in which the MLE is completely identical to the GLSE. In this case, statistical inferences based on the MLE in growth curve models becomes simpler. This special case is nothing but SCS, in which the dispersion component matrix  $\Sigma$  is decomposed as two orthogonal components. This point will be shown with illustrative examples. As an alternative to the MLE, restricted maximum likelihood (REML) estimates are studied in the context of growth curve models with SCS and random effects covariance structure in this chapter. Estimates of the dispersion components are unbiased in this case. Numerical studies are conducted to compare the GLSE, MLE and REML in growth curve models.

Within the likelihood framework in Chapter 4 we use the case deletion technique to explore the relationship between the multiple individual deletion model (MIDM) and the mean shift regression model (MSRM), to build up multiple outlier detection criteria, and to construct influence measurements based on the generalized Cook's distance and the confidence ellipsoid

volume. Also, influence measurements are used to assess a linear combination of regression coefficients. These diagnostic techniques are applied to GCMs with SCS and UC, respectively. For illustration, some biological, medical, and agricultural data sets are analyzed using these diagnostic techniques for outlier detection and influential observation identification.

Chapter 5 is devoted to discussing how Cook's (1986) likelihood-based local influence technique could be used to diagnose the applied of GCMs with SCS and UC, respectively. With these two specific covariance structures, the observed information matrix and the Hessian matrix are studied; the Hessian matrix serves as a basis of the local influence assessment in these models. As an ancillary result, the Hessian matrix is shown to be invariant under a one-to-one measurable transformation of parameters. Also, the practical data sets analyzed in the previous chapters are reanalyzed using local influence approach discussed in this chapter.

In Chapter 6, within the Bayesian framework, we discuss the influence of a subset of observations on growth fittings in terms of case deletion technique. Under a noninformative prior distribution, the posterior distributions of the parameters in GCMs with SCS and UC are considered, respectively. The Kullback-Leibler divergence is used to measure the change of posterior distributions when the subset of observations is removed from the model. The numerical examples addressed in the previous chapters are analyzed once again using the methods developed in this chapter.

Chapter 7 is devoted to discussion of the local influence approach in the GCM from a Bayesian point of view. The fundamental idea of *Bayesian local influence* is to replace the likelihood displacement of Cook's local influence with the Kullback-Leibler divergence. For the two commonly used covariance structures, SCS and UC, Bayesian Hessian matrices in the GCM are studied under an abstract perturbation. Those matrices play a pivotal role in the Bayesian local influence. Also, some properties of Bayesian Hessian matrix are considered as ancillary results, and the relationships between likelihood-based local influence and Bayesian local influence are studied. For illustration, the covariance-weighted perturbation is considered especially and employed to analyze several practical data sets.

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Keele University  
Hong Kong Baptist University

Jian-Xin Pan  
Kai-Tai Fang

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# Acronyms

AIC	Akaike Information Criterion
ANOVA	Analysis of Variance
BIC	Bayesian Information Criterion
BLUE	Best Linear Unbiased Estimate
BLUP	Best Linear Unbiased Prediction
CLS	Cyclic Lattice Squares
DFFITS	Difference between fitted values
EM	Expectation–Maximization algorithm
GCM	Growth Curve Model
GLM	Generalized Linear Model
GLMM	Generalized Linear Mixed Model
GLP	Good Lattice Points
GLSE	Generalized Least Square Estimate
GMANOVA	Generalized Multivariate Analysis-of-Variance
i.i.d.	Independent Identically Distributed random variable
KLD	Kullback–Leibler Divergence
LISREL	Linear structure regression equation analysis
LSE	Least Square Estimate
MAD	Median of Absolute Deviation from the median
MCMC	Markov Chain Monte Carlo
MD	Mahalanobis Distance
MIDM	Multiple Individual Deletion Model
MLE	Maximum Likelihood Estimate
MSRM	Mean Shift Regression Model
MVE	Minimum Volume Ellipsoid estimate
OMRM	Ordinary Multivariate Regression Model
p.d.	Positive Definite matrix
p.d.f.	Probability Density Function
PP	Projection Pursuit
PQL	Penalized Quasi-Likelihood estimator
REML	Restricted Maximum Likelihood
RSS	Residual Sum of Squares
SCS	Rao’s Simple Covariance Structure
SVD	Singular Value Decomposition
UC	Unstructured Covariance



# Notations

Matrices are denoted by upper case bold letters, column vectors by lower case bold letters, and scalars by lower case letters. For example,  $\mathbf{X}$ ,  $\mathbf{x}$  and  $x$  represent a matrix, a column vector, and a scalar, respectively.

## Space

$R^p$	$p$ -dimensional Euclidian space
$S^q$	unit sphere in the $q$ -dimensional Euclidian space $R^q$

## Scalar

$J(\mathbf{X} \rightarrow \mathbf{Y})$	Jacobian of the transformation from $\mathbf{X}$ to $\mathbf{Y}$
$\text{tr}(\mathbf{A})$	trace of the square matrix $\mathbf{A}$
$\det(\mathbf{A})$	determinant of the square matrix $\mathbf{A}$
$\Gamma_m(a)$	multivariate gamma function, i.e., $\Gamma_m(a) = \pi^{m(m-1)/4} \prod_{i=1}^m \Gamma(a - (i-1)/2)$

## Vector

$\mathbf{1}_p$	$\mathbf{1}_p = (1, 1, \dots, 1) \in R^p$ , i.e., the $p$ -variate vector of ones
$\mathbf{d}_{\max}$	unit eigenvector associated with the largest absolute eigenvalue of the Hessian matrix
$\text{vec}(\mathbf{A})$	direct operator of the matrix $\mathbf{A}$
$\text{vec}'(\mathbf{A})$	transpose of the vector $\text{vec}(\mathbf{A})$
$\text{svec}(\mathbf{A})$	symmetric direct operator of the symmetric matrix $\mathbf{A}$
$\text{svec}'(\mathbf{A})$	transpose of the vector $\text{svec}(\mathbf{A})$
$\text{diag}(\mathbf{A})$	vector formed by the diagonal elements of $\mathbf{A}$

## Matrix

$\mathbf{A}'$	transpose of the matrix $\mathbf{A}$
$\mathbf{A}^{-1}$	inverse of the nonsingular matrix $\mathbf{A}$
$\mathbf{A}^+$	Moore–Penrose generalized inverse of the matrix $\mathbf{A}$
$\mathbf{I}_p$	identity matrix with order $p \times p$

$E_{ij}(p, q)$	$p \times q$ matrix with $(i, j)$ th element being one and others being zero. in short, denoted $E_{ij}$
$K_{pq}$	permutation matrix with order $pq \times pq$ ; for $p = q$ , denoted $K_{p^2}$
$S_p$	duplication matrix with order $p^2 \times p(p+1)/2$
$P_A$	$P_A = A(A^T A)^{-1} A^T$ , the projection matrix of $A$
$Q_S$	$Q_S = S Q (Q^T S Q)^{-1} Q^T$ , a semiprojection matrix.
$A \otimes B$	Kronecker product of the matrices $A$ and $B$
$A * B$	Hadamard product of the matrices $A$ and $B$
$\Sigma > \mathbf{0}$	$\Sigma$ is a positive definite matrix
$\Sigma^{1/2}$	square root of the matrix $\Sigma$
$\text{Cov}(\mathbf{X})$	variance-covariance matrix of the random matrix $\mathbf{X}$ , i.e., $\text{Cov}(\mathbf{X}) = \text{Cov}(\text{vec}(\mathbf{X}))$

### Univariate distribution

$N(\mu, \sigma^2)$	univariate normal distribution with expectation $\mu$ and variance $\sigma^2$
$t_p$	Student's $t$ distribution with $p$ degrees of freedom
$\chi_p^2$	chi-square distribution with $p$ degrees of freedom
$F_{n,m}$	$F$ distribution with $n$ and $m$ as first and second degrees of freedom, respectively
$\text{Gamma}(a, b)$	gamma distribution with parameters $a$ and $b$
$\text{Beta}(a, b)$	beta distribution with parameters $a$ and $b$
$\Lambda(p, m, n)$	Wilk's distribution with three parameters $p, m$ , and $n$
$GT^2(m, r, n)$	Hotelling's generalized $T^2$ distribution with three parameters $m, r$ , and $n$

### Vector-variate distribution

$N_p(\mu, \Sigma)$	$p$ -dimensional normal distribution with expectation vector $\mu$ and dispersion matrix $\Sigma > \mathbf{0}$
$t_p(\mu, \Sigma, \nu)$	$p$ -dimensional $t$ distribution with location $\mu$ and dispersion $\Sigma > \mathbf{0}$ , and $\nu$ degrees of freedom

### Matrix-variate distribution

$N_{p,n}(\mathbf{M}, \Sigma, \Omega)$	matrix-variate normal distribution with location matrix $\mathbf{M}$ and dispersion matrices $\Sigma > \mathbf{0}$ and $\Omega > \mathbf{0}$
$W_m(n, \Sigma)$	Wishart distribution with parameters $n$ and $\Sigma > \mathbf{0}$
$t_{p,n}(\mathbf{M}, \Sigma, \Omega, \nu)$	matrix-variate $t$ distribution with location matrix $\mathbf{M}$ and dispersion matrices $\Sigma > \mathbf{0}$ and $\Omega > \mathbf{0}$ and $\nu$ degrees of freedom

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