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ALS ESTIMATION OF PARAMETERS IN A
STATE SPACE MODEL

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Abstract Asymptotic Least Squares is applied to the State Space model. In a limited subclass of models it leads to explicit estimators of variance parameters, while in the most general State Space model an ALS estimator is impractical. A small simulation study of the former situation indicates that the ALS estimator is an excellent approximation of the ML estimator.

Keywords State Space model, Kalman Filter, Asymptotic Least Squares.

ALS ESTIMATION OF PARAMETERS IN A STATE SPACE MODEL

Ivo J. Steyn[1]

1. Introduction

The State Space model, of which one of the many alternative forms is:

(1a) $\alpha_t = T.\alpha_{t-1} + \eta_t \qquad \eta_t \sim N(0,\sigma^2 Q)$

(1b) $y_t = Z_t.\alpha_t + \epsilon_t \qquad \epsilon_t \sim N(0,\sigma^2 R)$

encompasses vast classes of useful models, such as the standard linear regression model, all ARMA and ARIMA models, varying coefficient models, and many others. The State vector α_t (k x 1) contains all information needed to predict y_t (g x 1), as long as the measurement matrix Z_t (g x k) is known.

The problem of estimating the State vector α_t was solved as long as 28 years ago in two papers by Kalman and Kalman & Bucy[2]. Their estimation method - which has since become known as the Kalman Filter - does require two items of information before estimation can proceed : exact knowledge of all parameters in the model (i.e. those in T, R and S), and some estimate of the initial state α_0.

In this paper the former problem is examined. The unknown parameters are estimated with Asymptotic Least Squares, and, in a limited subclass of models, this yields explicit and simple estimators which can be calculated before a Kalman Filter is applied.
Section 2 reviews the ALS estimation technique, while section 3 is concerned with the application of ALS to the estimation of parameters in the Kalman Filter in a restricted subclass of models. Section 4 gives a numerical example of this, while in section 5 ALS is applied to the general State Space model (1a)-(1b). Section 6 attempts to draw conclusions.

2. Asymptotic Least Squares

Suppose we wish to estimate a vector of parameters θ by Maximum Likelihood but are unable to formulate an explicit estimator. However, we can estimate another vector β of parameters consistently, and β and θ are related through

(2) $f(\beta,\theta) = 0$

where f is a function from $\mathbb{R}^n \times \mathbb{R}^m$ to $\mathbb{R}^r$, n and m being the dimension of β and θ, respectively. We will also assume that β is estimated by $\hat{\beta}$, that

(3) $\sqrt{n}(\beta_0 - \hat{\beta}) \rightarrow N(0,\Omega(\beta_0))$

where β_0 is the true value of β, and that we have a consistent estimator $\hat{\Omega}$ for Ω.
We obtain the ALS estimator for θ by solving :

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1) Part of the research for this paper was carried out while I was a guest at Manchester University. I would like to thank Garry Phillips for the opportunity to work on this paper in an unfamiliar but stimulating environment. Heinz Neudecker provided inimitable guidance during some of the matrix calculations, for which many thanks.

2) The reader is referred to Harvey[1981] for an alternative derivation of this solution.

(4) $$\min_{\theta} \; f(\hat{\beta},\theta)' S \; f(\hat{\beta},\theta)$$.

where S is a suitably chosen weights matrix. If we define

(5a) $$F = f_{\theta}(\beta,\theta) \qquad \text{(a r x m matrix)}$$

(5b) $$K = f_{\beta}(\beta,\theta) \qquad \text{(a r x n matrix)}$$

then it can be proven (see Gouriéroux, Montfort & Trognon[1985]) that

(6) $$\sqrt{n}(\theta - \theta_{ALS}) \rightarrow N(0,[F'(K\Omega K')^{-1}F]^{-1})$$

and that the optimal choice for the weights matrix S is

(7) $$S = (K\hat{\Omega}K')^{-1}$$

Of course, the more efficient our estimator of β is, the more efficient our ALS estimator of θ is. If β is estimated by ML, the ALS estimator will be asymptotically equivalent to an ML estimate.

As an illustration, let us consider the case where the autocovariances $\gamma(k)$ are functions of a number of unknown parameters, collected in a vector θ:

(8) $$\gamma(k) = f_k(\theta) \qquad k = 0...r$$

The (r+1)-vector of autocovariances plays the part of β as described above, while the underlying parameters θ are the ones we wish to estimate. Clearly, K = I, and the ALS problem can be formulated as:

(9) $$\min_{\theta} \; [\hat{\gamma} - f(\theta)]'\Omega^{-1}[\hat{\gamma} - f(\theta)]$$

The asymptotic covariance matrix Ω of the estimated autocovariances can be found in Jenkins & Watts[1968] and is easily estimated. (9) can be solved by any numerical optimisation routine.

3. ALS and the State Space model

If all system matrices in (1a)-(1b) are time-invariant - even the measurement matrix Z - then the autocovariances of the data are relatively simple functions of the unknown parameters. This opens the way for an ALS estimation procedure as described in the previous section.

If we assume the vector process α_t is stationary (a necessary and sufficient condition for which is that all eigenvalues of T lie within the unit circle), then y_t is a stationary process. To express the autocovariances of the data in the unknown parameters, we realise that the covariance of α_t is the same as that of α_0 if the process is stationary. The unconditional variance matrix of α_0 (commonly denoted as P_0) satisfies the relation(see Harvey[1981, p.112]):

(10) $$vec(P_0) = (I_{k^2} - T\otimes T)^{-1}.vec(Q)$$

Since

(11) $$E[y_t y_{t-k}'] = E[Z\alpha_t\alpha_{t-k}'Z'] \qquad (k > 0)$$

$$E[y_t y_t'] = E[Z\alpha_t\alpha_t'Z'] + R$$

and

(12) $$\alpha_t = T^k\alpha_{t-k} + \sum_{i=0}^{k-1} T^i\eta_{t-i}$$

we get

(13) $$E[y_t y_{t-k}'] = ZT^kP_oZ' \qquad (k > 0)$$

$$E[y_t y_t'] = ZP_oZ' + R$$

If we denote $E[y_t y_{t-k}']$ by $\Gamma(k)$, we can then write

(14) $$\text{vec}(\Gamma(k)) = (Z\otimes Z)(I\otimes T^k)(I - T\otimes T)^{-1}\text{vec}(Q) \qquad (k > 0)$$

$$\text{vec}(\Gamma(0)) = (Z\otimes Z)(I - T\otimes T)^{-1}\text{vec}(Q) + \text{vec}(R)$$

If desired, these relations can also be written in terms of unique elements in $\text{vec}(\Gamma(k))$, vec(Q) and vec(R) by substituting $\text{vec}(A) = D_n v(A)$, where $v(A)$ contains the unique elements of the symmetric matrix A, and D_n is the so-called duplication matrix (see Magnus & Neudecker[1988, p.48-49]). For scalar measurements (g=1, Z is now a row vector, the matrix R becomes a scalar r), this simplifies slightly to

(15) $$\gamma(k) = (Z\otimes Z)(I\otimes T^k)(I - T\otimes T)^{-1}\text{vec}(Q) \qquad (k > 0)$$

$$\gamma(0) = (Z\otimes Z)(I - T\otimes T)^{-1}\text{vec}(Q) + r$$

where we can write $Z\otimes Z$ as $[\text{vec}(Z'Z)]'$ if we wish.
With (14) and (15) we have an explicit relation between the theoretical autocovariances of the y_t and the system matrices. Since the autocovariances of the data can be estimated easily, consistently and efficiently we can now estimate unknown parameters in Z, T, Q and R by ALS. Note that the derivatives of $\Gamma(k)$ with respect to the unknown parameters can also be calculated straightforwardly from (14), and these derivatives can then be used during the numerical minimalisation of (9).

A particularly simple case occurs if T is known. The theoretical autocovariances are then a simple linear function of the unknown parameters in Q, which we can summarise as

(16) $$c = M^*\text{vec}(Q) + re_1 = [M\ e_1][\varphi'\ r]' = K\theta$$

where e_1 is the first unit vector, φ contains the unique elements in vec(Q) and c is the vector containing all autocovariances. The structure of the matrix $M^* = M^*(Z,T)$ follows from (15), while $M = M^*D_n$. The final reformulation expresses the autocovariances in a matrix $K = K(Z,T)$ and a vector θ of parameters of interest. The ALS estimation problem (9) now becomes:

(17) $$\min_\theta\ [\hat{c} - K\theta]'\Omega^{-1}[\hat{c} - K\theta]$$

and the ALS estimator of θ is clearly

(18) $$\theta_{ALS} = (K'\Omega^{-1}K)^{-1}K'\Omega^{-1}\hat{c}$$

where Ω is the estimated asymptotic covariance matrix of the estimated autocovariances. That a closed form for the ALS estimator is possible when the relation between the parameters of interest and the estimated parameters is linear has been pointed out by Gouriéroux, Montfort & Trognon[1985]. While ALS has been applied to a State Space model from this subclass in

Gehring[1987], a numerical optimisation routine was applied to solve (17) in that paper. From the above, it is obvious this is both unnecessary and time-consuming.

The simple Aitken-type form of the ALS estimator in this class of models makes clear we can also estimate θ under restrictions like $B\theta = b$, to get

$$(19) \qquad \theta_{RALS} = \theta_{ALS} + (K'\Omega^{-1}K)^{-1}B'[B(K'\Omega^{-1}K)^{-1}B']^{-1}[b - B\theta_{ALS}]$$

a formula that will be familiar from GLS under linear restrictions.

(18) and (19) provide us with our first explicit estimators for unknown variance parameters, but only if Z is time-invariant, and if T is known. This is equivalent to stating we have a State Space model for an ARMA process in which all AR parameters are known. Although this may seem like a highly restricted subclass of State Space models, in fact useful models like structural time series models as in Harrison & Stevens[1976] can be written in this form. A considerable disadvantage of the estimators (18) and (19) is the fact that they do not lead to estimated variance matrices which are guaranteed positive definite. Theoretically, this could be remedied by reparametrising $Q = FF'$, but then explicit estimators are no longer feasible and we must resort to numerical approximation. However, we can put our faith in the asymptotic properties of the ALS estimator and hope the "true", positive definite variance matrices resurface in our estimators even in small samples. The sensitivity of the estimator to the number of autocovariances in γ and to the precision with which the matrix Ω is calculated also gives food for thought.

The question remains whether this procedure constitutes an improvement over numerical ML. In ALS we usually have to find the minimum of a function by numerical means, and the fact that said function is considerably simpler to calculate than a likelihood offers only limited solace. In practice, I would unhesitatingly recommend using ALS whenever possible, as long as recursivity is not a factor of importance. For every new observation, a considerable recalculation programme must be undertaken, with new estimates of the $\Gamma(k)$ and their asymptotic moments to be calculated, and a new function to be minimised, before a new estimate of the unknown parameters is found.
In the case where T is known, the ALS estimator can be calculated without any recourse to numerical optimisation, a considerable advantage.

4. A numerical example

We will apply the ALS procedure to the following simple trend model, adapted from Harrison & Stevens[1976] :

$$(20) \qquad d_t = d_{t-1} + b_{t-1} + \epsilon_t$$

$$(21) \qquad b_t = b_{t-1} + \eta_t$$

$$(22) \qquad y_t = d_t + u_t$$

where the three variances $\sigma^2(\epsilon)$, $\sigma^2(\eta)$ and $\sigma^2(u)$ are the unknown parameters of interest. We first transform the model (20)-(22) to a stationary model

$$(23) \qquad w_t = \Delta^2 y_t = \eta_t + \Delta\epsilon_t + \Delta^2 u_t$$

Although we could formulate a State Space model for (23) and construct the ALS estimator from there, this case is so simple we can express the autocovariances of w_t in the unknown parameters without the aid of a State Space model:

$$(24)\qquad \gamma(0) = \sigma^2(\eta) + 2\sigma^2(\epsilon) + 6\sigma^2(u)$$

$$\gamma(1) = -\sigma^2(\epsilon) - 4\sigma^2(u)$$

$$\gamma(2) = \sigma^2(u)$$

$$\gamma(k) = 0 \qquad (k > 2)$$

The autocovariances can be estimated in the usual manner from the w_t, and their asymptotic covariance matrix Ω can be estimated easily as well. We now face two questions :

1. How many covariances should I use for the ALS estimator ? (what is r in (8)?)
2. How many covariances should I use to calculate Ω? (we will denote this as R)

Data were generated by (20)-(22), and the ALS estimator (18) was calculated for different values of r and R. The values chosen for $\sigma^2(\epsilon)$, $\sigma^2(\eta)$ and $\sigma^2(u)$ were 0.1, 0.01 and 1, respectively. The results are given in Table 1.

TABLE 1 : SIMULATION RESULTS

		R = 5	R = 10	R = 15	R = 20
r = 3	$\sigma^2(\epsilon)$	0.355	0.341	0.337	0.320
	$\sigma^2(\eta)$	0.064	0.045	0.034	0.032
	$\sigma^2(u)$	1.032	0.885	0.881	0.791
r = 5	$\sigma^2(\epsilon)$	0.281	0.272	0.255	0.251
	$\sigma^2(\eta)$	0.033	0.030	0.030	0.028
	$\sigma^2(u)$	0.775	0.735	0.729	0.724
r = 10	$\sigma^2(\epsilon)$	0.200	0.167	0.133	0.122
	$\sigma^2(\eta)$	0.022	0.020	0.020	0.018
	$\sigma^2(u)$	0.335	0.300	0.245	0.201
r = 15	$\sigma^2(\epsilon)$	0.102	0.085	0.045	0.029
	$\sigma^2(\eta)$	0.016	0.013	0.008	0.008
	$\sigma^2(u)$	0.265	0.178	0.158	0.115
r = 20	$\sigma^2(\epsilon)$	0.023	0.012	0.004	0.000
	$\sigma^2(\eta)$	0.001	0.000	0.000	0.000
	$\sigma^2(u)$	0.101	0.045	0.040	0.027

For each parameter, the RMS difference between the ALS and the ML estimator over 500 replications is given.
The conclusions to be drawn from Table 1 must be accompanied with the usual disclaimer that such a limited simulation study can give only a first indication of the properties of the ALS estimator in this model. Nevertheless, it seems that for moderate values of r and R, estimators of satisfactory properties - virtually indistinguishable from ML estimators - were found. The computation time needed for the ALS estimator was around 10% of that usually needed for the ML estimator.

While the standard formula (18) could have been used to calculate the estimates above, the special structure of the matrix K allowed the use of a simpler formula. K can be partitioned as

$$K = \begin{bmatrix} B \\ 0 \end{bmatrix} \qquad \text{and, comformably } \Omega = \begin{bmatrix} Q & R \\ R' & S \end{bmatrix} \qquad \hat{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

where B is an invertible matrix. We will assume that Q and S are also invertible. Substituting the above into (18) and rearranging a few inversions leads to

(25) $$\theta_{ALS} = B^{-1}(c_1 - RS^{-1}c_2)$$

and it is this formula we have used to calculate the estimates in Table 1. It has greater numerical stability than (18), and can be used for any MA-model.

5. ALS in a general State Space model

While the results of the previous paragraphs are only applicable in a severely restricted State Space model, ALS can also be applied to the more general case (1a)-(1b). However, for this case we will be forced to choose a different approach, since a time-varying Z_t means y_t is no longer a stationary process, and autocovariances are thus of no use to us.
We will rewrite (1a)-(1b) in the following form, continuing to assume the process is stationary:

(25a) $$y_t = Z_t.\alpha_t + \epsilon_t \qquad \epsilon_t \sim N(0,R)$$

(25b) $$\alpha_t \sim N(0,P_o)$$

(25c) $$E[\alpha_t\alpha'_{t-k}] = T^kP_o$$

(25d) $$vec(P_o) = (I - T\otimes T)^{-1}.vec(Q)$$

This version of the State Space model - in which the scale factor σ^2 has been absorbed into the variance matrices for simplicity - is exactly equivalent to the standard form (1a)-(1b), as can be seen easily.
We now define

$$y = [y_1' \mid y_2' \mid .... \mid y_n']' \qquad \text{a s x 1 vector}$$

$$\alpha = [\alpha_1' \mid \alpha_2' \mid .... \mid \alpha_n']' \qquad \text{a nk x 1 vector}$$

$$\epsilon = [\epsilon_1' \mid \epsilon_2' \mid .... \mid \epsilon_n']' \qquad \text{a s x 1 vector}$$

$$Z = diag(Z_1, Z_2, ..., Z_n) \qquad \text{a s x nk matrix}$$

(n is the number of observations, s = gn) so that

(26a) $$y = Z\alpha + \epsilon$$

(26b) $$\alpha \sim N(0,P)$$

where P is a symmetric (nk x nk)-matrix with as (i,j)-th block $T^{i-j}P_o$ $(i > j)$. From (26a)-(26b) we find

(27) $$y \sim N(0, ZPZ' + I\otimes R)$$

Note that the variance matrix of y is a linear function of the parameters of interest (Q and R). We will thus base our ALS procedure on an estimate of the variance matrix of y, or rather, a vector containing the unique elements in that matrix.

We define

$$\beta = \text{the unique elements in } vec(E[yy']) = D_s^+ vec(E[yy'])$$

With only one observation on y available, the ML estimate of β is clearly $D_s^+ vec(yy')$. If we represent the variance of y in (27) by V, from Magnus & Neudecker (p.253, exc. 2) we get

$$E[D_s^+ vec(yy')] = D_s^+ vec(V)$$

$$var[D_s^+ vec(yy')] = D_s^+(I + K_s)(V \otimes V)(D_s^+)' = D_s^+(V \otimes V)(D_s^+)'$$

where K is the so-called Commutation matrix, again see Magnus & Neudecker. We thus have an unbiased estimator of β, an a consistent estimate of that estimator's variance matrix is also available : we can estimate V with yy' consistently, and hence $V \otimes V$ consistently with $(yy') \otimes (yy')$.

Which leaves the question of the relation between our vector of estimable parameters β and our parameters of interest, the unique elements in Q and R.
From (27) it is clear that

(28) $$\beta = D_s^+ E[vec(yy')] = D_s^+ vec(V) = D_s^+ vec(ZPZ' + I_n \otimes R)$$

To make the relation between $E[vec(yy')]$ and Q more specific, we will write P as

(29) $$P = B(I_n \otimes P_o) + (I_n \otimes P_o)B'$$

where B is a block-lower-triangular matrix whose (i,j)-th block is T^{i-j} (i > j), and whose diagonal blocks are $\frac{1}{2}I$. We can then write

(30) $$\beta = D_s^+ vec(V) = D_s^+\{(Z \otimes Z)(I_{nk} \otimes B + B \otimes I_{nk}) vec(I_n \otimes P_o) + vec(I_n \otimes R)\}$$

Since

(31) $$vec(I_n \otimes P_o) = (I_n \otimes K_{kn} \otimes I_k)\{vec(I_n) \otimes vec(P_o)\} = (I_n \otimes K_{kn} \otimes I_k)(vec(I_n) \otimes I_{k^2}) vec(P_o) =$$
$$(I_n \otimes K_{kn} \otimes I_k)(vec(I_n) \otimes I_{k^2})(I_{k^2} - T \otimes T)^{-1} vec(Q)$$

and

(32) $$vec(I_n \otimes R) = (I_n \otimes K_{gn} \otimes I_g)\{vec(I_n) \otimes vec(R)\} = (I_n \otimes K_{gn} \otimes I_g)(vec(I_n) \otimes I_{g^2}) vec(R)$$

we see that β is a linear function of the unique elements in Q and R. For simplicity's sake, let us stack these unique elements in a vector θ, and let

(33) $$\beta = K\theta$$

The ALS estimator of θ is once again of the form

(34) $$\theta_{ALS} = (K'\Omega^{-1}K)^{-1}K'\Omega^{-1}\hat{\beta}$$

where $\Omega = D_s^+(V \otimes V)(D_s^+)'$. To be sure, this estimator is not easily calculated, as the matrices involved in its calculation are of huge dimensions.

As an example let us examine a model in which the observations y_t are scalars, i.e. g = 1. The matrix R again becomes a scalar r, while the measurement matrices Z_t become row vectors. The vector y now contains n scalars, as does the vector ϵ. The number of unique elements in β is n(n+1)/2, while the number of unique elements in Q (including r) is $(k^2+k+2)/2$. The matrix K is thus $n(n+1)/2 \times (k^2+k+2)/2$. The matrix Ω (after removal of duplicated elements) is of dimensions n(n+1)/2 x n(n+1)/2. So we see the calculation of the ALS estimator involves the inversion of a [n(n+1)/2 x n(n+1)/2]-matrix, followed by the inversion of a $[(k^2+k+2)/2 \times (k^2+k+2)/2]$-matrix : no trivial calculation! For an ordinary trend model with 50 observations as used in the preceding paragraph, the first matrix involved is of dimensions 1275 x 1275... However, the first inversion can be reduced to more manageable dimensions, as

$$(35) \qquad \Omega^{-1} = \{D_s^+(V \otimes V)(D_s^+)'\}^{-1} = D_s'(V^{-1} \otimes V^{-1})D_s$$

which still leaves a 50 x 50 matrix to be inverted. One way to avoid this altogether is by neglecting the weight matrix Ω in (34) which leads to unbiased, but inefficient estimators of θ.

A more serious problem is that our estimate of V is noninvertible. Again, the simplest solution to this is to use a suboptimal estimate, while another possibility is the use of the Moore-Penrose inverse. In both cases, estimators with uncertain properties arise, so for the moment we must question the usefulness of the ALS estimator in a general State Space model.

6. Conclusions

We have seen that a simple ALS estimator for unknown variance parameters in a restricted State Space model can be derived, and that its small sample properties appear to be satisfactory in a simple example. In the more general State Space model, an ALS estimator can be derived, but its calculation involves the inversion of a matrix of formidable dimensions. For the moment, that estimator appears to be impractical.

If we confine our attention to the restricted subclass of State Space models used in paragraph 3, the ALS estimator appears to offer a simple and attractive alternative to tedious numerical optimisation of the likelihood. Final judgment on its suitability can only be passed after extensive study of its small sample properties.

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