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Optimization under nonlinear constraints

by

Leif Jansson and Erik Mellander

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Leif Jansson
The Ministry of Economic Affairs
103 33 Stockholm
Sweden

Erik Mellander
The Industrial Institute for Economic and Social Research
114 53 Stockholm
Sweden

In this paper a timesaving method is proposed for maximizing likelihood functions when the parameter space is subject to nonlinear constraints, expressable as second order polynomials. The suggested approach is especially attractive when dealing with systems with many parameters.

1. Introduction

In this note the implementation of second order polynomial constraints on a parameter matrix is given a simple algebraic form. First order partial derivatives of the constrained matrix are also given simple vector forms. The formulas presented are easily transformed into computer algorithms.

One area of special interest for the application of the above results is the maximization of the likelihood function of a system of simultaneous equations.

2. A maximum likelihood function

Consider a standard simultaneous equation system compactly written as

$$BY' + CZ' = AX' = E' \qquad (1)$$

where $A = (B|C)$ is the $n,(n+m)$ parameter matrix, $X' = (Y|Z)'$ is the $(n+m),T$ matrix of observations on the endogenous and predetermined variables and the columns of E', e_t $(t=1,2,\ldots,T)$ are vectors of unobservable random disturbances. The errors are assumed to have a time independent multivariate normal distribution, e_t NID(0,).

If the variance-covariance matrix is unconstrained the log-likelihood function can be concentrated with respect to giving

$$L = k + T \log B - 1/2\ T \log (AX'XA')$$

Koopmans and Hood (1953) where M denotes the determinant of matrix M.

A common way of maximizing the log-likelihood function L is to use an iterative gradient search method where the derivatives are numerically calculated. This approach allows for a flexible specification of the equations and makes it easy to specify nonlinear restrictions, but the number of evaluations of the log-likelihood function is in each iteration proportional to the number of parameters to be estimated. Thus, with many parameters to estimate there can be considerable gains in computing time if the first order derivatives instead can be given a simple analytical form.

The derivative of L with respect to a free parameter $_i$ can be written as

$$\frac{L}{\partial\Theta_i} = \text{vec} \quad \frac{A}{\partial\Theta_i})' \cdot \text{vec}\left((B^{-1'} \mid 0) - \phi\right) \qquad (2)$$

where $\phi = [AX'XA']^{-1} A(X'X)$

where vec M denotes the column vector whose elements are the columns of M put on top of each other.

Much of the calculations to achieve the complicated matrix ϕ is done to get the likelihood value L. So when the derivative vector $\partial A/\partial\Theta_i$ can be easily calculated also $\partial L/\partial\Theta_i$ is given with little extra computation.

3. Calculations of derivatives

The restricted parameters a_{ij} of the matrix A can be expressed as functions of k unrestricted parameters θ_ℓ. Second order polynomial restrictions on the parameters of the matrix A can then be written as

$$\text{vec}[A(\Theta)] = R1 \cdot F1 + R2 \cdot F2 + d$$

where

R1 = the [n(n+m),k] linear restriction matrix

F1 = the column vector containing the k free parameters

R2 = the [n(n+m),k(k+1)/2] non-linear restriction matrix

F2 = the column vector of the k(k+1)/2 possible different products of the k free parameters

i.e. $F2' = (\Theta_1^2, \Theta_1\Theta_2, \Theta_1\Theta_k, \ldots, \Theta_k^2)$

d = a column vector with n(n+m) constants

The first order derivatives of the linear part of the restricted parameters of the A' matrix with respect to Θ_i become

$$\frac{\partial}{\partial\Theta_i} R1 \cdot F1 = R1 \cdot \Delta 1_i$$

where $\Delta 1$ is a column vector with elements δ_j, $j = 1, \ldots, k$ and

$$\delta_j = \begin{cases} 0 & \text{if } j \neq i \\ 1 & \text{if } j = i \end{cases}$$

Thus, the first order derivatives of $R1 \cdot F1$ with respect to Θ_i are equal to the i:th column of the linear restriction matrix R1.

The non-linear part the derivatives becomes

$$\frac{\partial}{\partial\Theta_i} R2 \cdot F2 = R2 \cdot \Delta 2_i$$

where $\Delta 2$ is a column vector with element η_j, $j = 1, \ldots, k \cdot (k+1)/2$ and

$$\eta_j = \begin{cases} 0 & \text{if } \Theta_{j1} \text{ and } \Theta_{j2} \neq \Theta_i \\ \Theta_{j1} & \text{if } \Theta_{j2} = \Theta_i \\ \Theta_{j2} & \text{if } \Theta_{j1} = \Theta_i \\ 2\Theta_i & \text{if } \Theta_{j1} = \Theta_{j2} = \Theta_i \end{cases}$$

Thus, the first order derivative of the non-linear part become linear combinations of the columns of R2. The derivative of R2•F2 with respect to Θ_i, for instance, can alternatively be written as

$$\frac{\partial(R2 \cdot F2)}{\partial\Theta_i} = -2\Theta_i \cdot R2_i + \sum_{j \neq i} \Theta_j \cdot R2_j$$

In practice the R1, R2 and d matrices will contain mostly zeros and it would be practically impossible to set them up as in the formulas. They can, however, easily be packed into a dense form by storing only the nonzero elements of the R1 and R2 matrix together with their destination in the A matrix and the position of the free variable parameters they are associated with.

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