

PACKAGE ID - 000846MLTPL00 GREG

KWIC TITLE - Generalized REGression Package for Nonlinear
Parameter Estimation

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LIMITATION CODE -UNL **AUDIENCE CODE** - UNL

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DESCRIPTION - GREG computes modal (maximum-posterior-density) and interval estimates of the parameters in a user-provided Fortran subroutine MODEL, using a user-provided vector OBS of single-response observations or matrix OBS of multiresponse observations. GREG can also select the optimal next experiment from a menu of simulated candidates, so as to minimize the volume of the parametric inference region based on the resulting augmented data set.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes Source Code, User's Guide, Compilation and Linking Instructions, Sample Problem Input and Output;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - The objective function S , a weighted sum of squares deviations or sample covariance determinants, is minimized by successive quadratic programming steps. For each step, S is expanded as a quadratic function of the parameter vector O , around the initial point O_k of the step. The parametric sensitivities needed for this expansion can be computed by GREG as divided differences, or some or all of them can be provided by the user's subroutine MODEL. The quadratic approximation is minimized over a feasible trust parameter region; then a weak line search is conducted to establish an improved S value and initial parameter vector O_{k+1} for the next iteration. Ill-conditioned solutions are avoided by use of a threshold value ATOL for pivotal divisors in the quadratic minimization. Termination of the iterations controlled by the quadratic programming predictions of $\{\Delta\}S$ and $\{\Theta\}O$ for the current step. Marginal inference intervals and a covariance matrix for the estimable parameters are computed from the final quadratic expansion of $S(O)$.

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COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - GREG is in use on a wide variety of machines and operating systems.

PROGRAMMING LANGUAGES - Fortran and conforms largely to the Fortran 77 standard.

SOFTWARE LIMITATIONS - The user assigns the work array lengths and the output unit. Double precision is used for all floating-point calculations.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - The quadratic programming algorithm, upper and lower bounds, trust region, and pivoting threshold enable GREG to handle ill-conditioned or singular problems. The multiresponse code includes the objective functions of Box and Draper (1965, 1972) and some extensions described by Stewart, Caracotsios, and Sorensen (1992); it also includes automatic reduction of the working response set when necessary to keep the sample covariance matrix nonsingular. A search algorithm is provided to select additional experiments from a list of simulated candidates, when the user requests this option in the programs MAIN and MODEL.

RELATED SOFTWARE - LAPACK and BLAS codes used by GREG are provided in the LAPACK.FOR on the same diskette. Machine-optimized LAPACK and BLAS codes should be preferred where available.

OTHER PROG/OPER SYS INFO - The notation Filename.FOR on the diskette denotes a Fortran source file, and Filename.DAT denotes an output data file. The .FOR files, when compiled and linked, suffice for execution of the seven test problems given in the users manual, Appendix D. The .DAT files correspond to the printed outputs of the seven examples given in Appendix A. These results were computed on a VAXstation 3200.

HARDWARE REQS - No special hardware is required.

TIME REQUIREMENTS - Each example takes less than 3 seconds on a VAXstation 3200 computer.

REFERENCES - User's guide on media.

ABSTRACT STATUS - Submitted 5/15/95. Released screened 6/5/95.

SUBJECT CLASS CODE - P

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION
G CODES

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NONLINEAR PROBLEMS
REGRESSION ANALYSIS

EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/ER

PACKAGE TYPE - SCREENED