Usage of the Mori-Zwanzig method in time series analysis

Markus Niemann,[1,*] Thomas Laubrich,[1] Eckehard Olbrich,[2] and Holger Kantz[1]
[1]*Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany*
[2]*Max-Planck-Institut für Mathematik in den Naturwissenschaften, Inselstraße 22, D-04103 Leipzig, Germany*
(Received 17 July 2007; revised manuscript received 15 October 2007; published 16 January 2008)

The use of memory kernels stemming from a Mori-Zwanzig approach to time series analysis is discussed. We show that despite its success in determining properties from an analytical model, the kernel itself is not easily interpreted. We consider a recently introduced discretization of the kernel and show that its properties can be quite different from its continuous counterpart. We provide a rigorous analysis of the discrete case and show for several analytically calculated memory kernels of simple time series processes that their features are not readily detectable in the kernel. We show furthermore that practical relevant Mori-Zwanzig models with a finite kernel form a true subclass of the autoregressive moving average (ARMA) models. The fact that this approach already veils the properties of these simple time series gives rise to severe doubts about its applicability in more complex situations.

DOI: 10.1103/PhysRevE.77.011117 PACS number(s): 05.40.−a, 05.45.Tp, 05.10.Gg

I. INTRODUCTION

In the early years of the analysis of strongly and irregularly fluctuating time series data, linear stochastic models were used for their modeling and prediction [1]. When in the 1980s the phenomenon of deterministic chaos became more and more popular, the interpretation of strong fluctuations in terms of deterministic processes occurred as a charming alternative, resulting in a set of corresponding time series methods [2]. However, it soon became evident that purely deterministic and low-dimensional chaotic processes are usually not good candidates for processes in nature. Therefore, the inclusion of stochasticity into such nonlinear models was taken into account, resulting in time series methods to reconstruct Fokker-Planck equations from data [3]. Apart from some more technical restrictions, also such models are not able to explain long-range correlations and memory in data. Exactly this was reported in a huge number of more recent publications, such as in climate records [4], physiological data [5], economic data [6], and geophysical processes [7]. The method to detect such memory effects, the (detrended) fluctuation analysis, does not give any hint at the modeling of such data.

In this situation, the recently proposed modeling of time series data in terms of Mori-Zwanzig equations [8] appeared very promising. In the time-discrete Mori-Zwanzig approach, the time series model is a linear stochastic model in the spirit of an autoregressive AR(∞) model with correlated noises, where the AR coefficients, however, are interpreted as the values of a (linear) memory kernel. Hence, this model class seemed to be an appealing class to model infinite memory and hence non-Markovian behavior. In the same paper, a numerical procedure for the computation of the memory kernel from data was proposed.

In this contribution, we start by looking at the memory kernel of simple time-continuous processes and show that already the time-continuous memory kernel displays features which are hard to connect directly to the underlying physical process. Then, we review the above method and supply a comprehensive understanding of the memory kernel thus obtained and of the correlation of the produced residual forces, which are the correlated noise terms. We compute the kernels for several simple linear stochastic processes and for the process we considered in the continuous case sampled in discrete time steps. As results, we find that the discrete kernel can deviate substantially from the continuous counterpart and that simple processes generate kernels which are as long range and complicated as for other, genuinely non-Markovian processes. The memory kernels thus computed neither possess any straightforward interpretations in terms of the properties of the underlying processes nor reflect their complexity. Thus we have to draw the conclusion that this very compelling idea of modeling observed data by Mori-Zwanzig-like equations does not yield direct insight into the processes which generated the data.

In addition we show that the kernels with finite length which are interesting for data modeling result in a class of models which form a true subclass of antoregressive moving average (ARMA) models. Therefore, we conclude that this approach is not useful for data generation.

II. CONTINUOUS MORI-ZWANZIG KERNEL

The Mori-Zwanzig method [9–11] provides a projection formalism which is an exact equation for the time evolution of a set of "relevant" observables by putting the evolution of the neglected variables into a time kernel and residual terms. Its continuous-time version can be written for a set of observables $\mathcal{G}_\mu(t)$ as [[12], Eq. (11.2.14)]

$$\dot{\mathcal{G}}_\mu(t) = \sum_\nu \Omega_{\mu\nu}\mathcal{G}_\nu(t) - \int_0^t \sum_\nu \mathcal{K}_{\mu\nu}(t')\mathcal{G}_\nu(t-t')dt' + \mathcal{F}_\mu(t). \tag{1}$$

This splitting is done with respect to a scalar product on the space of observables which is invariant with respect to time translation. In general, this scalar product is constructed by

*niemann@mpipks-dresden.mpg.de

choosing an invariant probability measure μ on the phase space [13]:

$$\langle f,g\rangle = \langle fg\rangle_\mu = \int f(x)g(x)d\mu(x), \tag{2}$$

which corresponds to an ensemble of initial conditions. The noise terms $\mathcal{F}_\mu(t)$ are constructed in such a way that they stay orthogonal to the initial set of observables $\mathcal{G}_{0\mu} := \mathcal{G}_\mu(t=0)$ at all times:

$$\langle \mathcal{F}_\mu(t)\mathcal{G}_{0\nu}\rangle = 0. \tag{3}$$

Projecting on the initial set of observables, one gets rid of the "noise" terms:

$$\frac{d}{dt}\langle \mathcal{G}_\mu(t)\mathcal{G}_{0\nu}\rangle = \sum_\tau \Omega_{\nu\tau}\langle \mathcal{G}_\tau(t)\mathcal{G}_{0\mu}\rangle - \int_0^t \sum_\tau \mathcal{K}_{\mu\tau}(t')\langle \mathcal{G}_\tau(t-t')\mathcal{G}_{0\nu}\rangle dt', \tag{4}$$

$$\dot{\Gamma}_{\mu\nu}(t) = \sum_\tau \Omega_{\mu\tau}\Gamma_{\tau\nu}(t) - \int_0^t \sum_\tau \mathcal{K}_{\mu\tau}(t')\Gamma_{\tau\nu}(t-t')dt', \tag{5}$$

with $\Gamma_{\mu\nu}(t) := \langle \mathcal{G}_\mu(t)\mathcal{G}_{0\nu}\rangle$. Taking the Laplace transform, this equation reads (using matrix notation)

$$s\check{\Gamma}(s) - \Gamma(0) = [\Omega - \check{\mathcal{K}}(s)]\,\Gamma(s), \tag{6}$$

with

$$\check{\Gamma}(s) = \int_0^\infty e^{-st}\Gamma(t)dt \tag{7}$$

and

$$\check{\mathcal{K}}(s) = \int_0^\infty e^{-st}\mathcal{K}(t)dt \tag{8}$$

being the Laplace transforms of $\Gamma(t)$ and $\mathcal{K}(t)$. Using the fact that $\lim_{s\to\infty}\mathcal{K}(s)=\mathbf{0}$, Eq. (6) can be used to determine the kernel and Ω from a known correlation structure. Of course, the typical use of the Mori-Zwanzig formalism is to approximate the kernel for a given analytical model and to deduce the correlation structure or transport coefficients from it. But here we want to check if we can readily detect the properties of the system by looking solely at the kernel.

As a basis of the next two examples we will use the classical harmonic oscillator with the Hamilton function

$$H(q,p) = \frac{1}{2}q^2 + \frac{1}{2}p^2. \tag{9}$$

Invariant measures are given by [13]

$$d\mu(q,p) = Z(H(q,p))dqdp, \tag{10}$$

which contain as a special case the Boltzmann distribution

$$d\mu_{\mathrm{B}}(q,p) = \frac{\beta}{2\pi}\exp\left(-\frac{\beta}{2}(q^2+p^2)\right)dqdp. \tag{11}$$

Example (A): taking the observable $\mathcal{G}_0=q_0$. The time evolution is given by $\mathcal{G}(t)=q(t)=q_0\cos t - p_0 \sin t$ which gives

$$\Gamma(t) = \langle q_0^2\rangle\cos t. \tag{12}$$

Using Eq. (6) results in

$$\Omega = 0 \tag{13}$$

and

$$\mathcal{K}(t) = 1. \tag{14}$$

The nondecaying (infinite memory) kernel corresponds to the fact that the original second-order time derivative is replaced by a first-order derivative and an integration. The frequency of the oscillation does not enter through a periodicity of the kernel, but only as the scaling. We will come back to this example in the context of discrete sampling.

Example (B): taking the observable $\mathcal{G}_0=q_0^3$. This corresponds to the case of an observable where considering nonlinear transformations would be beneficial to the analysis. The Mori-Zwanzig formalism projects then the time evolution on the subspace spanned by q_0^3 which is equivalent to choosing one prefactor such that $q^3(t)$ is best (least mean square) approximated on the whole ensemble under consideration. The correlation function is

$$\Gamma(t) = \langle q_0^6\rangle\cos^3 t + 3\langle q_0^4p_0^2\rangle\cos t\,\sin^2 t. \tag{15}$$

Using Eq. (6) again gives

$$\Omega = 0 \tag{16}$$

and

$$\mathcal{K}(t) = \frac{9}{7+6\gamma} - \frac{12(\gamma+1)(3\gamma-1)}{7+6\gamma}\cos(\sqrt{7+6\gamma}t), \tag{17}$$

with $\gamma := \langle q_0^4p_0^2\rangle/\langle q_0^6\rangle$. In the case of a Boltzmann ensemble ($\gamma=1/5$), the kernel reduces to

$$\mathcal{K}(t) = \frac{45}{41} + \frac{144}{205}\cos\left(\sqrt{\frac{41}{5}}t\right). \tag{18}$$

Due to the high symmetry of the Hamilton function, it is possible to show that every distribution of the form described in Eq. (10) gives these numerical values. This kernel shows also infinite memory, but we see also an angular frequency of $\sqrt{41/5}$ which has no direct relation to the angular frequency 1 of the oscillator.

We see that it is hard to detect properties of the system directly from the kernel without processing it further. This observation will carry over to the discrete system.

III. DISCRETE MORI-ZWANZIG KERNEL

In [8] a discretized version of the Mori-Zwanzig equation is introduced and a method to determine the kernel elements from a time series is proposed. The space of relevant variables is taken to be the linear span of the measured observables. In the case of a multidimensional time series $[X_\alpha(t)]_{t=0,1,2,\ldots}$ the equation for $t\geqslant 0$ reads

$$X_{\alpha}(t+1) = -\sum_{\tau=0}^{t}\sum_{\gamma} K_{\alpha\gamma}(t-\tau)X_{\gamma}(\tau) + F_{\alpha}(t), \qquad (19)$$

where the $X_{\alpha}(t)$ are assumed to have zero mean. To simplify the equations given in [8] we made two changes: we assumed that the starting point of the time series is at 0 and the average is taken over an ensemble of processes, independently of whether this ensemble results from moving the origin over one realization of the process or considering different realizations of the process. Second, we subsumed the terms belonging to the current time (this is the oscillation term Ω and the difference term in [8]) into $K(0)$ since they lose their special meaning in the time-discrete case. These changes affect only the value of $K(0)$ and do not change any other results.

The $F_{\alpha}(t)$ terms describe again the fluctuations due to the complementary dynamics. They have the property $\langle X_{\beta}(0)F_{\alpha}(\tau)\rangle = 0$ for all times $\tau \geqslant 0$. This is used in [8] to determine the conditional equations for the kernel:

$$\Gamma_{\alpha\beta}(t+1) = -\sum_{\tau=0}^{t}\sum_{\gamma} K_{\alpha\gamma}(t-\tau)\Gamma_{\gamma\beta}(\tau) \quad \text{for } t \geqslant 0, \quad (20)$$

with $\Gamma_{\alpha\beta}(t) := \langle X_{\alpha}(t)X_{\beta}(0)\rangle$. Equations (19) and (20) in matrix notation are

$$X(t+1) + \sum_{\tau=0}^{t} K(t-\tau)\, X(\tau) = F(t) \qquad (21)$$

and

$$\Gamma(t+1) + \sum_{\tau=0}^{t} K(t-\tau)\, \Gamma(\tau) = 0 \quad \text{for } t \geqslant 1. \qquad (22)$$

From a time series analysis point of view Eqs. (21) and (22) form a linear model. We want to analyze them from this side and link them to the standard linear models.

Similarly to the continuous case one can use the unilateral z transform ([14], Chap. 3)—the discrete analog of the (unilateral) Laplace transform. The z transforms of the above series are defined as

$$\hat{X}(z) := \sum_{j=0}^{\infty} z^{-j}X(j) \qquad (23)$$

and

$$\hat{F}(z) := \sum_{j=0}^{\infty} z^{-j}F(j) \qquad (24)$$

for $z \in \{z \in \mathbb{C} : |z| > 1\}$

$$\hat{\Gamma}(z) := \sum_{j=0}^{\infty} z^{-j}\Gamma(j) \qquad (25)$$

and

$$\hat{K}(z) := \sum_{j=0}^{\infty} z^{-j}K(j) \qquad (26)$$

for $z \in \{z \in \mathbb{C} : |z| > \rho\}$ with some $0 < \rho < 1$. The ranges of convergence stem from the fact that the given series are stable and causal. In this paper we will not rely on this interpretation; the z transform can be rather seen as a formal power series in z^{-1} and regarded as a convenient tool for the bookkeeping of coefficients. Equations (21) and (22) can hence be written as

$$[1 + z^{-1}\hat{K}(z)]\, \hat{X}(z) = X(0) + z^{-1}\hat{F}(z) \qquad (27)$$

and

$$[1 + z^{-1}\hat{K}(z)]\, \hat{\Gamma}(z) = \Gamma(0). \qquad (28)$$

The first of these formulas contains on the right-hand side the part which would be considered as random in a model simulation (the initial condition and the "noise" terms). The extension of $\hat{K}(z)$ by the unit matrix [and therefore the appearance of $X(0)$ as a constant term on the right-hand side] in this form stems from the orthogonality condition between $X(0)$ and the noise terms: $\langle X_{\alpha}(0)F_{\beta}(\tau)\rangle = 0$.

Equation (28) shows that the autocovariance function contains exactly the same information as the kernel together with the covariance matrix. In the one-dimensional case the process of calculating the kernel components from the autocovariance function is (apart from a scaling factor) the same as the transformation of the coefficients of an (possibly infinite) AR model into the coefficients of a (possibly infinite) MA model and vice versa. It also shows that the kernel can be calculated by expanding

$$1 + z^{-1}\hat{K}(z) = \Gamma(0)\, \hat{\Gamma}^{-1}(z) \qquad (29)$$

as a power series in z^{-1} and reading off the coefficients.

Example (C): first-order autoregressive process [AR(1) process]. An AR(1) process is defined by

$$x(t) = ax(t-1) + \xi(t) \quad \text{with } -1 < a < 1, \qquad (30)$$

where $\xi(t)$ are independent and identically distributed (i.i.d.) normal random variables with mean 0 and variance 1. The autocovariance function of lag τ is ([1], Chap. 3.2.3) $\gamma_{\tau} = a^{|\tau|}/(1-a^2)$. Therefore, we get

$$\hat{\Gamma}(z) = \frac{1}{1-a^2}\sum_{j=0}^{\infty} z^{-j}a^{j} = \frac{1}{1-a^2}\frac{1}{1-z^{-1}a} \qquad (31)$$

and

$$1 + z^{-1}\hat{K}(z) = 1 - z^{-1}a. \qquad (32)$$

We can read off the kernel elements $K(0) = -a$ and $K(j) = 0$ for $j \geqslant 1$. This result coincides with the numerical findings in [8] since an Ornstein-Uhlenbeck process sampled at equidistant discrete time steps is an AR(1) process. Additionally, we implemented the numerical algorithm given in [8] [which essentially estimates the autocovariance function from the time series and calculates the kernel iteratively using Eq.

(20)]. Figure 1 displays the kernel $K(j)$ obtained numerically for a variety of AR(1) processes. Each series consisted of 10^6 points and was generated with a different parameter a. It can be seen that the numerical results are in perfect agreement with the analytical solution.

Example (D): second-order autoregressive process [AR(2)] with pseudoperiodic behavior. It is defined by

$$\begin{aligned} x(t) &= \phi_1 x(t-1) + \phi_2 x(t-2) + \xi(t) \\ &= 2D\cos(\omega)x(t-1) - D^2 x(t-2) + \xi(t), \end{aligned} \tag{33}$$

with $-1 < D < 1$, where the $\xi(t)$ have the same properties as in the last paragraph and $\phi_1 = 2D\cos(\omega)$, $\phi_2 = D^2$ with ω being the frequency of the oscillation and D the damping constant. The autocovariance function of lag τ is given by ([1], Chap. 3.2.4)

$$\gamma_\tau = \gamma_0 \frac{D^{|\tau|}\sin(\omega|\tau| + F)}{\sin(F)}, \tag{34}$$

with

$$\tan(F) = \frac{1+D^2}{1-D^2}\tan(\omega). \tag{35}$$

Writing the sine as a sum of exponentials and evaluating the geometric series gives

$$\hat{\Gamma}(z) = \gamma_0 \sum_{j=0}^{\infty} \frac{D^j \sin(\omega j + F)}{\sin(F)} z^{-j} = \gamma_0 \frac{1 - \frac{2D^3}{1+D^2}\cos(\omega)z^{-1}}{1 - 2D\cos(\omega)z^{-1} + D^2 z^{-2}} \tag{36}$$

and

$$\begin{aligned} 1 + z^{-1}\hat{K}(z) &= [1 - 2D\cos(\omega)z^{-1} + D^2 z^{-2}] \sum_{j=0}^{\infty} \left(\frac{2D^3}{1+D^2}\cos(\omega)\right)^j z^{-j} \\ &= 1 - \frac{2D\cos(\omega)}{1+D^2} z^{-1} + \left(\frac{1+D^2}{2D\cos(\omega)} - \frac{2D\cos(\omega)}{1+D^2}\right) z^{-1} \\ &\quad \times \sum_{j=1}^{\infty} \left(\frac{2D^3}{1+D^2}\cos(\omega)\right)^j z^{-j}. \end{aligned} \tag{37}$$

The kernel elements are therefore

$$K(0) = -\frac{2D\cos(\omega)}{1+D^2},$$

$$K(j) = \left(\frac{1+D^2}{2D\cos(\omega)} - \frac{2D\cos(\omega)}{1+D^2}\right)\left(\frac{2D^3}{1+D^2}\cos(\omega)\right)^j \quad \text{for } j \geq 1. \tag{38}$$

The oscillatory behavior with frequency ω has no counterpart in the kernel and the damping constant of the kernel $2D^3\cos(\omega)/(1+D^2)$ has no obvious physical interpretation, a phenomenon already encountered in the continuous case.

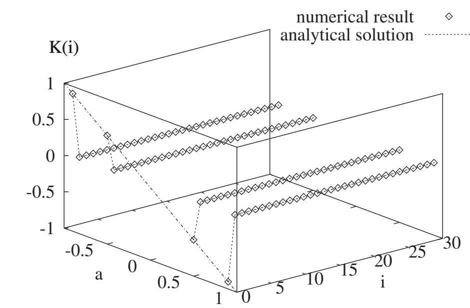

FIG. 1. Kernel $K(i)$ for four different AR(1) processes: $a \in \{-0.9, -0.5, 0.5, 0.9\}$. The numerical results are plotted with diamonds. The analytical solutions $K(0) = -a$ and $K(i) = 0$ for $i \geq 1$ are drawn with dotted lines for better visibility. The dot-dashed line corresponds to $K(0) = -a$.

Figure 2 shows both the numerically obtained kernels and the analytical solutions: a variety of AR(2) processes (each with 10^6 points) was generated and the corresponding kernels were computed according to the algorithm given in [8]. The numerical results were again in perfect agreement with the analytical solution.

Example (E): the harmonic oscillator, introduced in the last section [Eq. (9)], sampled at discrete time steps $t_j = \tau j$ with τ being the sampling interval. If we assume that $1/\tau$ is not rationally conjugated with the angular frequency (which is 1 in our example), the correlation function estimated from a time series will converge to the correlation function evaluated over the initial conditions of a microcanonical ensemble of the given energy; i.e., we will get using Eq. (12)

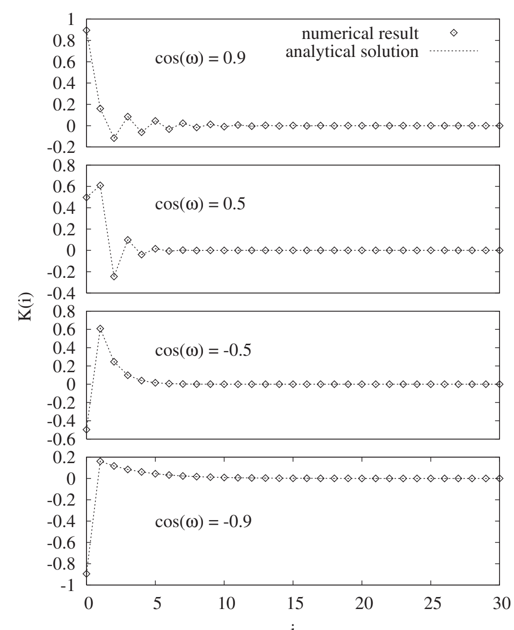

FIG. 2. Kernel $K(i)$ for four different AR(2) processes: $D = -0.9$ and $\cos(\omega) \in \{-0.9, -0.5, 0.5, 0.9\}$. The numerical results are plotted with diamonds. The analytical solutions, Eq. (38), are drawn with dotted lines for better visibility.

$$\Gamma(k) = \langle q_0^2 \rangle \cos(\tau k). \tag{39}$$

This generalizes to a set of time series representing an arbitrary ensemble corresponding to an energy distribution. Calculating the z transforms

$$\hat{\Gamma}(z) = \langle q_0^2 \rangle \frac{1 - z^{-1}\cos\tau}{1 - 2z^{-1}\cos\tau + z^{-2}} \tag{40}$$

and using Eq. (28)

$$\hat{K}(z) = -\cos\tau + \sin^2\tau \sum_{j=1}^{\infty} z^{-j}\cos^{j-1}\tau \tag{41}$$

gives the kernel elements

$$K(0) = -\cos\tau, \quad K(j) = \sin^2\tau\cos^{j-1}\tau. \tag{42}$$

This kernel looks similar to the kernel of an AR(2) process (in fact, the kernels coincide for $D \to 1$). It decays exponentially with a time constant $(-\ln\cos\tau)/\tau$ in contrast to the constant kernel in the continuous case. In particular, the time constant of the decay only depends on the sampling frequency and therefore does not reflect a property of the underlying process [e.g., $(-\ln\cos\tau)/\tau \sim \tau/2$ for $\tau \ll 1$]. This example shows that discretization can totally change the kernel which makes the interpretation even harder. Similarly to the continuous case the oscillating behavior of the original process is not directly visible in the kernel.

Example (F): the damped harmonic oscillator with stochastic driving and discrete sampling. We consider the damped harmonic oscillator with stochastic driving in continuous time

$$\frac{d^2x}{dt^2}(t) + g\frac{dx}{dt}(t) + \nu^2 x(t) = \eta(t), \tag{43}$$

which we assume to be in the oscillatory regime ($2\nu > g > 0$) and $\eta(t)$ constitutes white noise in continuous time $\langle \eta(t)\eta(s)\rangle = q\delta(t-s)$. The causal Green's function is given by

$$G(t) = \frac{1}{\omega}\Theta(t)e^{-\delta t}\sin(\omega t), \tag{44}$$

with $\delta = g/2$, $\omega = \sqrt{\nu^2 - \delta^2}$, and $\Theta(t)$ being the Heaviside step function. The solution to Eq. (43) can therefore be written as

$$x(t) = \int_{-\infty}^{\infty} G(t-t')\eta(t')dt'. \tag{45}$$

Combining this with $\langle \eta(t)\eta(s)\rangle = q\delta(t-s)$ enables us to determine the autocovariance function

$$\gamma(t-s) = \langle x(t)x(s)\rangle = \gamma(0)e^{-\delta|t-s|}\left(\cos(\omega|t-s|) + \frac{\delta}{\omega}\sin(\omega|t-s|)\right). \tag{46}$$

Similar to the previous example, we introduce the time discretization with time step τ and get for the z transform of the autocovariance function in discrete time

$$\hat{\Gamma}(z) = \gamma(0)\frac{1 - \left[\cos(\omega\tau) - \frac{\delta}{\omega}\right]e^{-\delta\tau}z^{-1}}{1 - 2\cos(\omega\tau)e^{-\delta\tau}z^{-1} + e^{-2\delta\tau}z^{-2}}. \tag{47}$$

Following now the analog calculation in example (D) we get for the kernel elements

$$K(0) = -\left(\cos(\omega\tau) + \frac{\delta}{\omega}\sin(\omega\tau)\right)e^{-\delta\tau},$$

$$K(j) = \left[1 + \left(\frac{\delta}{\omega}\right)^2\right]\sin^2(\omega\tau)\left(\cos(\omega\tau) - \frac{\delta}{\omega}\sin(\omega\tau)\right)^{j-2} e^{-\delta\tau j}. \tag{48}$$

For high sampling rates ($\tau \ll \omega, \delta$) we get for the time constant of the decay

$$-\frac{1}{\tau}\ln\left\{\left(\cos(\omega\tau) - \frac{\delta}{\omega}\sin(\omega\tau)\right)e^{-\delta\tau}\right\} = 2\delta + \frac{\omega^2 + \delta^2}{2}\tau + O(\tau^2), \tag{49}$$

while the scaling of the kernel is

$$\left[1 + \left(\frac{\delta}{\omega}\right)^2\right]\frac{\sin^2(\omega\tau)}{\left[\cos(\omega\tau) - \frac{\delta}{\omega}\sin(\omega\tau)\right]^2} = \left[1 + \left(\frac{\delta}{\omega}\right)^2\right](\omega\tau)^2 + O(\tau^3). \tag{50}$$

While we get the correct damping constant $g = 2\delta$ in zeroth order with a first-order correction (keeping in mind that one has to take the second order into account to see the kernel), the oscillatory behavior is not directly visible in the kernel and its frequency can only be determined by the properties of the kernel (e.g., the scaling) which are strongly sampling rate dependent.

IV. CORRELATIONS OF THE NOISE TERMS

In the time-continuous case, the memory kernel can also be found in the correlations of the noise terms [[12] Eq. (11.2.24)]:

$$\mathcal{K}_{\alpha\beta}(t) = \sum_{\gamma} g_{\beta\gamma}\langle F_\gamma(0)F_\alpha(t)\rangle, \tag{51}$$

with $g_{\alpha\beta}$ being the inverse of the covariance matrix: $\sum_\gamma g_{\alpha\gamma}\langle X_\gamma X_\beta\rangle = \delta_{\alpha\beta}$ [see [12] Eq. (11.2.3)]. We want to derive the corresponding equation for the time-discrete case. It will turn out to be useful to look at a two-dimensional generalization of the z transform containing all correlations of the noise terms at arbitrary times:

$$\hat{c}(z_1,z_2) := \langle \hat{F}(z_1)\hat{F}(z_2)^T\rangle = \sum_{i,j=0}^{\infty} c(i,j)z_1^{-i}z_2^{-j}, \tag{52}$$

with $c(i,j) := \langle F(i)F(j)^T\rangle$ being the covariance matrix between the noise terms at time steps i and j. Since we assume $X(i)$ to be stationary, we get

$$\langle \hat{X}(z_1)\hat{X}(z_2)^T\rangle = \left(\sum_{i=0}^{\infty}(z_1z_2)^{-i}\right)[\hat{\Gamma}(z_1)+\hat{\Gamma}(z_2)^T-\Gamma(0)]. \tag{53}$$

Combining this with Eqs. (27) and (28) gives

$$\hat{c}(z_1,z_2) = \frac{1}{1-(z_1z_2)^{-1}}[\Gamma(0)-\hat{K}(z_1)\,\Gamma(0)\,\hat{K}(z_2)^T]. \tag{54}$$

Defining the discrete counterpart of Eq. (51) as in Eqs. (4) and (10) in Ref. [8], i.e.,

$$\tilde{K}(t) \coloneqq \Gamma(0)^{-1}\,c(t,0), \tag{55}$$

we get from Eq. (54) by noting that $K(0)=-\Gamma(1)\,\Gamma(0)^{-1}$

$$\tilde{K}(0) = 1 + \Gamma(0)^{-1}\,K(0)\,\Gamma(1)^T,$$

$$\tilde{K}(i) = \Gamma(0)^{-1}\,K(i)\,\Gamma(1)^T \quad \text{for } i \geqslant 1. \tag{56}$$

In the one-dimensional case we get $\tilde{K}(i)$ for $i\geqslant 1$ by multiplying $K(i)$ by the autocorrelation of lag 1, $\rho_1=\gamma_1/\gamma_0$ (with γ_0 being the covariance and γ_1 the autocovariance of lag 1 of the process). This factor is a consequence of analyzing the calculation of $\tilde{K}(i)$ in the time-discrete formalism; it is missed by discretizing the corresponding continuous equation [which was done for Eq. (10) in [8]]. Because of Eq. (56), the calculation of $\tilde{K}(i)$ can only be used to check the integrity of the numerical implementation and not to test the applicability of the algorithm.

Example (G): first-order moving average process [MA(1) process]. This process is defined by

$$x(t) = \xi(t) + a\xi(t-1) \quad \text{with } a \in \mathbb{R}. \tag{57}$$

The kernel is easily calculated as [using Eq. (28)]

$$K(i) = \beta^{i+1}, \tag{58}$$

with the definition

$$\beta \coloneqq -\frac{a}{1+a^2}. \tag{59}$$

It should be noted that the kernel of this process can be distinguished from the kernel of a pseudoperiodic AR(2) process (38) only by $K(0)$ and a scaling factor. Using Eq. (54) we get for the correlations of the noise terms

$$c(i,j) = (1+a^2)\left(\delta_{ij} - \frac{\beta^{i+j}-\beta^{|i-j|-2}}{1-\beta^{-2}}\right)$$
$$\rightarrow (1+a^2)\left(\delta_{ij} - \frac{\beta^{|i-j|}}{1-\beta^2}\right) \tag{60}$$

for $i,j\rightarrow\infty$ with $i-j=$const. The elements of the time series itself are independent for time lags larger than 1. The longer exponentially decaying correlations of the noise terms are therefore compensated by the equally decaying kernel which is contrary to the behavior of the AR(1) process. The pseudoperiodic AR(2) process shows arbitrary intermediate behavior between these two. Therefore, it is hard to deduce the complexity of the process from the calculated kernel.

In general, the correlations of the noise terms decay similarly to the kernel [Eq. (54)], which makes it difficult to determine properties of the time series from the kernel.

V. MODELS WITH A FINITE KERNEL

In practical calculations one will always truncate the kernel to finitely many elements. Therefore, we want to identify the models corresponding to finite kernels. We will restrict this discussion to one-dimensional time series to keep the formalism simple, but the generalization is straightforward. Since it is general practice to consider time-delayed embeddings [2], we will look at such a d-dimensional embedding:

$$X(t) \coloneqq \begin{pmatrix} x(t+d-1) \\ x(t+d-2) \\ \vdots \\ x(t) \end{pmatrix}. \tag{61}$$

The covariance matrices $\Gamma(i)$ can be expressed in terms of the autocovariance function γ_i of the one-dimensional process:

$$(\Gamma(i))_{pq} = \gamma_{i-p+q}. \tag{62}$$

The *Yule-Walker estimates* $w_d(1),\ldots,w_d(d)$ of order d ([1], Chap. 3.2.2) are the parameters of an AR(d) model such that the power of the residuals is minimal. They can be determined by solving

$$\Gamma(0)\begin{pmatrix} w_d(1) \\ w_d(2) \\ \vdots \\ w_d(d) \end{pmatrix} = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_d \end{pmatrix}. \tag{63}$$

The *gapped function* $g_d(\kappa)$ ([14], Chap. 9.4.2) is defined as the covariance between the residuals and the time series:

$$g_d(\kappa) = \left\langle x(k-\kappa)\left(x(k) - \sum_{i=1}^{d} w_d(i)x(k-i)\right)\right\rangle_k$$
$$= \gamma_\kappa - \sum_{i=1}^{d} w_d(i)\,\gamma_{\kappa-i}. \tag{64}$$

Since the $w_d(i)$ are determined by Eq. (63), we have $g_d(i)=0$ for $1\leqslant i\leqslant d$, which explains the name "gapped function." Its value at the origin can be identified with the power of the residuals $\sigma_d^2=g_d(0)$. As this function is in general not symmetric, we can define two unilateral z transforms

$$\hat{g}_d^-(z) = \sum_{i=0}^{\infty} g_d(-i)z^{-i} \tag{65}$$

and

$$\hat{g}_d^+(z) = \sum_{i=0}^{\infty} g_d(d+1+i)z^{-i}. \tag{66}$$

With the notation N for the $d\times d$ matrix with 1 in the lower secondary diagonal and 0 elsewhere and e_1 for the first

d-dimensional unit vector, the kernel is given by [which can be checked by inserting it into Eq. (28)]

$$\hat{K}(z) = -N - e_1 \begin{pmatrix} -w_{d-1}(1) \\ \vdots \\ -w_{d-1}(d-1) \\ 0 \end{pmatrix}^T - \frac{\hat{g}^+_{d-1}(z)}{\hat{g}^-_{d-1}(z)} e_1 \begin{pmatrix} -w_{d-1}(d-1) \\ \vdots \\ -w_{d-1}(1) \\ 1 \end{pmatrix}^T . \tag{67}$$

By the Levinson-Durbin recursion ([14], Chap. 9.5), we know that the constant term of $\hat{g}^+_{d-1}(z)/\hat{g}^-_{d-1}(z)$ is $w_d(d)$ and

$$K(0) = -N - e_1 \begin{pmatrix} w_d(1) \\ \vdots \\ w_d(d) \end{pmatrix}^T . \tag{68}$$

If we want the kernel to vanish after p elements [i.e., $K(i)=0$ for $i>p$], we have $p+d$ parameters to specify the model.

The noise is concentrated in the first entry (which is, of course, due to the fact that the other components follow deterministicly from the previous time step):

$$\hat{F}(z) = \hat{f}(z) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} . \tag{69}$$

Using Eq. (54), the correlation structure of the $f(i)$ turns out to be

$$\hat{c}(z_1,z_2) = \frac{\sigma^2_{d-1}}{1-(z_1z_2)^{-1}} \left(1 - \frac{\hat{g}^+_{d-1}(z_1)}{\hat{g}^-_{d-1}(z_1)} \frac{\hat{g}^+_{d-1}(z_2)}{\hat{g}^-_{d-1}(z_2)} \right) . \tag{70}$$

For $i,j>p$ the correlation $\langle f(i)f(j)\rangle$ depends only on the difference $i-j$; $\gamma_{i-j}=\langle f(i)f(j)\rangle$ can be determined from the autocorrelation generating function $\hat{\gamma}(z)$ which follows from Eq. (70):

$$\hat{\gamma}(z) = \sum_{i=-\infty}^{\infty} \gamma_i z^{-i} = \sigma^2_{d-1} \left(1 - \frac{\hat{g}^+_{d-1}(z)\hat{g}^+_{d-1}(1/z)}{\hat{g}^-_{d-1}(z)\hat{g}^-_{d-1}(1/z)} \right) . \tag{71}$$

Therefore, $\gamma_k=0$ for $k>p$. Since we are dealing with a linear model and use only the first and second moments (i.e., the mean, the variance, and the correlations) for the calculation of the kernel, the calculations will be indistinguishable for any distribution which has the same first two moments. Therefore, we will assume for the moment that the $f(i)$ follow a Gaussian distribution with a covariance structure given by Eq. (71). Then Eq. (71) tells us that we can regard the $f(i)$ for $i>p$ as a MA(p) process. Putting this together with Eq. (67), we see that there are constants a_i, independent of t, such that for $t>p$

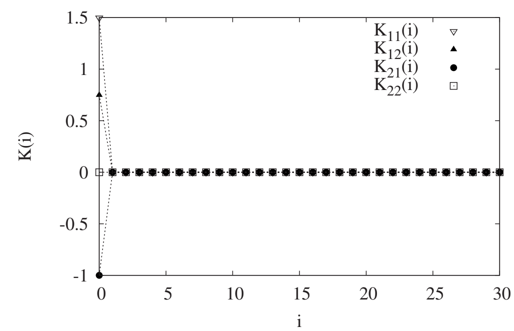

FIG. 3. Kernel $K_{\alpha\beta}(i)$ for a two-dimensional embedded AR(2) process with $\phi_1=-1.5$ and $\phi_2=-0.75$. The numerical result for each kernel element is plotted with points. The analytical solution, Eq. (74), is drawn with dotted lines for better visibility.

$$x(t+d) = \sum_{i=-p}^{d-1} a_i x(t+i) + f(t) . \tag{72}$$

This corresponds to an ARMA($p+d,p$) model where we are able to choose the $p+d$ coefficients of the autoregressive part, but the p coefficients of the moving average part are fixed by this. Describing it more intuitively, one can say that the finite kernel corresponds to a set of finite AR coefficients, while the same kernel imposes through Eq. (54) correlations on the noise terms for a finite lag which is equivalent to a MA model. Since the same kernel appears in the AR and MA parts, their coefficients are not independent. Therefore, considering models with a finite kernel is equivalent to considering a true subclass of the ARMA models.

As mentioned above, this analysis is not restricted to the case of Gaussian-distributed observables. Non-Gaussian behavior can be observed by checking the distributions of either the residuals in case of considering it from the ARMA model point of view or the distributions of the $f(t)$ in case of the Mori-Zwanzig point of view (which corresponds to the residuals of the model, when only the AR part is taken into account). Since the residuals of the ARMA model are already adjusted for the MA part, the residuals are "whiter" than the $f(t)$'s. In the context of data generation, allowing the $f(t)$'s to be non-Gaussian would correspond to driving the ARMA model with non-Gaussian noise.

Example (H): the AR(2) model embedded in two dimensions. The model is given by

$$x(t) = \phi_1 x(t-1) + \phi_2 x(t-2) + \xi(t) . \tag{73}$$

The first kernel element is

$$K(0) = \begin{pmatrix} -\phi_1 & -\phi_2 \\ -1 & 0 \end{pmatrix} , \tag{74}$$

while the other kernel elements vanish. Figure 3 shows the kernel elements $K_{\alpha\beta}(i)$ for a two-dimensional embedded AR(2) process: 10^6 points were generated with $\phi_1=-1.5$ and $\phi_2=-0.75$. The kernel was computed using the algorithm given in [8]. It can be seen that $K_{\alpha\beta}(i)=0$ for $i\geqslant 1$ and $K(0)$ coincides with Eq. (74).

VI. CONCLUSIONS

In this paper we discussed the use of the memory kernel of the Mori-Zwanzig formalism for data analysis. Despite its undisputed success in approximating the kernel in complex situations and deriving model parameters from it, we have shown with an example that the properties of the system are not directly reflected in the kernel. Furthermore, in data analysis one normally does not know that the time series has a linear relation to the "natural" variables of the underlying process. Being a linear analysis technique the Mori-Zwanzig approach is of course sensitive to nonlinear changes (a property it shares with a lot of other data analysis techniques). But we examplified with the harmonic oscillator that these transformations can lead to an oscillatory memory kernel with a frequency which is hard to relate to the frequency of the underlying process while in general nonlinear transformations induce changes in the autocorrelation function which have a defined relation to the base frequency (e.g., change in the harmonics, frequency doubling). Since the memory kernel is derived from the autocorrelation function, it does not contain more information, but instead of enhancing the information, it seems to veil them. In addition, if one wants to interpret the kernel in terms of memory, it is therefore better to think of the kernel not as *the* memory of the system, but of *a* memory of the observable depending on the given representation.

We focused then on a discrete Mori-Zwanzig formalism introduced in [8] and provided a rigorous formalism for the calculation of the kernel. We exemplified that the time discretization of the data can completely change the kernel such that the most prominent features are driven by the sampling time. A second example with a stochastically driven, dissipative, oscillatory system showed the correct damping constant in zeroth order in the kernel, but the oscillatory property was not directly detectable and the influence of its frequncy on the kernel was highly sensitive to the sampling time—both these quantities are directly accessible in the autocorrelation function. In addition we related the discrete Mori-Zwanzig formalism to standard models in linear time series analysis: namely, the ARMA models. We have calculated the kernels for some simple model processes of this type and have seen that it is hard to detect their features directly from the kernel while the connection is clear for the ARMA models: Why does a direct fit of AR coefficients for an AR(2) model yield the correct coefficients—i.e., a kernel which vanishes for $j \geqslant 2$—whereas the same data produce a slowly decaying model when the kernel is determined in accordance with the Mori-Zwanzig approach? The resulting models are both linear superpositions of past variables. The answer is that the Mori-Zwanzig approach enforces the residual forces to have an autocorrelation function which is identical to the kernel (apart from rescaling), whereas the residuals in the AR(2) model are uncorrelated. Therefore, the Mori-Zwanzig process is not only more complicated because of the long memory, but also because of a correlated noise driving it. In particular, modeling of the process by forward-in-time iteration of the model is not straightforward [as opposed to the AR(2) model], since one has to generate a correlated noise process. Therefore, the Mori-Zwanzig approach is not useful for data generation.

In addition we showed that the Mori-Zwanzig models with finite kernel form a true subclass of the ARMA models. In combination with the problems related to the interpretation of the kernel, this gives rise to severe doubts about the suitability of the Mori-Zwanzig approach for data analysis.

[1] G. E. Box, G. M. Jenkins, and G. C. Reinsel, *Time Series Analysis—Forecasting and Control*, 3rd ed. (Prentice-Hall, Englewood Cliffs, NJ, 1994).
[2] H. Kantz and T. Schreiber, *Nonlinear Time Series Analysis*, 2nd ed. (Cambridge University Press, Cambridge, UK, 2004).
[3] S. Siegert, R. Friedrich, and J. Peinke, Phys. Lett. A **243**, 275 (1998).
[4] R. B. Govindan, D. Vjushin, S. Brenner, A. Bunde, S. Havlin, and H.-J. Schellnhuber, Physica A **294**, 239 (2001).
[5] C.-K. Peng, S. Havlin, H. E. Stanley, and A. L. Goldberger, Chaos **5**, 82 (1995).
[6] K. Ivanova, Physica A **270**, 567 (1999).
[7] L. Telesca and M. Lovallo, Physica A **377**, 279 (2007).
[8] D. T. Schmitt and M. Schulz, Phys. Rev. E **73**, 056204 (2006).
[9] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).
[10] H. Mori, H. Fujisaka, and H. Shigematsu, Prog. Theor. Phys. **51**, 109 (1974).
[11] R. Zwanzig, Phys. Rev. **124**, 983 (1961).
[12] E. Fick and G. Sauermann, *The Quantum Statistics of Dynamic Processes*, Springer Series in Solid-State Sciences, Vol. 86 (Springer, Berlin, 1990).
[13] D. Givon, O. H. Hald, and R. Kupferman, Isr. J. Math. **145**, 221 (2005).
[14] K.-D. Kammeyer and K. Kroschel, *Digitale Signalverarbeitung—Filterung und Spektralanalyse mit MATLAB-Übungen* (Teubner, Wiesbaden, 2006).