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Rejoinder to Molenaar and Oud.

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0. Voorwoord.

Ongeveer anderhalf jaar geleden boden wij een manuscript aan ter publicatie in Kwantitatieve Methoden getiteld "A note on the calculation of latent trajectories in the quasi Markov simplex model by means of the regression method and the discrete Kalman filter". In dit manuscript wordt aangetoond dat de regressieschatter voor factorscores in een longitudinaal model beter is (in termen van mean square error) dan het recursieve Kalman filter. Enige tijd daarna ontvingen we het bericht van de redactie van Kwantitatieve Methoden, vergezeld van het betreffende referee rapport, dat werd afgezien van publicatie van het manuscript. Het opmerkelijke daarbij was, dat het referee rapport was gebaseerd op een stellingname die lijnrecht leek in te gaan tegen de belangrijkste conclusie van ons manuscript. Hoewel het volstrekt tegen onze gewoonte is om enige discussie aan te gaan omtrent de gronden waarop een ter publicatie aangeboden manuscript wordt geweigerd, was hier naar onze mening sprake van een bijzondere situatie. Immers, hier was sprake van een zakelijk verschil van inzicht omtrent de eigenschappen van het Kalman filter in relatie tot de regressieschatter voor factorscores in een longitudinaal factormodel. Aangezien dit verschil van inzicht objectief beslisbaar is, hebben we ons standpunt samengevat in een stelling en ons, zonder het redactionele besluit inzake de manuscripten ter discussie te stellen, gericht tot de redactie van Kwantitatieve Methoden met het verzoek deze stelling te mogen verdedigen tegenover een wetenschappelijk forum. We stellen het zeer op prijs dat ons nu deze gelegenheid wordt geboden.

Hieronder zal eerst de stelling worden herhaald waarop de discussie zich toespitst. De stelling waarin we onze positie hebben samengevat luidt:

> (S) "De regressieschatter voor factor scores in longitudinale factormodellen (welke schatter deel uitmaakt van de standaard LISREL output) is beter dan het Kalman filter (al dan niet in combinatie met de Bartlett schatter op t=1). De recursieve versie van de regressie schatter is niet het Kalman filter (al dan niet in combinatie mat de Bartlett schatter op t=1), maar de discrete fixed-interval smoother".

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Hoewel onze stelling geldt voor longitudinale factor modellen in het algemeen, zijn we in eerste instantie uitgaan van de meest eenvoudige variant: het quasi Markov simplex model. Dit maakte het mogelijk om, voor een gering aantal tijdstippen (twee), de exacte expressies voor het Kalman filter en de fixed-interval smoother te traceren.

Na deze situatie schets, gaan we nu over tot ons feitelijke antwoord op het commentaar van dr. Molenaar en dr. Oud.

1. Introduction.

Our paper concerning the estimation of latent trajectories in the quasi Markov simplex model contains two results. In the first place we find that the regression method yields factor scores which are characterized by a smaller mean square error variance than those obtained by means of the Kalman filter (KF). In the second place we note the equivalence of the Fixed Interval Smoother (FIS) and the regression method. These conclusion are based on the situation in which the longitudinal data have been recorded, that is to say off-line estimation (to use our term) or statical estimation (to use Molenaar and Oud's).

Molenaar and Oud offer a number of observations and comments concerning our findings which we will now discuss. In the interest of brevity, we adopt the definitions and notation used in our paper without repeating them here.

2. Consensus.

Let us first establish that Molenaar and Oud do not disagree with our findings. Firstly, they state that the FIS and the regression method yield identical results (section 2), echoing our statement that these methods use the same amount of information and an identical criterion (i.e. minimum error variance). Secondly, they agree that in the situation mentioned (off-line estimation), the KF yields estimates are characterized by a greater error variance than those obtained from the regression method. They write in section 2: 'Because the Kalman smoother (...) is based on more information (...) than the Kalman filter (...) it is quite clear that the smoothed estimate is more reliable than the filtered one, except for t_i = T'. This last estimate is identical whether it is obtained from the FIS (c.q. regression method) or from the KF. This finding is to be expected as explained in our paper and is evident in our simulation and in our appendix.

3. Preferences motivated by computational considerations.

This agreement notwithstanding Molenaar and Oud express certain preferences regarding the methods on calculating latent scores. In section 2, they state that the smoother should be preferred to the regression method because of its "efficiency". We take this to mean computational efficiency relating to computer memory requirements. We have no argument on this score. We are agreed that the regression method and the FIS yield identical results, so which one is used may quite rightly boil down to a matter of (computational) convenience. With regard to convenience, it is a lot easier in our experience to obtain the regression method matrix, a standard feature of LISREL output, than to write a computer program to carry out fixed interval smoothing.

In section 2, furthermore, a similar preference is expressed for short series, where the calculation of the regression matrix would presumably not pose any (computer memory) problem. This preference is supported by the fact that the error covariance matrices at each occasion can be calculated independent of the actual data. Finally the importance of dynamical estimation is stressed in favour of the KF.

It is clear from our results that the dynamical estimation using the KF yields an estimate of the factor score at the last measuremnet occasion that is identical to that obtained from the regression estimate. The last measurement (at T=10) in our simulation can be regarded as a dynamical estimate as there are no observations following it in time (see Molenaar and Oud's definition of dynamical estimation). Our simulation shows the equivalence of the KF estimate, the FIS estimate and the regression method estimate and we note that this equivalence is to be expected. On this ground clearly there is no reason to prefer any one of these methods, except again on the basis of computational convenience.

Secondly, it is obvious from Eq. 8.9 (reproduced in our paper as Eq. 5) in Lawley and Maxwell (page 109, 1971) that the error covariance matrix of the regression method estimates can be calculated prior to the actual estimation of factor scores. This then is a feature that the regression method shares with the KF and the FIS.

4. Bartlett initialisation.

An important theme in Molenaar and Oud concerns the initialisation of the KF (c.q. FIS) (see also Oud, van den Bercken, and Essers, 1990). This theme relates to the biasedness of the estimated factor scores.

Before continuing, we emphasize that we adopt the Lawley and Maxwell definition of conditional biasedness. That is we call an estimate, $\underline{\eta}$, conditionally biased if $E[\underline{\eta} \mid \eta] \neq \eta$, or to quote Lawley and Maxwell (1971, page 108): "(...) if we average $\underline{\eta}$ over all individuals whose true factor scores are given by η, the results differ from η".[1] As we touched on the subject of conditional bias only briefly in our paper by stating the regression method and the KF yield conditionally biased estimates, we will now consider this matter in more detail. The KF estimate of $\eta(t+1)$ is given by:

[1] Lawley and Maxwell use the symbol **f** and $\hat{\mathbf{f}}$ to denote a factor score and its estimate. To maintain a consistent notation we have changed this to η and $\underline{\eta}$.

(I) $\underline{\eta}(t+1 \mid t+1) = \underline{\eta}(t+1 \mid t) - \mathbf{K}_{t+1}\,[\Lambda(t+1)\underline{\eta}(t+1 \mid t) - \mathbf{y}(t+1)]$

To arrive at the expression for $E[\underline{\eta}(t+1 \mid t+1) \mid \eta(t+1 \mid t+1)]$, we require the conditional expectations of $\underline{\eta}(t+1 \mid t)$ and $\mathbf{y}(t+1)$ given $\eta(t+1 \mid t+1)$. We have

(II) $E[\underline{\eta}(t+1 \mid t) \mid \eta(t+1 \mid t+1)] = E[\underline{\eta}(t+1 \mid t)] + \Xi_{t+1}\,\{\eta(t+1 \mid t+1) - E[\eta(t+1 \mid t+1)]\}$

where the matrix Ξ_{t+1} contains slope parameters of the regression of $\underline{\eta}(t+1 \mid t)$ on $\eta(t+1 \mid t+1)$ (Anderson, 1958). As in our paper, we take $E[\eta(t)] = 0.0$ (t=1,2,...) so that this expression can be written:

(III) $E[\underline{\eta}(t+1 \mid t) \mid \eta(t+1 \mid t+1)] = \Xi_{t+1}\,\eta(t+1 \mid t+1)$

Furthermore,

(IV) $E[\mathbf{y}(t+1) \mid \eta(t+1 \mid t+1)] = \Lambda(t+1)\eta(t+1 \mid t+1)$,

as the measurement error of the observations $\varepsilon(t+1)$ (see Eq. 7) and the latent variables $\eta(t+1)$ are uncorrelated. Substituting these into Eq. I:

(V) $E[\underline{\eta}(t+1 \mid t+1) \mid \eta(t+1 \mid t+1)] =$
$\Xi_{t+1}\eta(t+1 \mid t+1) + \mathbf{K}_{t+1}\Lambda(t+1)\Xi_{t+1}\eta(t+1 \mid t+1) - \mathbf{K}_{t+1}\Lambda(t+1)\eta(t+1 \mid t+1)$

and rearranging we have:

(VI) $E[\underline{\eta}(t+1 \mid t+1) \mid \eta(t+1 \mid t+1)] = \Xi_{t+1}\eta(t+1 \mid t+1) +$
$\mathbf{K}_{t+1}\Lambda(t+1)[\Xi_{t+1}\eta(t+1 \mid t+1) - \eta(t+1 \mid t+1)]$.

We now ask when the following holds:

(VII) $\eta(t+1 \mid t+1) =$
$\Xi_{t+1}\eta(t+1 \mid t+1) + \mathbf{K}_{t+1}\Lambda(t+1)[\Xi_{t+1}\eta(t+1 \mid t+1) - \eta(t+1 \mid t+1)]$

or

(VIII) $\eta(t+1 \mid t+1) - \Xi_{t+1}\eta(t+1 \mid t+1) =$
$\mathbf{K}_{t+1}\Lambda(t+1)[\Xi_{t+1}\eta(t+1 \mid t+1) - \eta(t+1 \mid t+1)]$.

This is true when either $\Xi_{t+1} = \mathbf{I}$, or when $-\mathbf{K}_{t+1}\Lambda(t+1) = \mathbf{I}$. A perusal of Lawley and Maxwell (1971) and Molenaar and Oud's appendix reveals that the latter condition holds for t=1 when the KF is initialized by means of the Bartlett method. The estimate so obtained is therefore conditionally unbiased. For our initialisation this does not hold so that estimates at t=1 (and subsequent occasions) are minimum variance, but conditionally biased. For Ξ_{t+1} we have (e.g. Anderson, 1958):

(IX) $\Xi_{t+1} = B_{t+1,t}E[\eta(t)\eta(t)']B'_{t+1,t}\,\{B_{t+1,t}E[\eta(t)\eta(t)']B'_{t+1,t} + \Psi(t)\}^{-1}$

so that $\Xi_{t+1} = \mathbf{I}$ when $\Psi(t) = 0$, i.e. $\zeta(t) = 0$. In practice, $\Psi(t) = 0$ is highly restrictive and does not warrant serious consideration as a source of conditional unbiasedness.

The value of the Bartlett initialisation now depends on whether the conditional unbiasedness is retained at subsequent occasions (t=2,3,..). This will now be investigated. We obtain the Bartlett estimate of $\eta(1\,|\,1)$ and the associated error covariance matrix $\mathbf{V}(1)$ from Molenaar and Oud's appendix and derive the subsequent KF estimate of $\eta(2\,|\,2)$. The Kalman gain is (see Eq. 9):

(X) $\mathbf{K}_2 = \mathbf{V}(2\,|\,1)\,\Lambda'(2)[\Lambda(2)\,\mathbf{V}(2\,|\,1)\Lambda'(2) + \Theta(2)]^{-1}$

where (see Eq. 10)

(XI) $\mathbf{V}(2\,|\,1) = B_{2,1}[\Lambda'(1)\,\Theta(1)^{-1}\Lambda(1)]^{-1}B'_{2,1} + \Psi(1).$

In view of Eq. VIII, we require that $-\mathbf{K}_2\Lambda(2) = \mathbf{I}$ if the estimate of $\eta(2\,|\,2)$ is to be conditionally unbiased. Now from Eqs. X and XI it can be seen that $-\mathbf{K}_2\Lambda(2)$ approaches $\mathbf{I}$ when $\mathbf{V}(2\,|\,1)$ becomes large relative to $\Theta(2)$, or when $\Theta(2)$ approaches zero. Assuming that $\Theta(2)$ does not approach zero and that $\mathbf{V}(2\,|\,1)$ is not very large relative to $\Theta(2)$[2], the unbiasedness of the estimates at t=1 is lost at t=2 and, as t increases, the biasedness duely reaches the level of biasedness incurred by our initialisation[3]. The speed with which this happens is a nice problem to consider.

5. Illustration.

To illustrate, we simulate a trajectory consisting of 15 repeated measures according to the quasi Markov simplex model. Using the true parameter values given in our paper, we obtain estimates of the latent trajectory by means of the Kalman filter. Both initialisations are

[2] These assumptions boil down to the proposition that the reliability of the observations does not approach unity. If it did there would be no estimation problem at all, as $\eta(t) \approx \Lambda'(t)\,\mathbf{y}(t)$.

[3] Please note that Eqs. I to XI are general. That is to say they are not in any way specific to the quasi Markov simplex, although this model does constitute a special case.

used and, as can be seen in Table 1, the estimates obtained from the KF under each initialisation are indistinguishable after t=6.

Table 1: Kalman Filter estimates and standard errors under the standard and the Bartlett initialisations

t	KF estimates standard initialisation	KF estimates Bartlett initialisation	st.errors standard initialisation	st.errors Bartlett initialisation
1	-0.910	-1.365	5.774	7.069
2	-3.703	-4.028	5.270	5.430
3	1.103	1.021	5.210	5.229
4	-0.483	-0.513	5.203	5.205
5	-0.192	-0.193	5.202	5.202
6	-1.878	-1.881	5.202	5.202
7	-1.227	-1.227	5.202	5.202
8	-3.406	-3.406	5.202	5.202
9	-0.128	-0.128	5.202	5.202
10	1.145	1.145	5.202	5.202
11	-0.979	-0.979	5.202	5.202
12	-2.328	-2.328	5.202	5.202
13	-5.395	-5.395	5.202	5.202
14	-0.151	-0.151	5.202	5.202
15	-1.505	-1.505	5.202	5.202

Table 1, furthermore, contains the standard error of these estimate (i.e. the square root of the a-posteriori error variance - see Eq. 11). Here again we see a convergence of the standard errors using the Bartlett initialisation to those obtained from the standard initialisation. Although, in this particular illustration, the estimates are identical after t=6, it is stressed that the conditional unbiasedness which the Bartlett initialisations guarantees at t=1, is lost immediately at t=2.

6. Conclusions.

#1) There is one and only one reason to prefer the FIS to the regression method in the case of statical estimation and to prefer the KF to the FIS or the regression method in the case of dynamic estimation: computational convenience or, to use Molenaar and Oud's term, efficiency. As the length of the time series increases, this may become an increasingly important consideration.

#2) If one desires conditionally unbiased minimum variance estimates in the case of statical estimation, the Bartlett method can be used. If one desires conditionally unbiased minimum variance estimates in the case of dynamical estimation, the KF is not suitable (see conclusion #3).

#3) The Bartlett initialisation is suggested by Molenaar and Oud because they believe that this ensures conditional unbiasedness of the KF and the FIS estimates. The conclusions of Molenaar and Oud based on this belief are invalid because the conditional unbiasedness which is obtained at t=1 is, under general circumstances, immediately lost at t=2.

6. References.

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