FernUniversität in Hagen

SEM modeling with singular moment matrices

Part II: ML-Estimation of sampled stochastic differential equations

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Diskussionsbeitrag Nr. 442
August 2009

Diskussionsbeiträge der Fakultät für Wirtschaftswissenschaft
der FernUniversität in Hagen

Herausgegeben vom Dekan der Fakultät

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Abstract

Linear stochastic differential equations (SDE) are expressed as an exact discrete model (EDM) and estimated with structural equation models (SEM) and the Kalman filter (KF) algorithm. The SEM likelihood is well defined even for the times series case and the SEM and KF approach yield the same likelihood. The oversampling approach is introduced in order to formulate the EDM on a time grid which is finer than the sampling intervals. This leads to a simple computation of the nonlinear parameter functionals of the EDM. For small discretization intervals, the functionals can be linearized and software permitting only linear parameter restrictions can be used. However, in this case the SEM approach must handle large matrices leading to degraded performance and possible numerical problems. The methods are compared using coupled linear random oscillators with time varying parameters and irregular sampling times.

Key Words: Structural Equation Models (SEM); Kalman filtering (KF); Stochastic differential equations (SDE); Maximum Likelihood (ML) estimation; Nonlinear parameter restrictions; Oversampling; Coupled stochastic oscillators

1 Introduction

In a companion paper (I, Singer; 2009) it was shown that the structural equation model (SEM) representation of a discrete time state space model yields

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correct ML estimates even for one panel unit ($N = 1$), when the joint Gaussian distribution of the observations is used as likelihood function.
In this paper, the representation of sampled continuous time stochastic processes in terms of the exact discrete model (EDM; Bergstrom; 1976b, 1988) is discussed. This vector autoregression (VAR) involves nonlinear matrix restrictions for the parameter matrices, which must be handled by the software. A Kalman filter approach was given by Singer (1991, 1993, 1995, 1998). Nonlinear (w.r.t. the parameters) SEM software can implement such restrictions also (Oud and Jansen; 2000), but it may be worthwhile to find a representation which can be used in linear SEM and time series programs.
I propose the device of *oversampling* in order to linearize the EDM at a latent discretization level which is smaller than the sampling interval (Singer; 1995). The price to be payed is a larger dimension of the latent state, but now the parameter matrices are approximately linear with arbitrarily small error and the parameter functionals w.r.t. the exogenous variables are computed automatically by the SEM equations. The enlargement of the latent state dimension is unproblematic for the recursive Kalman approach, however (Singer; 1995).
Furthermore, oversampling yields a simple treatment of irregular sampling, since only the parameter matrices of the latent VAR recursion are involved. Time dependent parameters and arbitrary interpolation schemes of the exogenous variables are easily implemented in this approach.
This will be detailed in the further sections. Section 2 gives the definition of a SEM model including deterministic intercept terms and states the Gaussian likelihood function. In section 3 the SEM representation is applied to sampled stochastic differential equations (SDE). Using oversampling, linearized parameters with small errors are obtained, but the nonlinear restrictions are preserved. in section 4, the method is applied to coupled stochastic oscillators. In two appendices, oversampling and computational aspects are discussed.

2 SEM modeling

In the following the SEM model

$$\eta_n = B\eta_n + \Gamma x_n + \zeta_n \quad (1)$$
$$y_n = \Lambda\eta_n + \tau x_n + \epsilon_n \quad (2)$$

$n = 1, \ldots, N$, will be considered. The structural matrices have dimensions $B : P \times P,\ \Gamma : P \times Q,\ \Lambda : K \times P,\ \tau : K \times Q$ and $\zeta_n \sim N(0, \Sigma_\zeta)$, $\epsilon_n \sim N(0, \Sigma_\epsilon)$ are independent normally distributed error terms ($\Sigma_\zeta : P \times P,\ \Sigma_\epsilon : K \times K$).
In the structural and the measurement model, the variables x_n are *deterministic* control variables. They can be used to model intercepts and for dummy coding. Stochastic exogenous variables ξ_n are included by extending the latent

variables η_n. Since the error vectors are normally distributed, the indicators (2) are distributed as $N(\mu_{yn}, \Sigma_y)$, where

$$\begin{aligned} \eta_n &= B_1(\Gamma x_n + \zeta_n) && (3)\\ E[\eta_n] &= B_1\Gamma x_n && (4)\\ \mathrm{Var}(\eta_n) &= B_1\Sigma_\zeta B_1' && (5) \end{aligned}$$

$$\begin{aligned} E[y_n] &= \mu_{yn} = \Lambda E[\eta_n] + \tau x_n = [\Lambda B_1\Gamma + \tau]x_n := Cx_n && (6)\\ \mathrm{Var}[y_n] &= \Sigma_y = \Lambda\mathrm{Var}(\eta_n)\Lambda' + \Sigma_\epsilon = \Lambda B_1\Sigma_\zeta B_1'\Lambda' + \Sigma_\epsilon. && (7) \end{aligned}$$

In the equations above, it is assumed that $B_1 := (I - B)^{-1}$ exists.
Thus, the log likelihood function for the N observations $\{y_n, x_n\}$ is

$$l = -\tfrac{N}{2}\left(\log|\Sigma_y| + \mathrm{tr}[\Sigma_y^{-1}\ \ \tfrac{1}{N}\sum_n (y_n - \mu_{yn})(y_n - \mu_{yn})']\right). \quad (8)$$

In order to implement arbitrary restrictions on the structural matrices, it is assumed that they depend on an u dimensional parameter vector ψ, e.g. $\Sigma_\zeta = \Sigma_\zeta(\psi)$ etc. For example, the matrix exponential function in the definition of the exact discrete model (section 3) must be specified.
The likelihood function (8) is well defined for $N = 1$, since no log determinants of the moment matrices are involved, as is suggested by the ML fitting function of LISREL (cf. LISREL 8 reference guide, p. 21, eqns. 1.14, 1.15, p. 298, eqn. 10.8). The covariance matrix of the indicators, Σ_y (eqn. 7), must be nonsingular, however.[1] For a more detailed discussion of the likelihood function, see I.

3 Stochastic differential equations and continuous-discrete state space models

3.1 Stochastic differential equations

The stochastic differential equation (SDE)

$$dy(t) = A(t)y(t)dt + b(t)dt + G(t)dW(t); t \in [t_0, t] \quad (9)$$

is a linear dynamical model for the time evolution of the continuous time state vector $y(t) : p \times 1$. The matrix $A(t) : p \times p$ is called the drift, $b(t)$ is an inhomogenous term and $G(t) : p \times r$ is the strength of the process error $dW(t) : r \times 1$ where $W(t)$ is the r-dimensional Wiener process (Arnold; 1974). Formally one can divide by dt to obtain the white noise proecess $\zeta(t) = dW(t)/dt$, but $W(t)$ (a continuous time random walk) is not differentiable.

[1] Otherwise the singular normal distribution can be used (Mardia et al.; 1979, p. 41).

Models of this kind have a long tradition of applications in many fields, such as physics, mathematics, engineering, econometrics, finance, sociology, psychology etc.[2]
In applications, the inhomogeneous term $b(t)$ is usually parameterized as

$$b(t) \;=\; B(t)x(t);\; B(t) : p \times q$$

where $x(t)$ are deterministic control variables. In the panel case, one writes $b_n(t) = B(t)x_n(t)$. The parameter matrices are assumed to depend on a parameter vector ψ, which is supressed in most formulas.
The solution of (9) with initial value $y(t_0)$ is given by

$$y(t) \;=\; \Phi(t, t_0)[y(t) + \int_{t_0}^{t} \Phi(s, t_0)^{-1}[b(s)ds + G(s)dW(s)], \qquad (10)$$

(Arnold; 1974, ch. 8) where $\Phi(t, t_0)$ is the fundamental matrix of the system solving the deterministic matrix differential equation

$$\dot{\Phi}(t, t_0) \;=\; A(t)\Phi(t, t_0); \Phi(t_0, t_0) = I. \qquad (11)$$

It can be solved by a time ordered matrix exponential or as (time ordered) infinite product

$$\Phi(t, t_0) \;=\; \overleftarrow{T} \exp[\int_{t_0}^{t} A(s)ds] \qquad (12)$$

$$\;=\; \overleftarrow{T} \lim_{J\to\infty} \prod_{j=0}^{J-1} [I + A(\tau_j)\delta t], \qquad (13)$$

$\tau_j = t_0 + j\delta t; \delta t = (t - t_0)/J$, where $\overleftarrow{T}\,[A(t)A(s)] = A(s)A(t); t < s$ is the Wick time ordering operator (cf. Abrikosov et al.; 1963). The time ordering is essential, since the matrices $A(t)$ do not commute in general, i.e. $A(t)A(s) \neq A(s)A(t)$.

3.2 Exact discrete model (EDM)

The solution of the SDE (10) is the basis of the *exact discrete model* (EDM) introduced by (Bergstrom; 1976a, 1988), valid at the time points of measurement

[2] cf. e.g., Langevin (1908); Uhlenbeck and Ornstein (1954); Bartlett (1946, 1955, 1978); Itô (1951); Stratonovich (1960); Kalman and Bucy (1961); Schweppe (1965); Nelson (1967); Bergstrom (1976a); Coleman (1968); Jazwinski (1970); Black and Scholes (1973); Jennrich and Bright (1976); Phillips (1976); Doreian and Hummon (1976, 1979); Jones (1984); Möbus and Nagl (1983); Arminger (1986); Singer (1986, 1990, 1992b, 1998); Zadrozny (1988); Hamerle et al. (1991, 1993); Oud and Jansen (2000); Oud and Singer (2008a,b).

$\{t_0, t_1, \ldots, t_T\}$,

$$\begin{aligned} y(t_{i+1}) &= \Phi(t_{i+1}, t_i)y(t_i) \\ &+ \int_{t_i}^{t_{i+1}} \Phi(t_{i+1}, s)b(s)ds \\ &+ \int_{t_i}^{t_{i+1}} \Phi(t_{i+1}, s)G(s)dW(s), \end{aligned}$$

which is abbreviated as the VAR(1) system

$$y_{i+1} = A_i^* y_i + b_i^* + u_i;\ i = 0, \ldots, T-1. \tag{14}$$

The EDM is a Gaussian vector autoregression, but with nonlinear parameter restrictions involving the structural matrix $A(t)$ and the sampling intervals t_i. It is of the same form as the discrete time dynamical system (I, eq. 9-10).
An important special case is the system with constant coefficients $A(t) = A, b(t) = Bx(t), G(t) = G; \Omega = GG'$. In this case the parameter functionals are given explicitly as

$$\Phi(t_{i+1}, t_i) = A_i^* = \exp[A(t_{i+1} - t_i)] := \exp(A\Delta t_i) \tag{15}$$

$$b_i^* = \int_{t_i}^{t_{i+1}} \exp[A(t_{i+1} - s)]Bx(s)ds \tag{16}$$

$$\begin{aligned} \Omega_i^* &:= \mathrm{Var}(u_i) \\ &= \int_{t_i}^{t_{i+1}} \exp[A(t_{i+1} - s)]\Omega \exp[A'(t_{i+1} - s)]ds \end{aligned} \tag{17}$$

$$\mathrm{row}(\Omega_i^*) = [A \otimes I + I \otimes A]^{-1}[A_i^* \otimes A_i^* - I]\ \mathrm{row}(\Omega) \tag{18}$$

where row is the row-wise vector operator and $\otimes$ is the Kronecker product (McDonald and Swaminathan; 1973).
The estimation of the EDM (14) requires the implementation of the correct parameter restrictions, most importantly the matrix exponential function

$$\exp(A\Delta t_i) = \sum_{l=0}^{\infty} (A\Delta t_i)^l / l! \tag{19}$$

$$= \prod_{j=0}^{J_i - 1} \exp(A\Delta t_i / J_i) \tag{20}$$

$$= \lim_{J_i \to \infty} \prod_{J_i=0}^{J_i - 1} [I + A \cdot (\Delta t_i / J_i)]. \tag{21}$$

It contains the parameters $a_{mn}; m, n = 1, \ldots, p$ in a complicated nonlinear manner and is dependent on the sampling intervals Δt_i. Thus, even for constant dynamics A, the measurements depend on the sampling scheme. The product representation (21) shows, that the nonlinear transition matrix may be viewed as

the product of linear (in A) transition matrices $I + A \cdot (\Delta t_i / J_i) = I + A\, \delta t$ defined on smaller discretization intervals $\delta t = \Delta t_i / J_i$ (Singer; 1995, 1998). This introduction of a smaller discretization interval is called *oversampling*. It may be achieved by the definition of additional latent variables $y(t)$, where t is between the measurement times $\{t_0, t_1, \ldots, t_T\}$.
Summarizing the discussion,

- the crucial point is the computation of the parameter functionals (15–17). This point relates to any approach, either Kalman filter or SEM representations. In LSDE (Singer; 1990, 1991), the matrix exponential and its derivative was computed using the spectral decomposition of A (cf. also Jennrich and Bright; 1976; Jones; 1993; Najfeld and Havel; 1995; Moler and VanLoan; 2003).

- The influence of the exogenous variables $b(s) = Bx(s)$ is present during the whole sampling interval $[t_i, t_{i+1}]$ (see 16). Since the data $x(s)$ are usually only available at some time points t_i, approximations of $x(s)$ must be used, such as step functions, polygons or other interpolation schemes (cf. Phillips (1976); Singer (1995)). Alternatively, one can use stochastic variables (by extending the state vector) which are automatically interpolated by computing the smoothed states $E[x(t)|z_T, \ldots, z_0]$. For example, using the trivial dynamics $dx = GdW$, polygonal lines are obtained.

- The integral (16) must be solved explicitly to implement the restrictions. In the oversampling approach, these computations are done implicitly by the system equations.

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3.3 State space modelling

Usually the states $y(t_i)$ are not directly observable, therefore a measurement model

$$z_i = H(t_i)y(t_i) + d(t_i) + \epsilon_i; i = 0, \ldots, T,$$

$\mathrm{Var}(\epsilon_i) = R_i$ has to be added to the dynamic system model. Together with (9) one speaks of the *continuous-discrete state space model*

$$dy(t) = A(t)y(t)dt + b(t)dt + G(t)dW(t); t \in [t_0, t_T] \quad (22)$$

$$z_i = H_i y_i + D_i x_i + \epsilon_i, i = 0, \ldots, T. \quad (23)$$

As in the dynamical model, exogeneous variables $x(t) : q \times 1$ are used to specify the intercept terms $d(t) = D(t)x(t)$. In the panel case, one writes $d_n(t_i) = D_i x_{ni}$. All matrices depend on an u-dimensional parameter vector ψ and, if necessary, on lagged measurements $Z^{i-1} = \{z_{i-1}, \ldots, z_0\}$.

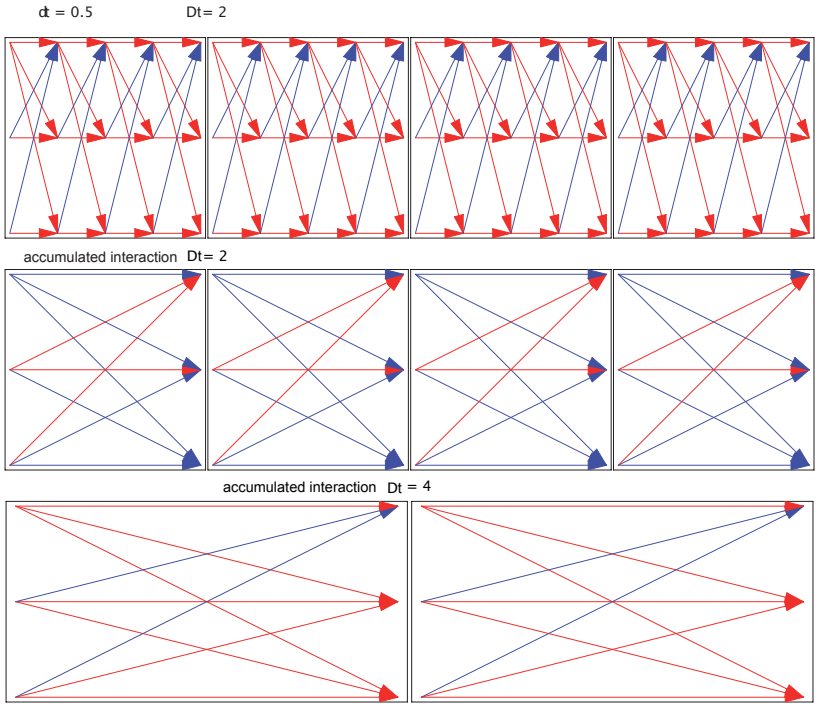

Figure 1: Oversampling of measurement intervals $\Delta t = 2$ and $\Delta t = 4$ with discretization interval $\delta t = 0.5$. The discrete time parameters $A^*(\Delta t) = \exp(A\Delta t)$ have different signs (red $= +$, blue $= -$) although the continuous time drift A is constant.

3.3.1 Oversampling

The dynamical EDM (14) is usually formulated for the measurement times t_i. Then, the computation of the parameter functionals in (14) requires the solution of the fundamental matrix and integrals of $x(s)$ over the sampling intervals Δt_i. To obtain an explicit solution, the exogenous variables must be interpolated between $x(t_i)$ and $x(t_{i+1})$. As mentioned, usually step or polygonal approximations are used. For the fundamental matrix Φ, one can use time ordered matrix exponentials (Singer; 1998) or a product representation (cf. eqn. 12–13).
In the oversampling approach (fig. 1), arbitrary interpolation schemes for $x(t)$ such as splines etc. can be used easily, since the integrals are obtained automatically by using a finer discretization scheme. The EDM is formulated at time points $\tau_j = t_0 + j\delta t, j = 0, \ldots, J$, such that all measurement times can be expressed on this grid with uniform spacing δt, i.e. $t_i = \tau_{j_i}$ with indices $j_0 = 0, \ldots, j_T = J = (t_T - t_0)/\delta t$.
This approach (cf. Singer; 1995, 2007) may be called *oversampling*, since more

latent states are inserted between the measurement times t_i. Thus one obtains

$$\begin{aligned} y_{j+1} &= A_j^* y_j + b_j^* + u_j; j = 0, \ldots, J && (24) \\ z_i &= H_{j_i} y_{j_i} + D_{j_i} x_{j_i} + \epsilon_{j_i}; i = 0, \ldots, T, && (25) \end{aligned}$$

where

$$\begin{aligned} A_j^* &= \Phi(\tau_j + \delta t, \tau_j) && (26) \\ b_j^* &= \int_{\tau_j}^{\tau_j + \delta t} \Phi(\tau_j + \delta t, s) B(s) x(s) ds && (27) \\ \Omega_j^* &:= \mathrm{Var}(u_j) = \int_{\tau_j}^{\tau_j + \delta t} \Phi(\tau_j + \delta t, s) \Omega(s) \Phi'(\tau_j + \delta t, s) ds && (28) \end{aligned}$$

In contrast to the usual EDM valid at fixed measurement times t_i, the interval δt can be made arbitrarily small. Then one obtains approximately by linearization[3]

$$\begin{aligned} A_j^* &\approx I + A_j \delta t && (29) \\ b_j^* &\approx b_j \delta t = B_j \hat{x}_j \delta t && (30) \\ \Omega_j^* &\approx \Omega_j \delta t && (31) \end{aligned}$$

and thus finds the Euler-Maruyama approximation of the SDE on the δt grid (times τ_j)

$$\begin{aligned} y_{j+1} &= (I + A_j \delta t) y_j + b_j \delta t + G_j \delta W_j \\ \delta W_j &= W(\tau_j + \delta t) - W(\tau_j). \end{aligned}$$

Summarizing,

- the oversampling approach yields a simple form of the parameter functionals, which can be solved explicitly on the interval $[\tau_j, \tau_{j+1}]$. If δt is small, they are approximately linear in the parameters $A(t), b(t)$ and $\Omega(t)$.

- Thus, also *linear* (in the parameters) KF and SEM software can be used to estimate the system (24).

  The linearization of $\exp(A_j \delta t) = I + A_j \delta t + O(A_j^2 \delta t^2)$ does introduce an approximation error, which must be kept small by choosing a δt, such that $||A_j^2|| \delta t^2$ is negligible. In applications A_j is not known before estimation, so the nonlinear specification (26–28; cf. appendix A) is preferable.

- The price to be payed is the introduction of more latent states y_j between the measurements. This is no problem in the recursive filtering approach, but the SEM states η and the structural matrices get large (cf. section 4.2 and I).

[3] The intercepts $b_j = B(\tau_j)\hat{x}(\tau_j) := B_j \hat{x}_j$ are obtained from the interpolated exogenous variables $\hat{x}(t)$. A more elaborated nonlinear treatment of (26–28) is given in appendix A.

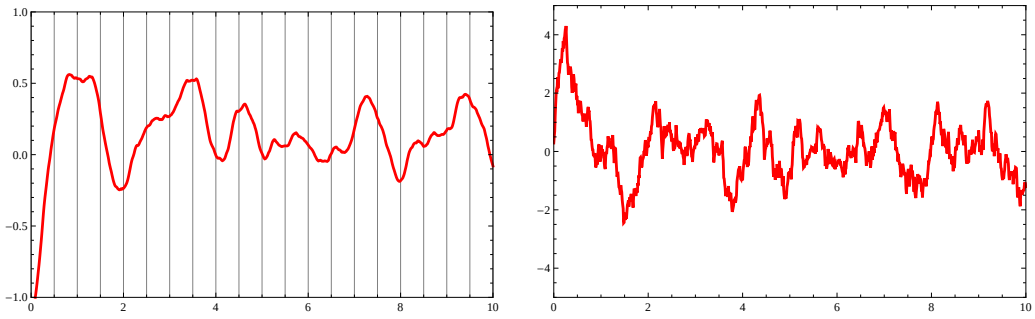

Figure 2: Simulation of the oscillator model with discretization interval $\delta t = 0.01$ in the interval $[t_0, t_T] = [0, 10]$. The sampling interval $\Delta t = 0.5$ is marked by vertical lines. Also visible is the roughness of the unobserved velocity process (right) which is not differentiable.

- The solution of the difference equation (24) for the indices $j = j_i, \ldots, j_{i+1}$ yields an approximation of the EDM (14) which is exact in the limit $\delta t \to 0$. One obtains the time ordered product representation of the fundamental matrix and approximations of the other integrals automatically and must only choose an interpolation $\hat{x}(t)$ of $x(t)$ on the oversampling grid points τ_j.

4 Applications

4.1 Numerical example 1: CAR(2) model

The random oscillator (also called Continuous time AR(2) process, mathematical pendulum, linear oscillator)[4] is defined by the second order differential equation

$$\ddot{y} + \gamma\dot{y} + \omega_0^2 y = bx(t) + g\zeta(t) \tag{32}$$

with the parameters $\gamma =$ friction, $\omega_0 = 2\pi/T_o =$ angular frequency, $T_o =$ period of oscillation, $g =$ strength of random force ζ and exogenous controls $x(t)$.
It is obtained from Newton's law

$$\text{Force} = \text{Mass} \times \text{Acceleration} = m\,\ddot{y}$$

by using a velocity dependent frictional force $\gamma\dot{y}$ and a linear restoring force $\omega_0^2 y$, where $\omega_0 = 2\pi\nu_0$ is the angular frequency of the undamped oscillation and ζ is a random force (white noise) with autocorrelation $E[\zeta(t)\zeta(s)] = \delta(t-s)$

[4] The model has numerous applications, for example the statistical analysis of sun spots (Bartlett; 1946; Arato et al.; 1962; Singer; 1993), in physics (for an overview see Gitterman; 2005) or in psychology (coupled oscillators, Boker and Poponak; 2004).

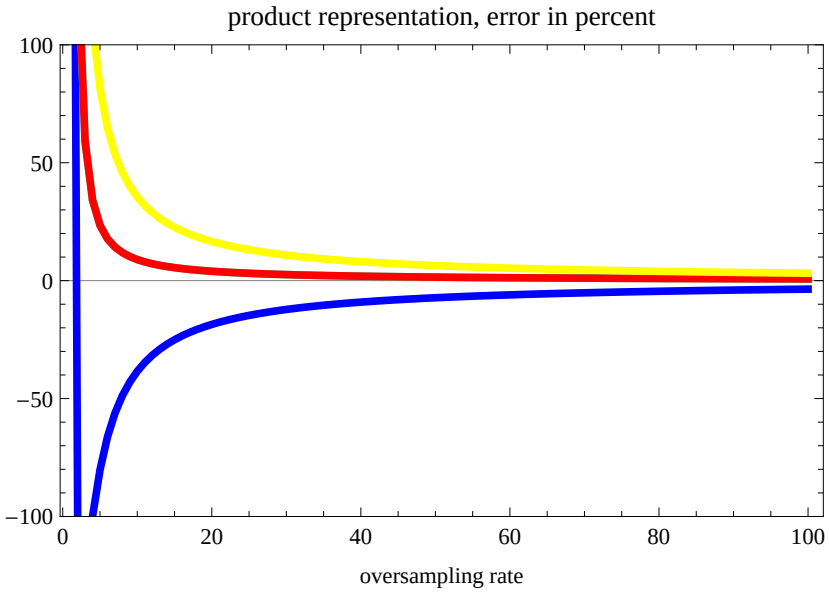

Figure 3: Oversampling of measurement interval $\Delta t = .5$ with sampling rate $L = 1, \ldots, 100$. Convergence of the product representation of the matrix exponential function (eqn. 21).

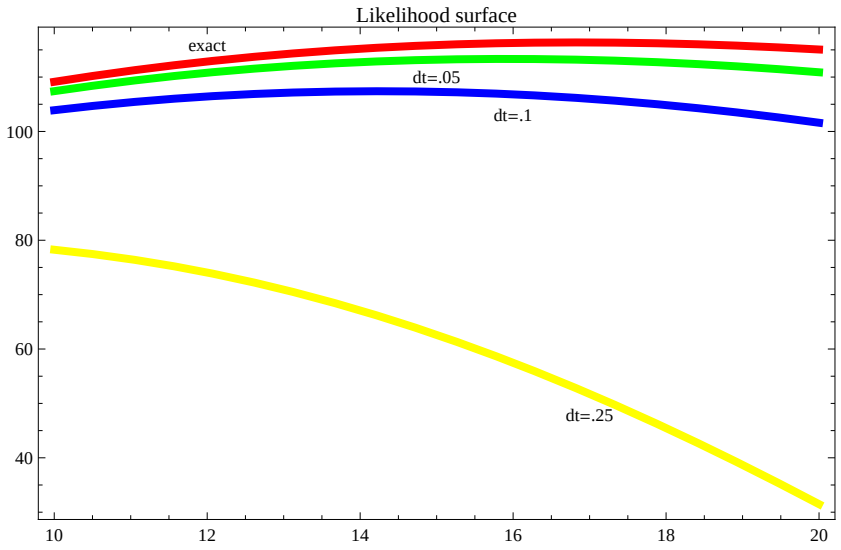

Figure 4: Likelihood surface for the parameter ω_0^2. Shown is the exact result and the functions using linearized oversampling $\delta t = .25, .1, .05$. The data z_i were simulated in the interval [0,50] using $\Delta t = 0.5, i = 0, \ldots, T = 100$.

parameters		SEM		KF	
	true	$\hat{\theta}$	std	$\hat{\theta}$	std
ω_0^2	16	12.1351	2.00838	12.1351	2.00834
γ	4	2.83901	0.719584	2.83901	0.719573
b	1	0.16749	0.219823	0.16749	0.219824
g	2	1.26954	0.26547	1.26954	0.265466
lik		121.341		121.341	
parameters		SEM, lin. oversampling, $J = 5$		KF, lin. oversampling, $J = 5$	
	true	$\hat{\theta}$	std	$\hat{\theta}$	std
ω_0^2	16	11.0852	1.72094	11.0852	1.72093
γ	4	3.63523	0.657319	3.63523	0.657312
b	1	0.147298	0.196889	0.147298	0.196888
g	2	1.12249	0.20603	1.12249	0.206028
lik		121.509		121.509	

Table 1: CAR(2) model, $T = 100$. Comparison of SEM and KF ML-estimates and likelihood. Top: exact EDM ($\Delta t = .5$), bottom: linearized EDM, oversampling ($J = 5; \delta t = .1$)

(Dirac delta-function).[5] The term $bx(t)$ represents external forces and can model intercepts. The force terms are scaled by the mass m.
The pendulum has state space representation

$$d\begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix} := \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -\gamma \end{bmatrix} \begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix} dt + \begin{bmatrix} 0 \\ b \end{bmatrix} x(t)dt + \begin{bmatrix} 0 & 0 \\ 0 & g \end{bmatrix} d\begin{bmatrix} W_1(t) \\ W_2(t) \end{bmatrix} \tag{33}$$

$$z_i := \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} y_1(t_i) \\ y_2(t_i) \end{bmatrix} + \epsilon_i; \; i = 0, \ldots, T. \tag{34}$$

Thus, the SDE of second order can be represented by a vector autoregression at the sampling times t_i. It is important to note that $dy_1 = y_2 dt$ or $dy_1/dt = \dot{y} = y_2$ is an unobserved velocity state which can be reconstructed by the Kalman filter or as smoothed latent vector $E[y_2(t)|Z^T]$. *No approximation of derivatives (e.g. numerical differences $\Delta y_1/\Delta t_i$) is necessary*. The velocity $\dot{y}(t_i) = y_2(t_i)$ at the measurement times t_i is unobserved (latent).
The eigenvalues of the drift matrix A are given by $\lambda_{1,2} = -\gamma/2 \pm i\sqrt{-\gamma^2/4 + \omega_0^2}$ $:= -\gamma/2 \pm i\omega$, thus the undamped frequency is lowered by the friction.
The stationary values are $\mu_s = A^{-1}Bx = \begin{bmatrix} bx/\omega_0^2 \\ 0 \end{bmatrix}$ and $\Sigma_s = (g^2/2\gamma)\begin{bmatrix} 1/\omega_0^2 & 0 \\ 0 & 1 \end{bmatrix}$, which is the solution of $A\Sigma_s + \Sigma_s A' + \Omega = 0$. Thus the friction $\gamma > 0$ is necessary to compensate for the random forces in order to admit a stationary solution (for constant $x(t) = x$).

[5] The formal derivative $\zeta(t) = dW(t)/dt$ is the white noise process; cf. Arnold (1974).

The EDM has the form

$$\begin{bmatrix} y_{1,i+1} \\ y_{2,i+1} \end{bmatrix} = \begin{bmatrix} a^*_{11} & a^*_{12} \\ a^*_{21} & a^*_{22} \end{bmatrix} \begin{bmatrix} y_{1,i} \\ y_{2,i} \end{bmatrix} + \begin{bmatrix} b^*_{1,i} \\ b^*_{2,i} \end{bmatrix} + \begin{bmatrix} u_{1i} \\ u_{2i} \end{bmatrix};\ i = 0, \ldots, T-1 \quad (35)$$

$$z_i = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} y_{1,i} \\ y_{2,i} \end{bmatrix} + \epsilon_i;\ i = 0, \ldots, T. \quad (36)$$

In this example only constant controls $x(t) = 1$ are considered. Thus, the matrices of the EDM are explicitly

$$\begin{aligned} A^*_i &= \exp(A\Delta t_i) && (37) \\ &= \exp(-\gamma/2\Delta t_i) \times \\ &\quad \begin{bmatrix} \gamma/(2\omega)\sin\omega\Delta t_i + \cos\omega\Delta t_i & (1/\omega)\sin\omega\Delta t_i \\ -(\omega_0/\omega)\sin\omega\Delta t_i & \cos\omega\Delta t_i - \gamma/(2\omega)\sin\omega\Delta t_i \end{bmatrix} \\ B^*_i &= A_i^{-1}(A^*_i - I)B && (38) \\ \mathrm{row}(\Omega^*_i) &= (A \otimes I + I \otimes A)^{-1}(A^*_i \otimes A^*_i - I)\mathrm{row}(\Omega). && (39) \end{aligned}$$

where

$$A = \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -\gamma \end{bmatrix}; B = \begin{bmatrix} 0 \\ b \end{bmatrix}; \Omega = \begin{bmatrix} 0 & 0 \\ 0 & g^2 \end{bmatrix}. \quad (40)$$

The true numerical values are set to $\psi = \{\omega_0^2, \gamma, b, g, \mu_1, \mu_2, \sigma_{11}, \sigma_{12}, \sigma_{22}\} = \{16, 4, 1, 2, 0, 0, 1, 0, 1\}$ where $\mu = E[y(t_0], \Sigma = \mathrm{Var}(y(t_0))$ are the parameters of the initial condition.

The matrices of the exact discrete model (37–39) are complicated nonlinear functions of the SDE matrices A, B, Ω and the sampling interval Δt_i. In particular, they loose the original restrictions. The numerical values are ($\Delta t_i = 0.5$)

$$\begin{aligned} A^*_i &= \begin{bmatrix} 0.150574 & 0.10482 \\ -1.67712 & -0.268705 \end{bmatrix} \\ B^*_i &= \begin{bmatrix} 0.0530891 \\ 0.10482 \end{bmatrix} \\ \Omega^*_i &= \begin{bmatrix} 0.0250479 & 0.0219744 \\ 0.0219744 & 0.376001 \end{bmatrix} \end{aligned}$$

From this it is easily seen that unrestricted estimation of the *-matrices does not work, since the restrictions on the SDE matrices (40) cannot be implemented.[6] Fig. 2 shows a part of the simulated trajectory in the interval $[0, 10]$ with discretization step $\delta t = 0.01$. The sampling interval $\Delta t = 0.5$ is marked by vertical lines. The first component is differentiable ($\dot{y}$ = velocity), but the second derivative (acceleration) $\ddot{y} = (d/dt)\dot{y}$ does not exist.

[6] The discussion on identification, embedding and aliasing is well known; cf. Singer and Spilerman (1976); Phillips (1976a); Hansen and Sargent (1983); Hamerle et al. (1991, 1993); Singer (1992a).

The simulation in fig. 2 was done with the SEM model (I, 11–12), where the EDM matrices were substituted for the discrete time matrices ($\alpha_j \to A_j^*$ etc.). The latent vector η contains the states $[y_j, \dot{y}_j], j = 0, \ldots, J$, but only the components $y_{j_i}, i = 0, \ldots, T$ are measured. Thus, in the measurement model (I, 12), only the components y_{j_i} are projected outside on measurements z_i.
The model can be estimated using the EDM on the measurement times $t_i = 0, 0.5, 1, 1.5, \ldots$ (nonlinear parameters $A^* = \exp(A\Delta t)$ etc.) or by using the linearized EDM $A^*(\delta t) \approx I + A\delta t$ etc. on an oversampled grid with $\delta t = 0.25, 0.1, .05$ etc. Fig. 3 displays the convergence of the product $(I + A\Delta t/L)^L$ for the oversampling rates $L = 1, \ldots, 100$. It shows that for the chosen true matrix A and sampling interval $\Delta t = 0.5$ at least 20 or more oversampling times must be used to hold the error reasonably small. On the other hand, no (explicit) matrix exponentials must be computed and linear (in the parameters) standard software can be used.
Fig. 4 shows the likelihood surface of parameter ω_0^2 for several oversampling intervals (linearized EDM matrices) and the true likelihood obtained by the EDM. Note that the same exact result is obtained when nonlinear oversampling is used (cf. eqn. 20)

4.2 Numerical example 2: Coupled oscillators with time varying parameters

Coupled CAR(2) processes are interesting models for the oscillatory behavior of individuals which are also in interaction (cf. Boker and Poponak; 2004). A physical picture are pendula which are connected by a spring, where the spring constant parametrizes the interaction. More generally, one could use coupled nonlinear physical pendula, which is equivalent to interacting particles moving in a periodic potential (cf. Gitterman; 2005, and the literature cited therein).[7] Models of this kind are well known in physics, e.g. for diffusing ions in superionic conductors, phonon fields, heat baths etc. In this article, the estimation of the system parameters and filtering and smoothing of the latent states is of central interest.
The random oscillator of example 1 is the basic ingredient. It is coupled to the other pendulum by a force proportional to the distance. More generally, a linear force $F(y_1, y_2) = \epsilon_1 y_1 + \epsilon_2 y_2 + \epsilon_3$ is introduced which may be time dependent as well. In a physical picture one can set $F(y_1, y_2) = K(y_1 - y_2 + c)$ with a coupling (spring) constant K and Kc is an initial tension.
The coupled oscillators are defined by (cf. 32)

$$\begin{aligned} \ddot{y}_1 + \gamma_1\dot{y}_1 + \omega_{01}^2 y_1 &= F(y_1, y_2) + g_1\zeta_1(t) \\ \ddot{y}_2 + \gamma_2\dot{y}_2 + \omega_{02}^2 y_2 &= -F(y_1, y_2) + g_2\zeta_2(t), \end{aligned}$$

[7] see also `http://www.fernuni-hagen.de/imperia/md/content/ls_statistik/sde.zip` for nonlinear filtering.

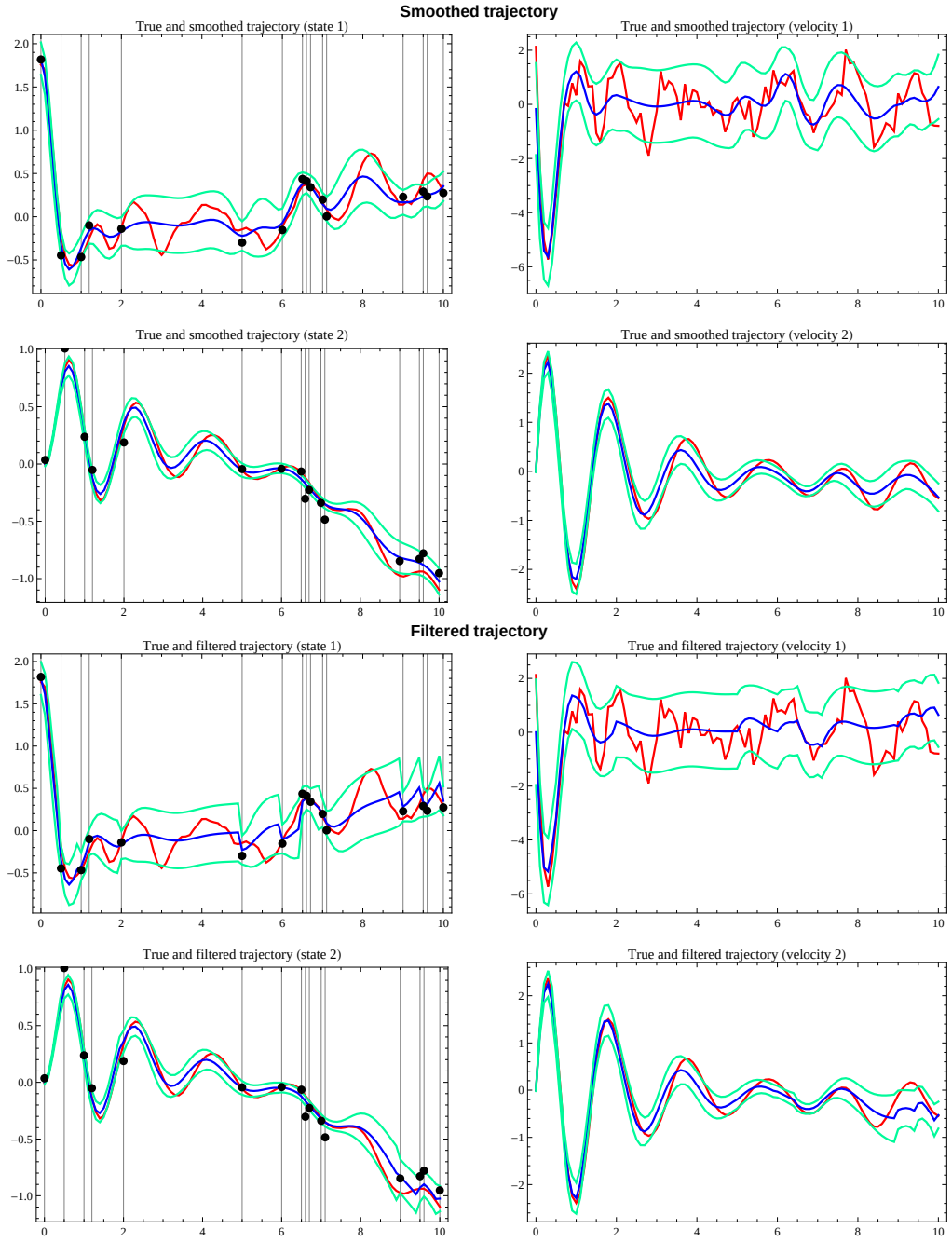

Figure 5: Coupled oscillators: smoothed and filtered trajectories and prediction bands using the true parameter values (see text). The dots represent measurements (error $\mathrm{Var}(\epsilon_i) = R = 0.01$).

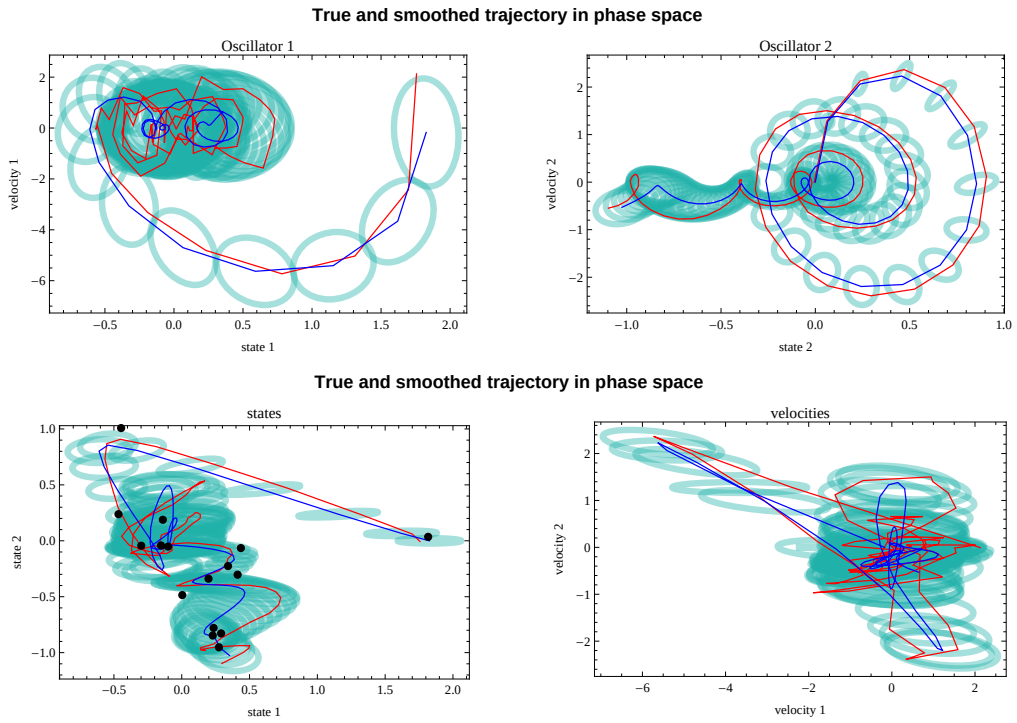

Figure 6: Coupled oscillators: true (red) and smoothed trajectories (blue) with 95% prediction ellipses in 4 dimensional phase space: state vs. velocity projections (top) and state vs. state, velocity vs. velocity (bottom). The dots represent measurements.

but more general specifications are possible (continuous time CVAR(2), including coupling via frictional forces).
For the purpose of filtering and estimation, the state space representation

$$d/dt \begin{bmatrix} y_1 \\ \dot{y}_1 \\ y_2 \\ \dot{y}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -\omega_{01}^2 + \epsilon_1 & -\gamma_1 & \epsilon_2 & 0 \\ 0 & 0 & 0 & 1 \\ -\epsilon_1 & 0 & -\omega_{02}^2 - \epsilon_2 & -\gamma_2 \end{bmatrix} \begin{bmatrix} y_1 \\ \dot{y}_1 \\ y_2 \\ \dot{y}_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \epsilon_3 \\ 0 \\ -\epsilon_3 \end{bmatrix} [1] + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & g_1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & g_2 \end{bmatrix} \begin{bmatrix} \zeta_{11} \\ \zeta_{12} \\ \zeta_{21} \\ \zeta_{21} \end{bmatrix}$$

is used. In order to model a changing interaction, the interaction parameters $\epsilon_l(t) = \epsilon_{l0} + \epsilon_{l1} t; l = 1, 2, 3$ are assumed to be time varying (other functional forms can be used as well). For the simulation of data I used the true parameter values $\omega_{01}^2 = 16, \gamma_1 = 4, \epsilon_1(t) = \epsilon_{10} + \epsilon_{11} t = -5 + 1t, g_1 = 2$ (first oscillator), $\omega_{02}^2 = 10, \gamma_2 = 0, \epsilon_2(t) = -\epsilon_1(t), g_2 = 0$ (second oscillator) and $\epsilon_3(t) = \epsilon_1(t)$. Thus the interaction force is $F(y_1, y_2, t) = (-5+1t)(y_1 - y_2 + 1)$. For $t = 0$, the

		nonlinear oversampling, $\delta t = .1$					
		SEM, inverse		SEM, g-inverse		KF	
parameter	true	$\hat{\psi}$	std	$\hat{\psi}$	std	$\hat{\psi}$	std
ω_{01}^2	16	19.5392	3.9437	19.5392	3.9435	19.5392	3.9437
γ_1	4	3.627	1.1126	3.627	1.1125	3.627	1.1126
ϵ_{10}	-5	-4.5474	0.6699	-4.5474	0.6699	-4.5474	0.6699
ϵ_{11}	1	0.9007	0.0919	0.9007	0.0919	0.9007	0.0919
g_1	2	2.0289	0.6753	2.0289	0.6752	2.0289	0.6752
ω_{02}^2	10	9.4755	1.0699	9.4755	1.0699	9.4755	1.0699
γ_2	1	1.0069	0.413	1.0069	0.413	1.0069	0.413
g_2	0	-0.2132	0.2914	0.2132	0.2914	0.2132	0.2914
time, likelihood		0.659547, 40.6223		0.659343, 40.6223		0.071734, 40.6223	

Table 2: Nonlinear oversampling: ML estimates for the irregularly sampled data (see fig. 5). Comparision of SEM (inverse, g-inverse) with KF. See text.

		nonlinear oversampling					
		$\delta t = .1$		$\delta t = .05$		$\delta t = .025$	
parameter	true	$\hat{\psi}$	std	$\hat{\psi}$	std	$\hat{\psi}$	std
ω_{01}^2	16	19.5392	3.9437	19.5381	3.9433	19.5378	3.9431
γ_1	4	3.627	1.1126	3.6266	1.1125	3.6265	1.1124
ϵ_{10}	-5	-4.5474	0.6699	-4.5685	0.6716	-4.5794	0.6725
ϵ_{11}	1	0.9007	0.0919	0.9005	0.0919	0.9004	0.0919
g_1	2	2.0289	0.6752	2.0287	0.6752	2.0287	0.6752
ω_{02}^2	10	9.4755	1.0699	9.4744	1.0695	9.4742	1.0694
γ_2	1	1.0069	0.413	1.007	0.4129	1.007	0.4129
g_2	0	0.2132	0.2914	0.2131	0.2913	-0.2131	0.2912
time, lik (SEM)		0.668482, 40.6223		2.7434, 40.3894		12.9137, 40.2625	
time, lik (KF)		0.068108, 40.6223		0.128167, 40.3894		0.241293, 40.2625	

Table 3: Nonlinear oversampling: ML estimates for irregularly sampled data. Oversampling times $\delta t = 0.1, 0.05, 0.025$. Numbers rounded to 4 digits. The likelihoods and evaluation times are shown in the last two rows.

		linear oversampling					
		$\delta t = .1$		$\delta t = .05$		$\delta t = .025$	
parameter	true	$\hat{\psi}$	std	$\hat{\psi}$	std	$\hat{\psi}$	std
ω_{01}^2	16	19.7074	4.5127	19.7774	3.8744	19.6349	4.0105
γ_1	4	5.9404	1.6527	4.7587	1.2193	4.1755	1.1857
ϵ_{10}	-5	-4.2604	0.6824	-4.2996	0.522	-4.4444	0.6463
ϵ_{11}	1	0.9093	0.1126	0.8921	0.0766	0.896	0.0838
g_1	2	2.277	0.7624	2.1573	0.6786	2.0899	0.6882
ω_{02}^2	10	10.0656	0.8584	9.8408	0.7096	9.6502	1.0415
γ_2	1	2.4442	0.9375	1.5869	0.3929	1.3007	0.4299
g_2	0	0	0.5892	0	0.9681	-0.1462	0.3856
time, lik (SEM)		0.64668, -16.9562		2.70384, 32.2323		12.9647, 39.0207	
time, lik (KF)		0.047711, -16.9562		0.080217, 32.2323		0.153833, 39.0207	

Table 4: Linear oversampling: ML estimates for irregularly sampled data. Oversampling times $\delta t = 0.1, 0.05, 0.025$. Numbers rounded to 4 digits. The likelihoods and evaluation times are shown in the last two rows.

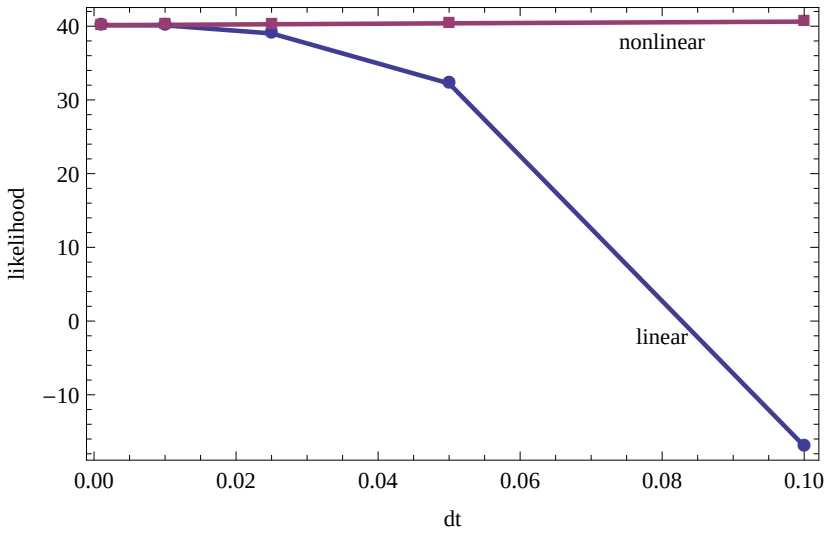

Figure 7: Coupled oscillators: Convergence of likelihoods (linearized and nonlinear parameter functionals) as a function of the oversampling intervals $\delta t = \{.1, .05, .025, .01, .001\}$.

term $F(y_1, y_2, 0)$ leads to an attraction of the oscillators, at $t = 5$ the interaction vanishes and for $t > 5$ increased repulsion takes part. The first oscillator is the same as in example 2, the second one is purely deterministic without random force and starts at $y_2 = 0$ at rest ($\dot{y}_2 = 0$). Due to the coupling it starts to move (first it is attracted by 1, but later it is indifferent and then repelled by 1; and vice versa).

Fig. 5 shows the true trajectories (state and velocity) of the oscillators together with approximate 95 % prediction intervals, computed with the true parameters. The filtered states (bottom) were computed with the Kalman filter and show $E[y(t)|Z^t]_i \pm 1.96\sqrt{\mathrm{Var}[y(t)|Z^t]_{ii}}$, $i = 1, \ldots, 4$. The smoothed state uses all information, i.e. $E[y(t)|Z^T]$. The results obtained by the SEM and the KF approach are very similar, although the recursive approach is much faster, both in simulation and filtering.

2-dimensional projections of the 4-dimensional movement in phase space are shown in fig. 6 (red lines). Also displayed is the (projected) smoothed state $E[(y_1, \dot{y}_1, y_2, \dot{y}_2)(t)|Z^T]$ (blue) and 95% prediction ellipses.

The parameters were estimated with the SEM-ML procedure with linear and nonlinear oversampling. Table 2 compares the results of the SEM (inverse and g-inverse of the covariance matrix Σ_y) with the Kalman filter. The results are almost identical, but the KF approach is much faster.

Tables 3–4 show the comparision of the ML estimates (nonlinear oversampling) with linearized oversampling ($\delta t = .1, 0.05, .025$). With increasing oversampling rate $L = 1, 2, 4$, the linearized ML estimates approach the nonlinear ones. The maximal dimensions $(J+1)p = (10/.025+1)4 = 1604$ of the SEM state η are quite big, however. Therefore, the likelihood evaluation is very slow in the SEM approach. The execution time for one likelihood evaluation is shown in the last lines of the tables.

Fig. 7 shows the convergence of the likelihoods as a function of oversampling interval $\delta t = \{.1, .05, .025, .01, .001\}$ for the nonlinear and linearized parameter functionals. It should be noted that due to the time dependence of the parameters, the nonlinear oversampling with $\exp(A(\tau_j)\delta t)$ leads to slightly different results depending on the oversampling interval (cf. appendix A).

5 Conclusion

Sampled linear stochastic differential equations can be represented by vector autoregressions, but the parameter functionals are nonlinearly dependent on the original SDE parameters. Both in the SEM and the KF approach, this must be implemented explicitly. Time dependent models can be treated by the oversampling device which corresponds to an Euler approximation of the SDE on a latent grid. Arbitrary interpolation schemes of the exogenous variables are permitted. If the grid spacing is small enough, linearized parameter functionals can be used.

Thus no eigenvalue computations or complex arithmetic is necessary. The price is a large SEM state, but the recursive KF approach still works. Both the SEM and the KF approach are valid for time series and panel data.

Appendix A: Nonlinear oversampling

The exact parameter functionals

$$\begin{aligned} A_j^* &= \Phi(\tau_j + \delta t, \tau_j) \\ b_j^* &= \int_{\tau_j}^{\tau_j+\delta t} \Phi(\tau_j + \delta t, s) B(s) x(s) ds \\ \Omega_j^* &= \int_{\tau_j}^{\tau_j+\delta t} \Phi(\tau_j + \delta t, s) \Omega(s) \Phi'(\tau_j + \delta t, s) ds \end{aligned} \tag{41}$$

of the oversampled model must be computed explicitly in order to perform simulation, ML estimation and filtering/smoothing explicitly.
If the time dependent matrices $A(t), \Omega(t)$ and vectors $b(t) = B(t)\hat{x}(t)$ etc. are approximated by step (simple) functions in the interval $[\tau_j, \tau_j + \delta t]$, i.e.

$$A(t) \approx \sum_j A_j \chi_{[\tau_j, \tau_j+\delta t)}(t)$$

etc. where

$$\chi_A(t) = \begin{cases} 1 & t \in A \\ 0 & else \end{cases}$$

(indicator function of A), the integrals can be solved explicity. One obtains

$$\begin{aligned} A_j^* &\approx \exp(A_j \delta t); \Phi(s, \tau_j) \approx \exp[A_j(s - \tau_j)] \\ b_j^* &\approx A_j^{-1}[\exp(A_j \delta t) - I] b_j \delta t \\ \Omega_j^* &\approx \int_{\tau_j}^{\tau_j+\delta t} \exp[A_j(\delta t + \tau_j - s)] \Omega_j \exp[A_j'(\delta t + \tau_j - s)] ds \end{aligned}$$

More complicated expressions are obtained by linear interpolation in $[\tau_j, \tau_j + \delta t]$ (cf. Hamerle et al.; 1993).
The last term can be written explicitly as (cf., e.g. Singer; 1990)

$$\text{row}(\Omega_j^*) \approx [A_j \otimes I + I \otimes A_j]^{-1}[\exp(A_j \delta t) \otimes \exp(A_j \delta t) - I]\text{row}(\Omega_j).$$

In order to avoid misunderstandings, note that the exogenous variables $x(t)$ are approximated twofold:
First they are interpolated between the measurement times t_i leading to $\hat{x}(t)$ (step functions, polygons, splines etc.). Then, they are evaluated at $\hat{x}_j = \hat{x}(\tau_j)$ and written as step (simple) functions $\hat{\hat{x}}(t) \approx \sum_j \hat{x}_j \chi_{[\tau_j, \tau_j+\delta t)}(t)$ to admit an evaluation of (41).

Appendix B: Numerical considerations

All computations were done using Mathematica 7, which is an interpreter language. The Kalman filter approach is implemented in the LSDE and SDE packages, whereas the SEM computations are obtained with the SEM equations of section 2.[8]

The ML estimator was obtained by using a quasi Newton algorithm with BFGS secant updates (Dennis Jr. and Schnabel; 1983) and numerical scores. At the end of the iteration the asymptotic standard errors were computed from the observed Fisher information $-(\partial^2 l/\partial\psi\psi')(\hat{\psi})$. In the SDE approach, analytical score functions were implemented also (Singer; 1990, 1993, 1995).

As mentioned, in the LSDE approach, the matrix exponential function and its derivative $\partial/\partial\psi \exp(A\Delta t)$ was calulated using the spectral representation $\exp(A\Delta t) = P\exp(\Lambda\Delta t)P^{-1}$ where P contains the eigenvectors and Λ is the diagonal matrix of (complex) eigenvalues. In rare cases a Jordan canonical form may be necessary, but we assume that all eigenvalues are distinct (cf. Jennrich and Bright; 1976; Singer; 1990).

In the SEM approach, the Mathematica kernel function MatrixExp was utilized. According to the online help, it uses variable-order Padé approximation, evaluating rational matrix functions using Paterson-Stockmeyer methods, or Krylov subspace approximations.[9] For a thourough discussion of the matrix exponential and its derivative, see Wilcox (1967); Najfeld and Havel (1995); Moler and VanLoan (2003).

The software permits arbitrary nonlinear matrix restrictions since all matrices are functions of a parameter vector ψ (e.g. $\exp(A(\psi)\Delta t)$).

In the oversampling approach (Euler approximation), the linearized $\exp(A\delta t) \approx I + A\delta t$ can be used with error controlled by δt. Thus one could work with linear (in the parameters) programs like LISREL, at least for $N > 1$ to avoid singularity of the moment matrices (but cf. Hamerle et al.; 1991). The oversampling (better approximation for $\exp(A\delta t)$) leads to larger state dimensions $(J+1)p; J = (t_T - t_0)/\delta t$, however.

In the SEM program, the structural matrices (of order $(J+1)p \times (J+1)p$) are computed automatically by block matrix operations, which may be somewhat tedious in other systems.

Generally, in my experience, the SEM approach only works satisfactorily (in terms of numerical stability and speed) if $(J+1)p \leq 100$. The KF approach is only limited by the dimensions p and k of the state variables.

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[8] see:
http://www.fernuni-hagen.de/imperia/md/content/ls_statistik/sde.zip,
http://www.fernuni-hagen.de/imperia/md/content/ls_statistik/publikationen/semarchive.exe

[9] http://reference.wolfram.com/mathematica/note/SomeNotesOnInternalImplementation.html#14568).

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