**maximize** — Details of iterative maximization

Description Option for set maxiter Methods and formulas Syntax Remarks and examples References Maximization options Stored results Also see

# Description

Title

All Stata commands maximize likelihood functions using moptimize() and optimize(); see *Methods and formulas* below. Commands use the Newton-Raphson method with step halving and special fixups when they encounter nonconcave regions of the likelihood. For details, see [M-5] moptimize() and [M-5] optimize(). For more information about programming maximum likelihood estimators in ado-files and Mata, see [R] ml and Gould, Pitblado, and Poi (2010).

set maxiter specifies the default maximum number of iterations for estimation commands that iterate. The initial value is 16000, and # can be 0 to 16000. To change the maximum number of iterations performed by a particular estimation command, you need not reset maxiter; you can specify the iterate(#) option. When iterate(#) is not specified, the maxiter value is used.

## Syntax

Maximum likelihood optimization

mle\_cmd ... [, options]

Set default maximum iterations

```
set maxiter # [, permanently]
```

#### 2 maximize — Details of iterative maximization

options	Description	
<u>dif</u> ficult	use a different stepping algorithm in nonconcave regions	
<pre>technique(algorithm_spec)</pre>	maximization technique	
<u>iter</u> ate(#)	perform maximum of # iterations; default is iterate(16000)	
$[\underline{no}]\underline{log}$	display an iteration log of the log likelihood; typically, the default	
<u>tr</u> ace	display current parameter vector in iteration log	
gradient	display current gradient vector in iteration log	
showstep	report steps within an iteration in iteration log	
<u>hess</u> ian	display current negative Hessian matrix in iteration log	
<u>showtol</u> erance	report the calculated result that is compared to the effective convergence criterion	
<u>tol</u> erance(#)	tolerance for the coefficient vector; see Options for the defaults	
<u>ltol</u> erance(#)	tolerance for the log likelihood; see Options for the defaults	
<u>nrtol</u> erance(#)	tolerance for the scaled gradient; see Options for the defaults	
<pre>qtolerance(#)</pre>	when specified with algorithms bhhh, dfp, or bfgs, the $q - H$ matrix is used as the final check for convergence rather than nrtolerance() and the H matrix; seldom used	
<u>nonrtol</u> erance	ignore the nrtolerance() option	
<pre>from(init_specs)</pre>	initial values for the coefficients	

where *algorithm\_spec* is

```
algorithm [ # [ algorithm [#] ]...]
```

```
algorithm is { nr | bhhh | dfp | bfgs }
```

and *init\_specs* is one of

matname [, skip copy]
{ [eqname:]name = # | /eqname = # } [...]
# [# ...], copy

### **Maximization options**

difficult specifies that the likelihood function is likely to be difficult to maximize because of nonconcave regions. When the message "not concave" appears repeatedly, ml's standard stepping algorithm may not be working well. difficult specifies that a different stepping algorithm be used in nonconcave regions. There is no guarantee that difficult will work better than the default; sometimes it is better and sometimes it is worse. You should use the difficult option only when the default stepper declares convergence and the last iteration is "not concave" or when the default stepper is repeatedly issuing "not concave" messages and producing only tiny improvements in the log likelihood.

technique (*algorithm\_spec*) specifies how the likelihood function is to be maximized. The following algorithms are allowed. For details, see Gould, Pitblado, and Poi (2010).

technique(nr) specifies Stata's modified Newton-Raphson (NR) algorithm.

technique(bhhh) specifies the Berndt-Hall-Hall-Hausman (BHHH) algorithm.

technique(dfp) specifies the Davidon-Fletcher-Powell (DFP) algorithm.

technique(bfgs) specifies the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm.

The default is technique(nr).

You can switch between algorithms by specifying more than one in the technique() option. By default, an algorithm is used for five iterations before switching to the next algorithm. To specify a different number of iterations, include the number after the technique in the option. For example, specifying technique(bhhh 10 nr 1000) requests that ml perform 10 iterations with the BHHH algorithm followed by 1000 iterations with the NR algorithm, and then switch back to BHHH for 10 iterations, and so on. The process continues until convergence or until the maximum number of iterations is reached.

- iterate(#) specifies the maximum number of iterations. When the number of iterations equals iterate(), the optimizer stops and presents the current results. If convergence is declared before this threshold is reached, it will stop when convergence is declared. Specifying iterate(0) is useful for viewing results evaluated at the initial value of the coefficient vector. Specifying iterate(0) and from() together allows you to view results evaluated at a specified coefficient vector; however, not all commands allow the from() option. The default value of iterate(#) for both estimators programmed internally and estimators programmed with ml is the current value of set maxiter, which is iterate(16000) by default.
- log and nolog specify whether an iteration log showing the progress of the log likelihood is to be displayed. For most commands, the log is displayed by default, and nolog suppresses it. For a few commands (such as the svy maximum likelihood estimators), you must specify log to see the log.
- trace adds to the iteration log a display of the current parameter vector.
- gradient adds to the iteration log a display of the current gradient vector.
- showstep adds to the iteration log a report on the steps within an iteration. This option was added so that developers at StataCorp could view the stepping when they were improving the ml optimizer code. At this point, it mainly provides entertainment.
- hessian adds to the iteration log a display of the current negative Hessian matrix.
- showtolerance adds to the iteration log the calculated value that is compared with the effective convergence criterion at the end of each iteration. Until convergence is achieved, the smallest calculated value is reported.
- shownrtolerance is a synonym of showtolerance.

Below we describe the three convergence tolerances. Convergence is declared when the nrtolerance() criterion is met and either the tolerance() or the ltolerance() criterion is also met.

- tolerance(#) specifies the tolerance for the coefficient vector. When the relative change in the coefficient vector from one iteration to the next is less than or equal to tolerance(), the tolerance() convergence criterion is satisfied.
  - tolerance(1e-4) is the default for estimators programmed with ml.

tolerance(1e-6) is the default.

ltolerance(#) specifies the tolerance for the log likelihood. When the relative change in the log
likelihood from one iteration to the next is less than or equal to ltolerance(), the ltolerance()
convergence is satisfied.

ltolerance(0) is the default for estimators programmed with ml.

ltolerance(1e-7) is the default.

nrtolerance(#) specifies the tolerance for the scaled gradient. Convergence is declared when  $gH^{-1}g' < nrtolerance()$ . The default is nrtolerance(1e-5).

qtolerance(#) when specified with algorithms bhhh, dfp, or bfgs uses the q - H matrix as the final check for convergence rather than nrtolerance() and the H matrix.

Beginning with Stata 12, by default, Stata now computes the **H** matrix when the q-H matrix passes the convergence tolerance, and Stata requires that **H** be concave and pass the nrtolerance() criterion before concluding convergence has occurred.

qtolerance() provides a way for the user to obtain Stata's earlier behavior.

nonrtolerance specifies that the default nrtolerance() criterion be turned off.

from() specifies initial values for the coefficients. Not all estimators in Stata support this option. You
can specify the initial values in one of three ways: by specifying the name of a vector containing
the initial values (for example, from(b0), where b0 is a properly labeled vector); by specifying
coefficient names with the values (for example, from(age=2.1 /sigma=7.4)); or by specifying
a list of values (for example, from(2.1 7.4, copy)). from() is intended for use when doing
bootstraps (see [R] bootstrap) and in other special situations (for example, with iterate(0)).
Even when the values specified in from() are close to the values that maximize the likelihood,
only a few iterations may be saved. Poor values in from() may lead to convergence problems.

- skip specifies that any parameters found in the specified initialization vector that are not also found in the model be ignored. The default action is to issue an error message.
- copy specifies that the list of values or the initialization vector be copied into the initial-value vector by position rather than by name.

### Option for set maxiter

permanently specifies that, in addition to making the change right now, the maxiter setting be remembered and become the default setting when you invoke Stata.

### **Remarks and examples**

#### stata.com

Only in rare circumstances would you ever need to specify any of these options, except nolog. The nolog option is useful for reducing the amount of output appearing in log files.

The following is an example of an iteration log:

```
Iteration 0:
               log likelihood = -3791.0251
               log likelihood = -3761.738
Iteration 1:
Iteration 2:
               log likelihood = -3758.0632
                                             (not concave)
               log likelihood = -3758.0447
Iteration 3:
               log likelihood = -3757.5861
Iteration 4:
Iteration 5:
               \log likelihood = -3757.474
Iteration 6:
               \log likelihood = -3757.4613
Iteration 7:
               \log likelihood = -3757.4606
Iteration 8:
               \log likelihood = -3757.4606
  (table of results omitted)
```

At iteration 8, the model converged. The message "not concave" at the second iteration is notable. This example was produced using the heckman command; its likelihood is not globally concave, so it is not surprising that this message sometimes appears. The other message that is occasionally seen is "backed up". Neither of these messages should be of any concern unless they appear at the final iteration.

If a "not concave" message appears at the last step, there are two possibilities. One is that the result is valid, but there is collinearity in the model that the command did not otherwise catch. Stata checks for obvious collinearity among the independent variables before performing the maximization, but strange collinearities or near collinearities can sometimes arise between coefficients and ancillary parameters. The second, more likely cause for a "not concave" message at the final step is that the optimizer entered a flat region of the likelihood and prematurely declared convergence.

If a "backed up" message appears at the last step, there are also two possibilities. One is that Stata found a perfect maximum and could not step to a better point; if this is the case, all is fine, but this is a highly unlikely occurrence. The second is that the optimizer worked itself into a bad concave spot where the computed gradient and Hessian gave a bad direction for stepping.

If either of these messages appears at the last step, perform the maximization again with the gradient option. If the gradient goes to zero, the optimizer has found a maximum that may not be unique but is a maximum. From the standpoint of maximum likelihood estimation, this is a valid result. If the gradient is not zero, it is not a valid result, and you should try tightening up the convergence criterion, or try ltol(0) tol(1e-7) to see if the optimizer can work its way out of the bad region.

If you get repeated "not concave" steps with little progress being made at each step, try specifying the difficult option. Sometimes difficult works wonderfully, reducing the number of iterations and producing convergence at a good (that is, concave) point. Other times, difficult works poorly, taking much longer to converge than the default stepper.

### Stored results

Maximum likelihood estimators store the following in e():

S	calars		
	e(N)	number of observations	always stored
	e(k)	number of parameters	always stored
	e(k_eq)	number of equations in e(b)	usually stored
	e(k_eq_model)	number of equations in overall	usually stored
		model test	
	e(k_dv)	number of dependent variables	usually stored
	e(df_m)	model degrees of freedom	always stored
	e(r2_p)	pseudo-R-squared	sometimes stored
	e(11)	log likelihood	always stored
	e(11_0)	log likelihood, constant-only model	stored when constant-only model is fit
	e(N_clust)	number of clusters	stored when vce(cluster <i>clustvar</i> ) is specified; see [U] <b>20.21 Obtaining robust variance estimates</b>
	e(chi2)	$\chi^2$	usually stored
	e(p)	significance of model of test	usually stored
	e(rank)	rank of e(V)	always stored
	e(rank0)	rank of $\texttt{e(V)}$ for constant-only model	stored when constant-only model is fit
	e(ic)	number of iterations	usually stored
	e(rc)	return code	usually stored
	e(converged)	1 if converged, 0 otherwise	usually stored

Macros e(cmd) name of command always stored e(cmdline) command as typed always stored e(depvar) names of dependent variables always stored e(wtype) weight type stored when weights are specified or implied e(wexp) weight expression stored when weights are specified or implied e(title) title in estimation output usually stored by commands using ml e(clustvar) name of cluster variable stored when vce(cluster *clustvar*) is specified; see [U] 20.21 Obtaining robust variance estimates Wald or LR; type of model  $\chi^2$  test e(chi2type) usually stored e(vce) vcetype specified in vce() stored when command allows (vce()) e(vcetype) title used to label Std. Err. sometimes stored e(opt) type of optimization always stored e(which) max or min; whether optimizer is to always stored perform maximization or minimization e(ml\_method) type of ml method always stored by commands using ml e(user) name of likelihood-evaluator program always stored e(technique) from technique() option sometimes stored sometimes stored1 e(singularHmethod) m-marquardt or hybrid; method used when Hessian is singular e(crittype) optimization criterion always stored1 e(properties) estimator properties always stored e(predict) program used to implement predict usually stored Matrices e(b) coefficient vector always stored e(Cns) constraints matrix sometimes stored e(ilog) iteration log (up to 20 iterations) usually stored e(gradient) gradient vector usually stored e(V) variance-covariance matrix of always stored the estimators e(V\_modelbased) model-based variance only stored when e(V) is neither the OIM nor OPG variance Functions e(sample) marks estimation sample always stored

1. Type ereturn list, all to view these results; see [P] return.

See *Stored results* in the manual entry for any maximum likelihood estimator for a list of returned results.

### Methods and formulas

Optimization is currently performed by moptimize() and optimize(), with the former implemented in terms of the latter; see [M-5] **moptimize()** and [M-5] **optimize()**. Some estimators use moptimize() and optimize() directly, and others use the ml ado-file interface to moptimize().

Prior to Stata 11, Stata had three separate optimization engines: an internal one used by estimation commands implemented in C code; ml implemented in ado-code separately from moptimize() and used by most estimators; and moptimize() and optimize() used by a few recently written

estimators. These days, the internal optimizer and the old version of ml are used only under version control. In addition, arch and arima (see [TS] arch and [TS] arima) are currently implemented using the old ml.

Let  $L_1$  be the log likelihood of the full model (that is, the log-likelihood value shown on the output), and let  $L_0$  be the log likelihood of the "constant-only" model. The likelihood-ratio  $\chi^2$  model test is defined as  $2(L_1 - L_0)$ . The pseudo- $R^2$  (McFadden 1974) is defined as  $1 - L_1/L_0$ . This is simply the log likelihood on a scale where 0 corresponds to the "constant-only" model and 1 corresponds to perfect prediction for a discrete model (in which case the overall log likelihood is 0).

Some maximum likelihood routines can report coefficients in an exponentiated form, for example, odds ratios in logistic. Let b be the unexponentiated coefficient, s its standard error, and  $b_0$  and  $b_1$  the reported confidence interval for b. In exponentiated form, the point estimate is  $e^b$ , the standard error  $e^bs$ , and the confidence interval  $e^{b_0}$  and  $e^{b_1}$ . The displayed Z (or t) statistics and p-values are the same as those for the unexponentiated results. This is justified because  $e^b = 1$  and b = 0 are equivalent hypotheses, and normality is more likely to hold in the b metric.

### References

Gould, W. W., J. S. Pitblado, and B. P. Poi. 2010. *Maximum Likelihood Estimation with Stata.* 4th ed. College Station, TX: Stata Press.

McFadden, D. L. 1974. Conditional logit analysis of qualitative choice behavior. In *Frontiers in Econometrics*, ed. P. Zarembka, 105–142. New York: Academic Press.

## Also see

[R] ml — Maximum likelihood estimation

[SVY] ml for svy — Maximum pseudolikelihood estimation for survey data

[M-5] **moptimize**() — Model optimization

[M-5] optimize() — Function optimization