Example Problems and Software Extensions

to accompany

Nonlinear Parameter Estimation Methods: an Integrated System in BASIC

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References

The diskette also includes the public-domain nonlinear parameter determination software subset NLPDEX. This is in a self-unloading program NLPDEX.EXE. This collection includes an errata list for Nonlinear Parameter Estimation: an Integrated System in BASIC.

Program code segments on this diskette

BASS1.FN: liver function in rats
BASS2.DTA: data for BASS2 problem
BASS2.RES: Hepatitis patient liver function
CAL4H.MRG: merge into CAL4.FN to produce problem file for Newton method
CGG.MRG: merge into CG.BAS for global minimization
CGS.BAS: shortened form of CG (conjugate gradients)
CYQ.RES: the Chebyquad test problems
DELETER.BAS: remove derivative code
DRIVEX.BAS: a generic driver program (in NLPDEX)
ENZYMX.RES: progress curve enzyme kinetics with
ENZYME.DTA: a data file for ENZYMX
EROBUST.SRC: source form of EROBUST.BAT robust estimation BATch command
ESHL.RES: heat loss from experimental houses
FOUROUT.BAS: answers for testing Newton’s iteration on FOURTH.HSN
FOURTH.HSN: fourth power function with Hessian for Newton’s method
FUNGI.RES: fungicide effectiveness problem
GDRIVE.BAS: global minimization driver
GENROSEH.HSN: generalized Rosenbrock test with Hessian for Newton’s method
GERALD.RES: two simultaneous nonlinear equations
GFIRE.RES: fire damage to building supports
GMMIX.FN: a mixture of statistical distributions
GMMIXD.DTA: data for GMMIX.FN
GOLDPR.FN: a test function for global minimization
GRID.BAS: global minimization by grid search
HARTMAN.FN: a test function for global minimization
HESBUILD.BAS: build Hessian from .JSD file information

HIEBERT.RES : the Hiebert examples
HJFAIL.FN - a test problem which causes axial search to miss minimum
HJG.MRG: merge into HJ.BAS for global minimization
HJS.BAS: shortened form of the Hooke and Jeeves code HJ
HOBBSJ.JSD: HOBBS logistic fit with Jacobian 2nd derivative for Newton
KANNAN.RES: modelling MEFSET transistors
L1LINF.FN: test functions for L1 & Linfinity modelling
LOADMSG.BAS: displays message while programs loading
LOCN.RES: simple measures of location to test robust estimation
MAXLIK.FN: location and dispersion of a data series
MLADINE2.RES: a test function for global minimization
MLADINEO.FN: a test function for global minimization
MOTHJM.HSN: poroporo moth capture model by maximum likelihood
MRTG.MRG: merge into MRT.BAS for global minimization
MRTS.BAS: shortened form of Marquardt code MRT
NASHH.FN: a test function for global minimization
NLCONFIG.BAS: program to adapt batch files to your computer
NLERRATA: errata for NLPE (in NLPDEX)
NLGOX.BAS: a program consolidator in BASIC (in NLPDEX)
NLGRID.SRC: source form of batch file to run grid search
NLPDEX.DOC: instructions for unloading NLPDEX.EXE
NLPDEX.TXT: documentation for NLPDEX subset
NLRAN.SRC: source form of batch file to run random search
NLRRG.SRC: source form of batch file to run random restarts
NLX.SRC: source form batch file to replace NL.BAT (included Newton)
NMG.MRG: merge into NM.BAS for global minimization
NMS.BAS: shortened form of Nelder Mead polytope code NM
NTN.BAS: safeguarded Newton minimizer
POSTNTN.BAS: post-solution analysis for NTN
QUADSNH.MRG: merge into QUADSN.FN to provide Hessian for Newton
RANMIN.BAS: random search for global minimization
RCOS.FN: a test function for global minimization
RCOS2.RES: a test function for global minimization
RDELETE.BAS: to delete unwanted code for robust estimation
RESAVE.BAS: save residuals (in NLPDEX)
RESAVE.MRG: merge into RESSAVE.BAS to give RESAVE.BAS (generic code)
RESAVE.XTR: possible extra code in RESAVE.BAS
RNG.BAS: Wichmann-Hill random number generator
ROBUST.FN: a loss function generator for robust estimation
ROBUSTE.MRG: piece of code for robust estimation
ROBUSTT.MRG: piece of code to test robust estimation function
SD.MRG: merge into CG.BAS to give steepest descents code
SHEKEL.FN: a test function for global minimization
SORTER.BAS: source code of program code line sorter
STRETCH.RES: Stress-Deformation of Rubber
STRLIN.MRG: merge into STRETCH.RES --> STRLIN.FN
STRPOL.MRG: merge into STRETCH.RES to allow polynomial modelling
TABITOH.HSN: the Tabata and Ito test functions with Hessian for Newton
TESTGOX.BAS: a test consolidator in BASIC
TESTX.SRC: source code batch file to replace TEST.BAT
TNG.MRG: merge into TN.BAS for global minimization
TNS.BAS: shortened form of truncated Newton code TN
TROBUST.SRC: source code batch file to test robust estimation codes
TSORTER.BAS: to sort program code in robust estimation
VMG.MRG: merge into VM.BAS for global minimization

VMS.BAS: shortened form of variable metric minimizer VM
WOODH.MRG: merge into WOOD.FN to compute Hessian for Newton
XF.BAS: a BASIC cross-reference utility
ZIDEK.FN: estimating both n and p for Binomial processes

Chapter 1: Introduction

This work was conceived when we realized that the size of our primary monograph (Nonlinear Parameter Estimation: an Integrated System in BASIC, Marcel Dekker Inc., New York, 1987, hereafter abbreviated as NLPE) was becoming unreasonably large with details of the software and problems. The extra material which is included in this work is, however, of some interest to practitioners. We have included, in particular:

- minimization and nonlinear least squares program codes which have been stripped of extra features such as mask and bounds constraints, console image file output, and REMark statements;

- source codes for the "clean-up" programs DELETER.BAS and SORTER.BAS which have been provided in executable form on the distribution disk;

- generic driver and residual saving program code segments DRIVEX.BAS and RESAVE.BAS which allow the methods to be used in personal computers which are not IBM PC compatible, albeit with some possible changes in program statement syntax;

- program builders NLGOX.BAS and TESTGOX.BAS which can be used to run the nonlinear estimation problems entirely in a BASIC environment;

- a Newton's method minimization program code NTN.BAS with extension to the program builder NLX.BAT to allow the use to Jacobian (.JSD) and Hessian (.HSN) problem files;

- a selection of additional test and parameter estimation problems to further illustrate how the program codes in NLPE can be applied to a wide variety of problem types in many different application areas.

Note that the "generic" program segments and program builders extend the range of machines for which our programs are suitable. We believe that many environments are suitable for our methods, though we cannot claim to have conducted more than very cursory tests on a few sample systems. Some possible environments are:

CP/M 80 systems which use Microsoft BASIC

Atari 520ST and 1040ST systems in Atari BASIC

Apple IIxx under Applesoft BASIC

Apple Macintosh under Microsoft BASIC

Tandy (Radio Shack) RS 100 (BASIC is only language)

Digital Equipment Corp. VAX systems in BASIC

Commodore 64 and Amiga computers under various BASIC translators

The BASICs of these systems are not entirely equivalent to that used on IBM PCs and compatible machines. One of the most common differences is that commands to open and close files may be quite different. In some cases, only the syntax is altered (as with BASIC-80 or MBASIC for CP/M machined), while with others, for example the Radio Shack Model 100 portable, the syntax is the same, but the file naming convention is different. In the latter case, BASIC programs are usually tokenized and there are a number of other peculiarities. We have run many nonlinear parameter estimation problems on the RS 100, but must admit to consolidating the programs on a PC clone and downloading the resulting file.

We would very much like to know of user experiences, both happy and unhappy, in transferring the programs to other environments. Furthermore, we are willing to engage in correspondence with users to assist them to carry out their work. Our policy in this regard is quite straightforward:

> We aim to exchange ideas with anyone who may help us to improve our understanding and our techniques for solving computational problems in the area of optimization and parameter estimation. Within the constraints of our own time and according to our interest we will tackle problems sent to us as a tool for learning. Beyond this, and in particular if there are time deadlines or requests for what may be called 'production' calculations, we ask that a contract be set up for our services. We try to acknowledge all sources of problems, data, or advice, and expect a similar professional courtesy to be shown by those we deal with.

Before proceeding further, we would like to acknowledge the assistance of those who have provided the problems and data which appear in this work; they are named in the various sections which present the problems. We are also highly appreciative of the editorial assistance of Mary M. Nash, founder of Nash Information Services Inc.

1-1 How to print and extract information

Each chapter of this problem book is stored in the self-unloading archive, EXBOOK.EXE as a text file called EX-Cnn where nn refers to the number of the chapter. EX-C00 contains the table of contents. EX-APP contains appendices to this work, principally the bibliography and references. All the text in this work is set up so that it has a maximum line width of 75 characters. This width allows the text to be printed on almost all printers while maximizing the information contained on a screen. Straight ASCII text with no special characters has been chosen for machine-independent printing. Text files are already formatted so that they may be printed directly at the printer in page form. Each page ends with a formfeed character to take account of the possibility of different page lengths. We assume your printer can accommodate at least 66 lines per page (or can be put in a mode which will take pages at least this long). Furthermore, we assume the printer is set so that formfeeds will move to the top of the page.

The self-unloading archive EXPROG.EXE includes all program code segments associated with this book. These codes have NOT been edited for printing but rather have been left in a form for immediate use.

1-2 Errata list for Nonlinear Parameter Estimation (NLPE)

The errata list can be found in NLPDEX.EXE, a self-unloading archive of the public domain subset of our nonlinear parameter determination work. NLPDEX.EXE may be freely copied and distributed provided that no charge is made.

1-3 A comment on computational precision

Commentary in NLPE on page 398 may be taken to imply that some of the yield/density models may be difficult to estimate. This is misleading in a certain sense which is described below. The following summary of calculations using MRT with the LONION.RES problem file shows the effect of running the consolidated program

```
          1. as is (referred to as SPSP results)
          2. after adding the statement
                  1 DEFDBL A-H,O-Z
             but loading the program into gwbasic.
             (referred to as DPSP results)
          3. after adding the statement
                  1 DEFDBL A-H,O-Z
             but loading the program into gwbasic/d.
             (referred to as DPDP results)
```

See Appendix D of NLPE for some discussion of peculiarities in the interpreted Microsoft BASIC computing environment.

```
Calculations performed at 13:35:21 on 11-06-1987
LONION.RES -- Ratkowsky (1983) yield/density models
  for White Imperial Spanish Onions at Purnong Landing
    851105  -- Using log of deviations.
Results are presented in the order
SPSP = SINGLE PRECISION THROUGHOUT
DPSP = DOUBLE PRECISION VARIABLES BUT SP FUNCTION EVALUATIONS
       (i.e. gwbasic called without /d option)
DPDP = DOUBLE PRECISION WITH DP FUNCTION EVALUATIONS
       (i.e. gwbasic/d has been invoked)
with captioning only on the SPSP result.

which model is to be used  1
models: 1. y=(b(1)+b(2)*x)^(-1/b(3))
           Bleasdale and Nelder
  ELAPSED SECS= 278  AFTER 13  GRAD & 24  FN EVAL
           618+306+286     25         47
                551        18         31
```



```
CALCULATED FUNCTION MINIMUM =  .2833198
                               .2833193139825332
       (after twice finding lower points in axial search)
                               .2833200322947878

PARAMETER CORRELATION ESTIMATES
ROW  1  :   1.00000
ROW  2  :   0.99258  1.00000
            0.99258  1.00000
            0.99258  1.00000
ROW  3  :  -0.99790 -0.99813  1.00000
           -0.99791 -0.99813  1.00000
           -0.99791 -0.99813  1.00000

           Parameter      Std. Err.       Gradient
B( 1 ) =  3.824575E-03    .0044026      -.2283635
          3.842159D-03    .0044193      -.0002121
          3.842145D-03    .0044190      -4.028550D-10
B( 2 ) =  1.298609E-04   7.505212E-05   -15.99707
          1.301707D-04   7.518662D-05   -1.106590D-02
          1.301705D-04   7.518155D-05    1.680891D-08
B( 3 ) =  .9061568        .1578974      -1.374608E-02
          .9055268        .1578435      -1.082998D-05
          .9055273        .1578330      -5.725212D-12


for B( 1 )  R. OF CURV. =  3.515E-06   tilt =   25.10388
                           3.713D-05           -89.89187
                           2.605D-06             0.00001
for B( 2 )  R. OF CURV. =  1.463E+00   tilt =   89.95573
                           1.565D-08           -89.87126
                           6.796D-10            -0.00049
for B( 3 )  R. OF CURV. =  8.526E-04   tilt =    3.04514
                           8.479D-04             0.00124
                           8.479D-04             0.00000


which model is to be used  2
        2. y=1/(b(1)+b(2)*x+b(3)*x*x)
           Holliday

  ELAPSED SECS= 36  AFTER 1  GRAD & 5  FN EVAL
              173        5        18
              243        7        16
CALCULATED FUNCTION MINIMUM =  .2861091
                               .2841802695259617
                               .2841806547804453
PARAMETER CORRELATION ESTIMATES
ROW  1  :   1.00000
ROW  2  :  -0.95128  1.00000
           -0.95155  1.00000
           -0.95155  1.00000
ROW  3  :   0.86266 -0.96124  1.00000
            0.86279 -0.96125  1.00000
            0.86279 -0.96125  1.00000
```

```
             Parameter      Std. Err.       Gradient
B( 1 ) =  .001883         3.884385E-04     .261219
          2.05411D-03     3.897276D-04    -1.60438D-04
          2.05411D-03     3.897275D-04    -4.80147D-09
B( 2 ) =  9.159E-05       1.190481E-05     12.20847
          8.571236D-05    1.193202D-05    -9.767651D-03
          8.571240D-05    1.193202D-05     7.666254D-07
B( 3 ) =  0               7.381472E-08     -50143.59
          3.807744D-08    7.416836D-08     -.665118
          3.807719D-08    7.416838D-08     -6.46618D-05

for B( 1 )  R. OF CURV. =  1.649E-06   tilt =  -24.98111
                           4.066D-05           -89.92606
                           1.222D-06             0.00000
for B( 2 )  R. OF CURV. =  1.758E+01   tilt =   89.98462
                           2.201D-03           -89.99786
                           3.430D-10            -0.00062
for B( 3 )  R. OF CURV. =  1.476E+18   tilt =   89.99999
                           3.569D-01           -89.99998
                           3.469D-14            -0.49886

which model is to be used  3
        3. y=1/(b(1)+b(2)*x^b(3))
           Farazdaghi and Harris

  ELAPSED SECS= 278  AFTER 11  GRAD & 21  FN EVAL
                348        11         28
                713        14         26
CALCULATED FUNCTION MINIMUM =  .2828563
                               .2828561592391452
                               .2828563079480075
PARAMETER CORRELATION ESTIMATES
ROW  1  :   1.00000
ROW  2  :  -0.96738  1.00000
           -0.96736  1.00000
           -0.96736  1.00000
ROW  3  :   0.95454 -0.99843  1.00000
            0.95451 -0.99843  1.00000
            0.95451 -0.99843  1.00000

             Parameter      Std. Err.       Gradient
B( 1 ) =  2.293134E-03   6.175835E-04   -5.817676E-02
          2.294295D-03   6.172849D-04   -3.087303D-04
          2.294294D-03   6.172971D-04   -2.039749D-10
B( 2 ) =  6.039201E-05   3.862849E-05   -5.098023
          6.031844D-05   3.857717D-05   -1.987834D-02
          6.031853D-05   3.857804D-05   -9.567884D-10
B( 3 ) =  1.079781       .1227842       -1.440823E-03
          1.080017       .1227740       -4.698483D-06
          1.080017       .1227766        4.184389D-12

for B( 1 )  R. OF CURV. =  1.288E-06   tilt =    9.84343
                           1.000D+35             0.00000
                           1.224D-06             0.00000
```



```
for B( 2 )  R. OF CURV. =  2.092E+02   tilt =   89.99467
                           1.110D-03            89.99693
                           1.702D-10             0.00019
for B( 3 )  R. OF CURV. =  2.389E-03   tilt =   -0.17349
                           1.569D-07           -27.38825
                           2.390D-03            -0.00000
```

The above data show the importance of extended precision to obtaining small gradients and tilts at the solution point for the models and data in question. They also point to the need for care in interpreting single precision results, in that the influence of the computing environment may hide true statistical information.

1-4 NLQUICK -- fast setup for nonlinear estimation

General: readers may welcome a recipe for quickly trying some of the software on the NLPE diskette. The following brief instructions may be useful:

NLQUICK - a short-cut to running the Nash & Walker-Smith nonlinear parameter estimation software.

1. Use a 2-drive PC or compatible with at least 512K memory.

2. Configure the PC to boot with a RAMdisk (VDISK) of as large a size as you can afford. We suggest 360K in a 640K system. To do this, include a line

```
     device=VDISK.SYS 360 256 100
```

in the CONFIG.SYS file on the system disk of your PC, and make sure the file VDISK.SYS is also on this disk. Reboot the system to install the RAMdisk. Copy gwbasic.exe to the RAMdisk (c:), or ensure the active PATH points to a directory containing gwbasic.exe. BASICA users will need to alter the batch file nl.bat, replacing 'gwbasic' with 'basica'.

3. Put the Nash/Walker-Smith disk (or preferably a copy for security) in drive b:

4. Try the following commands

```
     c:    <-- to log in drive c:, the ramdisk
     copy b:nl.bat    <-- puts the main batch file on c:
     nl mrt hobbs <-- estimates the parameters of a logistic model using
                      Marquardt's method.  We suggest starting values of
                      2, 5, and 3 for the parameters.
```

Good luck.

- -