## Maximum Likelihood Estimation and Nonlinear Least Squares in Stata

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July 2007



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ML / NL in Stata

## Maximum likelihood estimation

A key resource is the book *Maximum Likelihood Estimation in Stata*, Gould, Pitblado and Sribney, Stata Press: 3d ed., 2006. A good deal of this presentation is adapted from that excellent treatment of the subject, which I recommend that you buy if you are going to work with MLE in Stata.

To perform maximum likelihood estimation (MLE) in Stata, you must write a short Stata program defining the likelihood function for your problem. In most cases, that program can be quite general and may be applied to a number of different model specifications without the need for modifying the program.



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Let's consider the simplest use of MLE: a model that estimates a binomial probit equation, as implemented in official Stata by the probit command. We code our probit ML program as:

```
program myprobit_lf
version 10.0
args lnf xb
quietly replace `lnf' = ln(normal( `xb' )) ///
if $ML_y1 == 1
quietly replace `lnf' = ln(normal( -`xb' )) ///
if $ML_y1 == 0
end
```



This program is suitable for ML estimation in the **linear form** or lf context. The local macro lnf contains the contribution to log-likelihood of each observation in the defined sample. As is generally the case with Stata's generate and replace, it is not necessary to loop over the observations. In the linear form context, the program need not sum up the log-likelihood.



Several programming constructs show up in this example. The args statement defines the program's *arguments*: lnf, the variable that will contain the value of log-likelihood for each observation, and xb, the linear form: a single variable that is the product of the "X matrix" and the current vector **b**. The arguments are local macros within the program.

The program replaces the values of lnf with the appropriate log-likelihood values, conditional on the value of  $ML_y1$ : the first dependent variable or "y"-variable. Thus, the program may be applied to any 0–1 variable as a function of any set of X variables without modification.



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Given the program—stored in the file myprobit\_lf.ado on the ADOPATH—how do we execute it?

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webuse auto, clear
gen gpm = 1/mpg
ml model lf myprobit_lf ///
   (foreign = price gpm displacement)
ml maximize
```

The ml model statement defines the context to be the linear form (lf), the likelihood evaluator to be myprobit\_lf, and then specifies the model. The binary variable foreign is to be explained by the factors price, gpm, displacement, by default including a constant term in the relationship. The ml model command only defines the model: it does not estimate it. That is performed with the ml maximize command.



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You can verify that this routine duplicates the results of applying probit to the same model. Note that our ML program produces estimation results in the same format as an official Stata command. It also stores its results as ereturns, so that postestimation commands—such as test and lincom—are available.

Of course, we need not "roll our own" binomial probit. To understand how we might apply Stata's ML commands to a likelihood function of our own, we must establish some notation, and explain what the linear form context implies.



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The log-likelihood function can be written as a function of variables and parameters:

$$\ell = \ln L\{(\theta_{1j}, \theta_{2j}, \dots, \theta_{Ej}; y_{1j}, y_{2j}, \dots, y_{Dj}), j = 1, N\}$$
  
$$\theta_{ij} = \mathbf{x}_{ij}\beta_i = \beta_{i0} + x_{ij1}\beta_{i1} + \dots + x_{ijk}\beta_{ik}$$

or in terms of the whole sample:

$$\ell = \ln L(\theta_1, \theta_2, \dots, \theta_E; \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_D)$$
  
$$\theta_i = \mathbf{X}_i \beta_i$$

where we have *D* dependent variables, *E* equations (indexed by *i*) and the data matrix  $X_i$  for the *i*<sup>th</sup> equation, containing *N* observations indexed by *j*.



In the special case where the log-likelihood contribution can be calculated separately for each observation and the sum of those contributions is the overall log-likelihood, the model is said to meet the *linear form restrictions*:

$$\ln \ell_j = \ln \ell(\theta_{1j}, \theta_{2j}, \dots, \theta_{Ej}; y_{1j}, y_{2j}, \dots, y_{Dj})$$
$$\ell = \sum_{j=1}^N \ln \ell_j$$

which greatly simplify the task of specifying the model. Nevertheless, when the linear form restrictions are not met, Stata provides three other contexts in which the full likelihood function (and possibly its derivatives) can be specified.



One of the more difficult concepts in Stata's MLE approach is the notion of ML *equations*. In the example above, we only specified a single equation:

(foreign = price gpm displacement)

which served to identify the dependent variable  $ML_y1$  to Stata) and the X variables in our binomial probit model.

Let's consider how we can implement estimation of a linear regression model via ML. In regression we seek to estimate not only the coefficient vector **b** but the error variance  $\sigma^2$ . The log-likelihood function for the linear regression model with normally distributed errors is:

$$\ln L = \sum_{j=1}^{N} [\ln \phi\{(y_j - x_j\beta)/\sigma\} - \ln \sigma]$$

with parameters  $\beta$ ,  $\sigma$  to be estimated.



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Writing the conditional mean of y for the  $j^{th}$  observation as  $\mu_i$ ,

 $\mu_j = E(\mathbf{y}_j) = \mathbf{x}_j \beta$ 

we can rewrite the log-likelihood function as

$$\theta_{1j} = \mu_j = x_{1j}\beta_1$$
  

$$\theta_{2j} = \sigma_j = x_{2j}\beta_2$$
  

$$\ln L = \sum_{j=1}^{N} [\ln \phi\{(y_j - \theta_{1j})/\theta_{2j}\} - \ln \theta_{2j}]$$



This may seem like a lot of unneeded notation, but it makes clear the flexibility of the approach. By defining the linear regression problem as a two-equation ML problem, we may readily specify equations for both  $\beta$  and  $\sigma$ . In OLS regression with homoskedastic errors, we do not need to specify an equation for  $\sigma$ , a constant parameter; but the approach allows us to readily relax that assumption and consider an equation in which  $\sigma$  itself is modeled as varying over the data.

Given a program mynormal\_lf to evaluate the likelihood of each observation—the individual terms within the summation—we can specify the model to be estimated with

ml model lf mynormal\_lf ///
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In the homoskedastic linear regression case, this might look like

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ml model lf mynormal_lf ///
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where the trailing set of () merely indicate that nothing but a constant appears in the "equation" for  $\sigma$ . This ml model specification indicates that a regression of mpg on the weight and displacement is to be fit, by default with a constant term.

We could also use the notation

```
ml model lf mynormal_lf ///
    (mpg = weight displacement) /sigma
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where there is a constant parameter to be estimated.



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#### But what does the program mynormal\_lf contain?

```
program mynormal_lf
version 10.0
args lnf mu sigma
quietly replace `lnf' = ///
ln(normalden( $ML_y1, `mu', `sigma' ))
end
```

We can use Stata's normalden (x, m, s) function in this context. The three-parameter form of this Stata function returns the Normal[m, s] density associated with x divided by s. m,  $\mu_j$  in the earlier notation, is the conditional mean, computed as  $\mathbf{X}\beta$ , while s, or  $\sigma$ , is the standard deviation. By specifying an "equation" for  $\sigma$  of (), we indicate that a single, constant parameter is to be estimated in that equation.



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What if we wanted to estimate a heteroskedastic regression model, in which  $\sigma_j$  is considered a linear function of some variable(s)? We can use the same likelihood evaluator, but specify a non-trivial equation for  $\sigma$ :

```
ml model lf mynormal_lf ///
   (mpg = weight displacement) (price)
```

This would model  $\sigma_j = \beta_4 \text{ price} + \beta_5$ . If we wanted  $\sigma$  to be proportional to price, we could use

```
ml model lf mynormal_lf ///
  (mu: mpg = weight displacement) ///
  (sigma: price, nocons)
```

which also labels the equations as mu, sigma rather than the default eq1, eq2.

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A better approach to this likelihood evaluator program involves modeling  $\sigma$  in log space, allowing it to take on all values on the real line. The likelihood evaluator program becomes

```
program mynormal_lf2
version 10.0
args lnf mu lnsigma
quietly replace `lnf' = ///
ln(normalden( $ML_y1, `mu', exp(`lnsigma' )))
end
```

It may be invoked by

ml model lf mynormal\_lf2 ///
 (mpg = weight displacement) /lnsigma, ///
 diparm(lnsigma, exp label("sigma"))

Where the diparm ( ) option presents the estimate of  $\sigma$ .



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Where the diparm ( ) option presents the estimate of  $\sigma$ .



We have illustrated the simplest likelihood evaluator method: the linear form (lf) context. It should be used whenever possible, as it is not only easier to code (and less likely to code incorrectly) but more accurate. When it cannot be used—when the linear form restrictions are not met—you may use methods d0, d1, or d2.

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Stata's ML routines provide a variety of optimization methods. The default method is the Newton–Raphson algorithm (technique(nr)), which relies on a computed Hessian matrix of second partials to guide its search for the optimum. The method used by Stata is a modified version of Newton–Raphson incorporating improvements by Marquardt.

A related set of methods are the quasi-Newton methods, which avoid explicit computation of the Hessian. A popular choice is the Berndt, Hall, Hall and Hausman algorithm (technique (bhhh)). Other quasi-Newton methods are those of Davidon, Fletcher and Powell (technique (dfp)) and Broyden, Fletcher, Goldfarb and Shanno (technique (bfgs)). The BHHH method is not available with method d0, as it relies upon gradients (first derivatives).



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A method lf likelihood evaluator program will look like:

```
program myprog
  version 10.0
  args lnf thetal theta2 ...
  tempvar tmp1 tmp2 ...
  qui gen double `tmp1' = ...
  qui replace `lnf' = ...
end
```



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Just as linear regression may be applied to many nonlinear models (e.g., the Cobb–Douglas production function), Stata's *linear form restrictions* do not hinder our estimation of a nonlinear model. We merely add equations to define components of the model. If we want to estimate

$$\mathbf{y}_j = \beta_1 \mathbf{x}_{1j} + \beta_2 \mathbf{x}_{2j} + \beta_3 \mathbf{x}_{3j}^{\beta_4} + \beta_5 + \epsilon_j$$

with  $\epsilon \sim N(0, \sigma^2)$ , we can express the log-likelihood as

$$\begin{aligned} \ln \ell_j &= \ln \phi \{ (y_j - \theta_{1j} - \theta_{2j} x_{3j}^{\theta_{3j}}) / \theta_{4j} \} - \ln \theta_{4j} \\ \theta_{1j} &= \beta_1 x_{1j} + \beta_2 x_{2j} + \beta_5 \\ \theta_{2j} &= \beta_3 \\ \theta_{3j} &= \beta_4 \\ \theta_{4j} &= \sigma \end{aligned}$$

#### The likelihood evaluator for this problem then becomes

```
program mynonlin_lf
version 10.0
args lnf theta1 theta2 theta3 sigma
quietly replace `lnf' = ln(normalden( $ML_y1, ///
`theta1'+`theta2'*$X3^`theta3', `sigma' ))
end
```

This program evaluates the LLF using a *global macro*, X3, which must be defined to identify the Stata variable that is to play the role of  $x_3$ .

By making this reference a global macro, we avoid hard-coding the variable name, so that the same model can be fit on different data without altering the program.



(a)

We could invoke the program with

```
global X3 bp0
ml model lf mynonlin_lf (bp = age sex) ///
   /beta3 /beta4 /sigma
ml maximize
```

Thus, we may readily handle a nonlinear regression model in this context of the linear form restrictions, redefining the ML problem as one of four equations.

If we need to set starting values, we can do so with the ml init command. The ml check command is very useful in testing the likelihood evaluator program and ensuring that it is working properly. The ml search command is recommended to find appropriate starting values. The ml query command can be used to evaluate the progress of ML if there are difficulties achieving convergence.



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# If the l f method cannot be used, Stata's ML routines require the use of methods tt d0, d1 or d2. In any of those methods, several additional responsibilities are borne by the programmer:

In contrast to lf, where the likelihood evaluator's arguments include  $\theta_{ij}$  expressions incorporating both  $x_{ij}$  and  $\beta_i$ , these methods pass the coefficient vector as a single argument. You must generate  $\theta_{ij}$  expressions with the help of the utility command mleval.



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In the lf approach, the likelihood evaluator computes the value of log-likelihood for each observation, storing it in variable lnf. In these methods, you must sum the log-likelihood values over observations and store it in a *scalar*lnf, an argument to the likelihood evaluator. The utility command mlsum may be used.

In the lf approach, the program respects the estimation sample and deals with impossible values where the log-likelihood function cannot be calculated. In these methods, you must handle those matters in your likelihood evaluator.



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In the lf approach, the program respects the estimation sample and deals with impossible values where the log-likelihood function cannot be calculated. In these methods, you must handle those matters in your likelihood evaluator.



A prototype d0, d1 or d2 likelihood evaluator:

```
program myprog
   version 10.0
   args todo b lnf g negH
11
                calculate scalar 'lnf' = ln L
   if ('todo' == 0 \mid 'lnf' >= .) exit
11
                 for a d1 program, calculate q,
11
                the gradient vector: d ln L / d beta
   if ('todo' == 0 | 'lnf' >= .) exit
11
                 for a d2 program, calculate negH,
11
                the negative Hessian:
11
                 -d2 \ln L / d beta d beta'
end
```



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The todo argument is 0 if lnf must be calculated, 1 if the row vector g must also be calculated, and 2 if the matrix negH must also be calculated. Thus, for methods d1 and d2, the program may be called with todo=1, requesting only calculation of the log-likelihood.



The argument  ${\rm b}$  is the current value of the vector of coefficients as a row vector. If you specify

ml model d0 myprog (foreign = mpg weight)

b will contain three values:

$$\theta_i = \beta_1 mpg_i + \beta_2 weight_i + \beta_3$$

The constant term (if included) is always the last coefficient.



### If you specify

ml model d0 myprog (foreign = mpg weight) ///
 (displ = weightsq) /sigma

b will contain six values:

$$\begin{aligned} \theta_{1j} &= \beta_1 mpg_j + \beta_2 weight_j + \beta_3 \\ \theta_{2j} &= \beta_4 weightsq_j + \beta_5 \\ \theta_{3j} &= \beta_6 \end{aligned}$$



To form the combinations of coefficients and data, we use mleval in our likelihood evaluator:

```
tempvar theta1 theta2 ...
tempname theta3 ...
mleval `theta1' = `b', eq(1)
mleval `theta2' = `b', eq(2)
mleval `theta3' = `b', eq(3) scalar
```

We specify each theta as a tempvar (if a variable) or a tempname (if a scalar, such as  $\sigma$ ). These theta macros may then be used in writing the likelihood function, just as in method lf.



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To generate the total log-likelihood of the sample, we should use mlsum in our likelihood evaluator:

mlsum `lnf' = ...

Use of mlsum automatically includes only observations specified in the estimation subsample (those for which  $ML_samp==1$ ), applies weights if specified, and ensures that there are no missing values of observations' likelihood. If there are missing values, it sets the scalar lnf to missing to signal that the current coefficient values in tt b are not feasible.



If the likelihood function meets the linear form restrictions (but we wish to use method d0, d1 or d2), we may use the mlvecsum and mlmatsum commands in our likelihood evaluator to produce the appropriate formulas for the gradient vector g and negative Hessian negH.

Stata recommends that the routine is tested as a method d0 evaluator before making use of the first or first and second derivatives. Methods d1debug and d2debug assist you in determining whether the derivatives have been coded properly.



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We have presented interactive use of Stata's ML facilities, in which commands ml model, ml search and ml maximize are used to perform estimation. If you are going to use a particular maximum likelihood evaluator extensively, it may be useful to write an ado-file version of the routine, using ML's noninteractive mode.

An ado-file version of a ML routine can implement all the features of any Stata estimation command, and itself becomes a Stata command with a *varlist* and options, as well as the ability to replay results.



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An ado-file version of a ML routine can implement all the features of any Stata estimation command, and itself becomes a Stata command with a *varlist* and options, as well as the ability to replay results.



To produce a new estimation command, you must write two ado-files: newcmd.ado and newcmd\_ll.ado, the likelihood function evaluator. The latter ado-file is unchanged from our previous discussion. The newcmd.ado file will characteristically contain references to two programs, internal to the routine: Replay and Estimate. Thus, the skeleton of the command ado-file will look like:

```
program newcmd
version 10.0
if replay() {
    if ("`e(cmd)'" != "newcmd") error 301
      Replay `0'
}
else Estimate `0'
end
```



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If newcmd is invoked by only its name, it will execute the Replay subprogram if the last estimation command was newcmd. Otherwise, it will execute the Estimate subprogram, passing the remainder of the command line in local macro 0 to Estimate.

The Replay subprogram is quite simple:

```
program Replay
   syntax [, Level(cilevel), other-display-options ]
   ml display, level(`level') other-display-options
end
```



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end
```



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The Estimate subprogram will contain:

```
program Estimate, eclass sortpreserve
  syntax varlist [if] [in] [, vce(passthru) ///
  Level(cilevel) other-estimation-options ///
  other-display-options ]
```

```
marksample touse
```

```
ml model method newcmd_ll if `touse', ///
`vce' other-estimation-options maximize
```

```
ereturn local cmd "newcmd"
Replay, 'level' other-display-options
end
```



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The Estimate subprogram is declared as eclass so that it can return estimation results. The syntax statement will handle the use of if or in clauses, and pass through any other options provided on the command line. The marksample touse ensures that only observations satisfying the if or in clauses are used.

On the ml model statement, method would be hard-coded as lf, d0, d1, d2. The if `touse' clause specifies the proper estimation sample. The maximize option is crucial: it is this option that signals to Stata that ML is being used in its noninteractive mode. With maximize, the ml model statement not only defines the model but triggers its estimation.

The non-interactive estimation does not display its results, so ereturn and a call to the Replay subprogram are used to produce output.



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Additional estimation options can readily be added to this skeleton. For instance, cluster-robust estimates can be included by adding a CLuster(varname) option to the syntax statement, with appropriate modifications to ml model. In the linear regression example, we could provide a set of variables to model heteroskedasticity in a HEtero(varlist) option, which would then define the second equation to be estimated by ml model.

The mlopts utility command can be used to parse options provided on the command line and pass any related to the ML estimation process to ml model. For instance, a HEtero(varlist) option is to be handled by the program, while an iterate(#) option should be passed to the optimizer.



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## Nonlinear least squares estimation

Besides the capabilities for maximum likelihood estimation of one or several equations via the ml suite of commands, Stata provides facilities for single-equation nonlinear least squares estimation with nl and the estimation of nonlinear systems of equations with nlsur.

The nl and nlsur commands may be invoked in three ways: interactively, using a "programmed substitutable expression", and using a "function evaluator program". We discuss the first and third methods here. The function evaluator program is quite similar to the likelihood function evaluators we have discussed.



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In the interactive mode, you specify the nonlinear least squares expression, including starting values if necessary, on the command line. For example, consider the two-factor CES production function:

$$\ln Q_i = \beta_0 - \frac{1}{\rho} \ln \left( \delta K_i^{-\rho} + (1-\delta) L_i^{-\rho} \right) + u_i$$

### with the parameters $\beta_0, \rho, \delta$ .

This could be estimated with:

nl (lnQ={b0}-1/{rho=1}\*ln({delta=0.5}\*K^(-1\*{rho}) + (1-{delta}\*L^(-1\*{rho})))

Note that the parameters are enclosed in { }, with initial values given if needed. The entire equation must be enclosed by ( ). You may use options such as robust and cluster (*varname*) with nl.



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The standard apparatus for any estimation command is available after invoking tt nl. For instance, we might want to calculate the elasticity of substitution for the CES function, defined as  $\sigma = 1/(1 + \rho)$ . The nlcom command can provide point and interval estimates of this expression via the delta method:

#### nlcom (sigma: 1 / ( 1 + [rho]\_b[\_cons] ))

where we refer to the "constant" in the rho equation, and label the resulting expression sigma in the output.

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If you want to use nl extensively for a particular problem, it makes sense to develop a *function evaluator program*. That program is quite similar to any Stata ado-file or ml program. It must be named nl*func*.ado, where *func* is a name of your choice: e.g., nlces.ado for a CES function evaluator.

The stylized function evaluator program contains:

program nlfunc version 10.0 syntax varlist(min=n max=n) if, at(name) // extract vars from varlist // extract params as scalars from at matrix // fill in dependent variable with replace end



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    // extract params as scalars from at matrix
    // fill in dependent variable with replace
end
```



The *varlist* contains all Stata variables referenced in the program, both dependent and independent. Their names are passed to the program, so that different variables may be used without modifying the program.

The *if* argument should be used, as a local macro, on all generate or replace statements within the program to restrict analysis to the estimation sample.

The *at(name)* contains the name of a Stata matrix—a row vector—containing the current values of the parameters. The parameters must be extracted from this matrix when referenced in the program.



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To retrieve the Stata variables from the *varlist*, use statements such as:

local logoutput : word 1 of 'varlist'

and reference logoutput as a local macro within the program.

To retrieve the parameters from the matrix specified in *at(name)*, use:

```
tempname b0 rho delta
scalar 'b0' = `at'[1,1]
scalar `rho' = `at'[1,2]
scalar `delta' = `at'[1,3
```

and reference the parameters as local macros within the program.



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If any additional variables are needed, define them as tempvars of type double and respect the *if* condition:



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To use the program nlces, call it with the nl command, but only include the unique part of its name, followed by @:

nl ces @ lnQ cap lab, parameters(b0 rho delta) ///
initial(b0 0 rho 1 delta 0.5)

You could restrict analysis to a subsample with the *if exp* qualifier:

nl ces @ lnQ cap lab if industry==33, ...



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### Two alternative syntaxes for invoking the program exist:

```
nl ces @ lnQ cap lab, nparameters(3) ///
initial(b0 0 rho 1 delta 0.5)
```

In this case, you need not spell out the parameter names in the parameters option, but merely indicate how many there are in nparameters.

You can also pass the parameter values, in the order that they appear in the function evaluator program, in a row vector:

matrix startv = (0, 1, 0.5)
nl ces @ lnQ cap lab, nparameters(3) initial(startv)



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The techniques for estimating a system of nonlinear equations (for instance, cost share equations for a transcendental logarithmic cost function) are similar to those described above for single-equation nonlinear least squares. You must write a function evaluator program that generates values for each of the LHS variables, working with the entire parameter vector. For more details see [R] nlsur. Note, however, that this command does not implement estimation of a nonlinear system of simultaneous equations.

