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Statistical inference of stochastic differential equations under colored noise excitation

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Statistical inference and SDE's

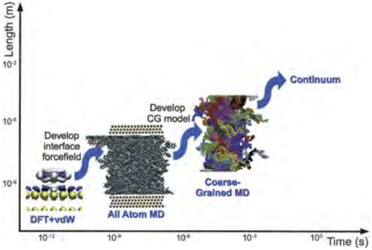

Figure: Multiscale modelling of polymer solid interfaces [Johnston and Harmandaris, 2013]

- Methods for statistical inference of stochastic differential equations have become especially important lately that the enhanced availability of data and computational power allows for rich datasets from different scales and mechanisms of system interactions.

Stochastic Differential Equations

Let $(\Omega, \mathcal{F}, P)$ be a probability space and let us consider the system of SDE's :

$$\dot{x}(\,t\,;\,\omega\,) = K\,\left(\,x(t;\omega),\ y(t;\omega)\,\right)$$

$$\dot{x}(\,0\,;\,\omega\,) = x_0(\,\omega\,), \quad t > 0, \quad \omega \in \Omega$$

where:
$x(t;\omega)$: the response, $y(t;\omega)$: the excitation.

- A data driven approach: Given data from $x(t,\omega)$ (and $y(t\omega)$) we want to find the operator K and the characteristics of random noise $y(t,\omega)$.
- Many methods have been developed for the statistical inference of diffusion processes that follow the Markovian property, have independent increments, and are completely characterized by their transition probability e.g. approximate, pseudo likelihood (Euler, Eulerian, local linearization) and simulated likelihood methods.

Random Differential Equation

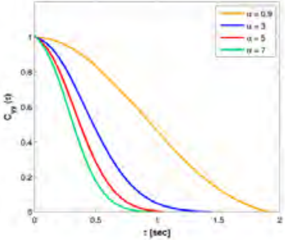

Figure: The low -pass Gaussian filter excitation covariance $C_{yy}(\tau) = \sigma^2 exp(-a(\tau))^2$ for $\sigma = 1$

- In many systems encountered in engineering, finance, and biology when the correlation time of the excitation is of the same order of magnitude as the system's relaxation time it is not a plausible simplification to assume that the system is excited by a delta correlated process (white noise).
- Such cases can be more realistically modeled by correlated random functions, also known as colored random noises.
- SDE's with colored random noise excitation are also referred to as Random Differential Equetions (RDEs).

Response- Excitation (RE) theory

- The Response-Excitation theory for RDEs :
  - Proposes the joint treatment of the probabilistic structure of the response and the excitation, leaving the space for their stochastic dependence to be determined during the solution of the problem
  - Involves two separate time variables- one for the excitation and one for the response
  - Uses functional averages over the response realizations and the excitation
  - References e.g.: *Sapsis and Athanassoulis [2008], Venturi, Sapsis, Cho, and Karniadakis [2012], Athanassoulis, Tsantili, and Kapelonis [2015], Tsantili [2014], Mamis, Athanassoulis, and Kapelonis [2019]*.
- In the context of the Response-Excitation theory two-time RE moment equations were developed along with suitable closures for non-linear systems.
  - References e.g.: *Athanassoulis, Tsantili, and Kapelonis [2013], Tsantili [2014], Athanassoulis, Tsantili, and Kapelonis [2015], see also Joo and Sapsis [2016]* .

Outline

- Review of the derivation of the two-time RE moment equations.
- Present a Gaussian two-moment approach for the statistical inference of RDE's using the two-time RE moment equations.
- Examine the use of simple, surrogate models for the data-driven description of non-Markovian processes.

RDEs under colored noise excitation

We consider random differential equations:

$$\dot{x}(t;\omega) = K\left(x(t;\omega),\ y(t;\omega)\right)$$
$$x(0;\omega) = x_0(\omega)$$

Where K is a linear or non-linear operator with polynomial non-linearities, $y(t;\omega)$ is a colored noise excitation, e.g.:

- A shifted OU (sOU) process with $m_y = 0$ and thus $C_{yy} = R_{yy}$, where :

$$R_{yy}(t,s) = \sigma^2 \cdot \exp\left(-\alpha \cdot |t-s|\right) \cdot \cos\left(\omega_0 \cdot (t-s)\right)$$

with correlation time:

$$\tau_{yy}^{\mathrm{corr}} = \frac{\alpha}{\alpha^2 + \omega_0^2} + \frac{e^{-\alpha\pi/(2\omega_0)}}{1 - e^{-\alpha\pi/(\omega_0)}} \cdot \frac{2\omega_0}{\alpha^2 + \omega_0^2}, \quad \omega_0 > 0$$

- A low pass Gaussian Filter (lpGF):

$$R_{yy}(t,s) = \sigma^2 \cdot \exp\left(-\alpha(t-s)^2\right)$$

$$\tau_{yy}^{\mathrm{corr}} = \sqrt{\pi}/(2\sqrt{\alpha})$$

RDEs under colored noise excitation

We consider random differential equations:

$$\dot{x}(\, t\,;\,\omega\,) = K\ (\, x(t;\omega),\ y(t;\omega)\,)$$
$$x(\,0\ ;\ \omega\,) = x_0(\,\omega\,)$$

Where K is a linear or non-linear operator with polynomial non-linearities, $y(t;\omega)$ is a colored noise excitation, e.g.:

- The methodology proposes the derivation of a system of four moment equations directly from the dynamical system:
- One-time diagonal moment equations for the $m_x(t)$ and $R_{xx}(t)$
- Two-time moment equations for $R_{xy}(t,s)$ and $R_{xx}(t,s)$

Moment equations for linear RDEs

From the linear RDE:

$$\dot{x}(t\,;\,\omega) \;=\; -A\cdot x(t\,;\omega) + B\cdot y(t\,;\,\omega)$$

The solution of the two-time RE moment system is given by:

$$m_x\,(t) = e^{A\cdot t}\cdot B\cdot \int_{t_0}^{t} m_y\,(s)\cdot e^{-A\cdot s} ds + e^{A\cdot(t-t_0)}\cdot m_{x_0},\quad \forall\, t \geq t_0$$

$$R_{x\,y}\,(t,s) = e^{A\cdot t}\cdot \int_{t_0}^{t} B\cdot R_{y\,y}\,(t_1,s)\cdot e^{-A\cdot t_1} d\,t_1 + e^{A\cdot(t-t_0)}\cdot m_{x_0}\cdot m_y\,(s)\quad,\quad \forall\, t \geq t_0, \forall\, s \geq t_0$$

$$\begin{aligned} R_{x\,x}\,(t,s) = B\cdot e^{A\cdot(s+t)} \int_{t_0}^{t} & \left(e^{-A\cdot t_1}\cdot \int_{t_0}^{s} B\cdot R_{y\,y}\,(t_2,t_1)\cdot e^{-A\cdot t_2} d\,t_2 \right) d\,t_1 + \\ & e^{A\cdot(t+s-t_0)} B\cdot m_{x_0}\cdot \int_{t_0}^{t} m_y\,(t_1)\, e^{-A\cdot t_1} d\,t_1 + \\ & e^{A\cdot(t+s-t_0)}\cdot B\cdot m_{x_0}\cdot \int_{t_0}^{s} m_y\,(s_1)\cdot e^{-A\cdot s_1} d s_1 + e^{A\cdot(t+s-2\cdot t_0)}\cdot R_{x_0 x_0}, \end{aligned}$$

The equation for $R_{x\,x}(t,t)$ is obtained taking the limit $s \to t$.

Remark on RE moment equations of non-linear systems

- When $K(x(t,\omega), Y(t,\omega))$ is non-linear the (truncated) moment system is not closed and, thus, some closure scheme should be invoked.
- For non-linear systems a suitable two-fold closure (moment and time closure) closure was introduced in Athanassoulis et al. [2013], Tsantili [2014], Athanassoulis et al. [2015],.
- For a mono-stable scalar system, the moment closure was obtained by applying the standard Gaussian closure to the two-time RE moments. For a bi-stable cubic non-linear half oscillator a bi-Gaussian moment closure scheme was discussed in [Tsantili, 2014]. The time closure was achieved by using an exact non-local (in time) condition for the one-time moments. Athanassoulis et al. [2013], Tsantili [2014], Athanassoulis et al. [2015]
- A moment-equation-copula-closure method for non linear vibrational systems subjected to correlated noise was introduced in Joo and Sapsis [2016]

Maximum Likelihood of discrete observations

Let us denote a random process $X(t) = x(t;\omega)$ and consider the RDE :

$$\dot{X}(\, t\,) = K\, \Big(X(t),\ Y(t, \theta^{(2)}); \theta^{(\mathbf{1})}\Big)$$

$$\dot{X}(\,0\,;\ \,) = X_0, \quad t > 0, \quad \omega \in \Omega$$

- Let us assume a parametric K with parameters $\theta^{(1)}$ and let $\theta^{(2)}$ be the parameters of the random excitation. We assume that $\phi = \{\theta^{(1)}, \theta^{(2)}\}$ lay on the parametric space Φ.
- Given a discrete sample set $\mathbf{d}_N = \{d_i = X(t_i)\}_{i=1}^{N}$ associated to the process $X(t)$ we can infer the model parameters ϕ by maximizing the (exact) likelihood function

$$L(\theta; \mathbf{d_N}) = p(\mathbf{d}_N; \phi)\,,$$

where $p(X(t_1), \ldots, X(t_N); \phi)$ denotes the finite-dimensional joint density of the sample $X(t_1), \ldots, X(t_N)$.

MLE RE Gaussian approximation

- If we consider a Gaussian approximation $G(t)$ of the original process $X(t)$. The exact likelihood function is approximated by the likelihood function that corresponds to a multivariate Gaussian density.
- Within this approximation we consider the following observation equation to incorporate the measurement error

$$\mathbf{D}(t) = \mathbf{G}(t) + \epsilon(t)\, t > 0.$$

- Given the observed data the corresponding likelihood function is

$$L(\phi|\mathbf{d_N}) = (\mathbf{2}\pi)^{-\mathbf{N}/2} |\mathbf{\Sigma}(\phi)|^{-1/2} \exp\left[-(\mathbf{1}/\mathbf{2})(\mathbf{d} - \mu(\phi))^{\mathbf{T}} [\mathbf{\Sigma}(\phi)]^{-\mathbf{1}} (\mathbf{d} - \mu(\phi))\right],$$

where $\mu(\phi) = (\mathbf{m(t_1)}, \ldots, \mathbf{m(t_N)})$, $\mathbf{\Sigma}(\phi) = \mathbf{V}(\phi) + \mathbf{\Sigma}^{\epsilon}$ and $\mathbf{V}(\phi)$ is the variance-covariance matrix with elements :

$$[\mathbf{V}]_{kl} \;=\; v(t_k, t_l) \;=\; R_{xx}(t_k, t_l) \;-\; m_x(t)\, m_x(s), \quad k, l \;=\; 1, \ldots N$$

  - The elements are obtained by the solution of two time RE moment that incorporate all the history of the excitation.
  - The system parameters and the correlation structure of the response appear in the Likelihood function.

MLE 2D RE Gaussian approximation

Given observed data $d^{(1)} = \{X_{1:N}\} = \{X_1, \dots, X_N\}$ for the response, and $d^{(2)} = \{Y_{1:N}\} = \{Y_1, \dots, Y_N\}$ for the excitation we are given the choice to consider the two-dimensional process $\Psi = [X(t) \;\; Y(t)]^{tr}$ with mean

$$\mu(\phi) = \mathbf{E}\left[\Psi\right] = \left[\mu_X(t) \;\; \mu_Y(t)\right]^{tr},$$

and covariance

$$\boldsymbol{\Sigma}(\phi) = \mathbf{E}\left[(\mathbf{X}(t) - \mu_X(t)) \otimes (\mathbf{Y}(s) - \mu_Y(s))\right] = \begin{bmatrix} v_{XX}(t,s) & v_{XY}(t,s) \\ v_{XY}(t,s) & v_{YY}(t,s) \end{bmatrix}.$$

Given the observed data the Likelihood will be given by:

$$L_c(\phi|\mathbf{d}^{(1)}, \mathbf{d}^{(2)}) = \frac{1}{(2\pi)^{2N}|\mathbf{V}_N|} \exp\left\{-\frac{1}{2}\left(\Psi_{1:N} - \mu_N\right)^{tr} \mathbf{V}_N^{-1} \left(\Psi_{1:N} - \mu_N\right)\right\}$$

where $\mu_{\mathbf{N}} = \mu_{\mathbf{N}}(\phi)$ is the vector with $2N$ elements

$$\mu_N = \left[\mu^{tr}(t_1) \;\; \dots \;\; \mu^{tr}(t_N)\right]^{tr}$$

and $\mathbf{V}_N = \mathbf{V}_N(\phi)$ is a $2N \times 2N$ matrix with block-elements

$$\boldsymbol{\Sigma}(t_i, t_j) = \begin{bmatrix} v_{XX}(t_i,t_j) & v_{XY}(t_i,t_j) \\ v_{XY}(t_i,t_j) & v_{YY}(t_i,t_j) \end{bmatrix}, \quad i,j = 1, \dots, N.$$

Benchmarks in steady state

- In what follows we shall consider the long-time, statistical equilibrium limit of the system and infer the system parameter there for some benchmark examples.
- We obtain sample paths of the excitation $y(t, \omega)$ considering the K-L expansion [Tsantili and Hristopulos, 2016] of its covariance $C_{yy}(t, s)$, then we solve the linear scalar RDE:

$$\dot{x}(t\,;\,\omega) \;=\; -A \cdot x(t\,;\omega) + B \cdot y(t\,;\,\omega)$$

- To learn the model parameters we estimate the variance-covariance matrix of the Gaussian likelihood function from the long-time limits of analytical solutions [Tsantili, 2014] of the two-time RE moment equations.

Benchmarks in steady state - OU process

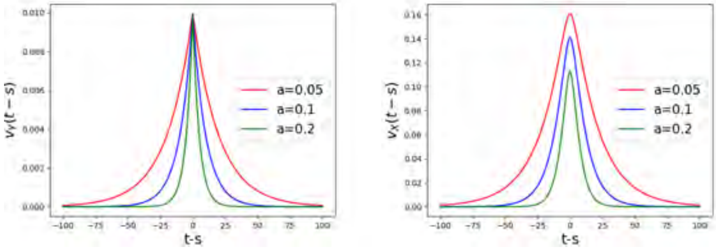

Figure: a. Covariance of the OU process for different values of the correlation length $t_{corr} = 1/\alpha$. b. Long-time stationary response of the linear system for $(A, B, \sigma) = (0.3, 1.3, 0.1)$

The long time response correlation (here for $m_y = 0, C_{xx}(t,s) = R_{xx}(t,s)$) of a linear system excited by an OU process

$$C_{xx}^{(\infty)}(t,s) = \frac{B^2 \cdot \sigma^2}{(\alpha - A)^2 \cdot (A+\alpha)^2} \times (-e^{A\cdot|t-s|} \frac{\alpha \cdot (\alpha^2 - A^2)}{A}) + e^{-\alpha|t-s|} (-\alpha^2 + A^2))$$

Benchmarks in steady state -OU process

Parameter	A	B	α
Exact values	0.3	1.3	0.1
OU Excitation	0.297	1.26	0.108
95% CI	[0.276, 0.32]	[1.206, 1.321]	[0.099, 0.117]

Table: Approximation of the a linear system with OU excitation, using the Gaussian MLE and solving the two-time moment equations. The confidence intervals (CI) for the obtained parameters are also denoted. Results from 100 paths of 100 data points of observation each.

Benchmarks in the steady state - Shifted OU process

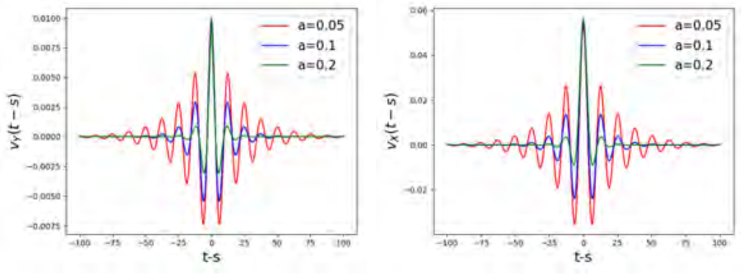

Figure: a. Covariance for the shifted OU process excitation for different values of α and $\omega_0 = 0.5$.b. Long-time stationary response of the linear system for $(A, B, \omega_0, \sigma) = (0.3, 1.3, 0.5, 0.1)$.

$$C_{xx}^{(\infty)}(t,s) = \frac{B^2 \cdot \sigma^2}{\left((\alpha - A)^2 + \omega_0^2\right) \cdot \left((A+\alpha)^2 + \omega_0^2\right)} \times$$

$$\left[-e^{A \cdot |t-s|} \frac{\alpha \cdot \left((\alpha^2 - A^2) + \omega_0^2\right)}{A} + e^{-\alpha \cdot |t-s|} \times\right.$$

$$\left.\left[\left(-(\alpha^2 - A^2) + (\omega_0)^2\right) \cdot \cos\left(\omega_0 \cdot |t-s|\right) + 2 \cdot \alpha \cdot \omega_0 \cdot \sin\left(\omega_0 \cdot |t-s|\right)\right]\right].$$

Benchmarks in the steady state - Shifted OU process

Parameter	A	B	α	ω_0
Exact values	0.3	1.3	0.1	0.5
OU Excitation	0.3003	1.3886	0.0985	0.50144
95% CI	[0.279, 0.322]	[1.284, 1.374]	[0.092, 0.106]	[0.493, 0.510]

Table: Approximation of the linear system for shifted OU excitaion with $(A, B, \alpha, \sigma, \omega_0) = (0.3, 1.3, 0.1, 0.1, 0.5)$ using the Gaussian MLE and solving the two-time moment equations . The confidence intervals (CI) for the obtained parameters are also denoted. Results from 100 paths of 100 data points of observation each.

Benchmarks in the steady state - Low Pass Gaussian Filter

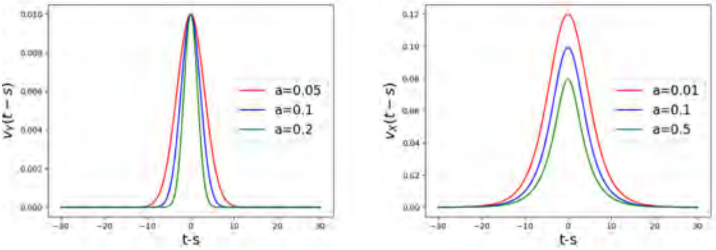

Figure: a. Covariance of the lpGF process for different values of the parameter α and for $\omega = 0.5$. b. Long-time stationary response of the linear system for $(A, B, \alpha, \sigma) = (0.3, 1.3, 1, 0.1)$.

$$
\begin{aligned}
C_{xx}^{(\infty)}(t-s) &= \\
&= \frac{\sqrt{\pi}}{4\sqrt{a}} \cdot \frac{B^2 \cdot \sigma^2}{(-A)} \cdot e^{\frac{A^2}{4 \cdot \alpha}} \times \left(e^{A \cdot (s-t)} \cdot \left(erf\left(\sqrt{\alpha} \cdot (s-t) + \frac{A}{2 \cdot \sqrt{\alpha}} \right) + 1 \right) + \right. \\
&+ \quad \left. e^{A \cdot (t-s)} \left(erf\left(\sqrt{\alpha} \cdot (t-s) + \frac{A}{2 \cdot \sqrt{a}} \right) + 1 \right) \right)
\end{aligned}
$$

Benchmarks in the steady state - Low Pass Gaussian Filter

Parameter	A	B	α
Exact values	0.3	1.3	1
OU Excitation	0.301	1.335	0.98
95% CI	[0.2802, 0.322]	[1.307, 1.364]	[0.938, 1.0194]

Table: Approximation of a low pass Gaussian Filter excitation with $(A, B, \alpha, \sigma) = (0.3, 1.3, 1, 0.1)$ using the Gaussian MLE and solving the two-time moment equations . The confidence intervals (CI) for the obtained parameters are also denoted. Results from 100 paths of 100 data points of observation each.

Generalized Langevin Equation (GLE)

Let us now consider the GLE describing the movement of one particle in a box

$$\begin{cases} dQ_t = P_t dt, \\ \frac{dP_t}{dt} = -\alpha_1 Q_t - [\eta^2 \int_0^t \exp\left(\frac{t-s}{\tau}\right) P_s ds] + F_t^{rn}, \quad t > 0, \\ Q_{t=0} = q_0, P_{t=0} = p_0, \end{cases}$$

where the auto-correlation of the random force F^{rn} is given by

$$R_{F^{rn}}(t-s) = \beta^{-1} \eta^2 \exp\left(\frac{t-s}{\tau}\right), \quad t > s.$$

- We use the extended dynamics of the GLE to obtain approximate sample paths $\bar{Q}_t, \bar{P}_t$ of Q_t, P_t .

Time-dependent potential for the transient -time dynamics

From the obtained data we infer the parameters of a (Markovian) Langevin equation with a time-dependent potential and a white noise excitation [Baxevani et al.]:

$$\begin{cases} d\tilde{Q}_t = \tilde{P}_t dt \\ d\tilde{P}_t = -D(t;\theta_{(1)})\, B(\tilde{Q}_t,\theta_{(2)})dt - \gamma \tilde{P}_t dt + \sigma dW_t, \quad t > 0, \\ \tilde{Q}_{t=0} = p_0 \quad \tilde{P}_{t=0} = p_0 \,. \end{cases}$$

Let us denote the total force of the GLE as

$$F_{tot}(Q_t) = -\alpha_1 Q_t - [\eta^2 \int_0^t \exp\big(\frac{t-s}{\tau}\big) P_s ds] + F_t^{rn},$$

and let

$$F_{CG}(Q,t;\phi) = -D(t;\theta^{(1)})\, B(Q_t,\theta^{(2)})\,.$$

To estimate the parameters $\phi = \{\theta^{(1)}, \theta^{(2)}\}$ we solve the Force Matching problem given by

$$argmin_\phi \frac{1}{n_t}\frac{1}{n_p}\sum_{n=1}^{n_p}\sum_{i=1}^{n_t} |F_{tot}(Q_{t_i},P_{t_i},t_i) - F_{CG}(Q_{t_i},t_i,\phi)|^2\,,$$

Transient time mean values

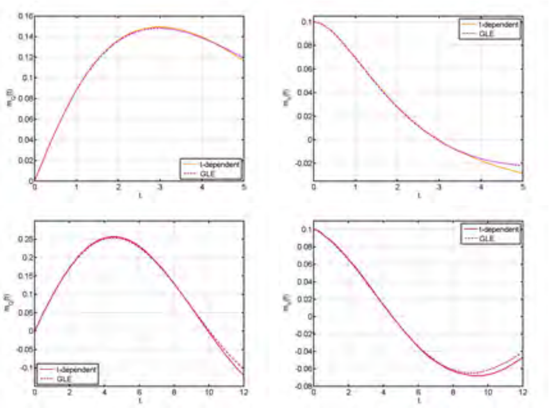

Figure: Comparison of the (sample) mean values of Q_t and P_t of the GLE with the sample mean values $\tilde{Q}_t, \tilde{P}_t$ of the Langevin Equation with time-dependent potential(for $n_p = 2000$ paths and $n_t = 100$ data points). We consider two different correlation times of F^{rn}, i.e. for $\tau = 0.5$ (upper panel) and $\tau = 0.1$ (lower panel). The other parameters are $\alpha = 0.1, \eta = 1, \beta = 1000,\ q_0 = 0,\ p_0 = 0.1$.

Transient time variances

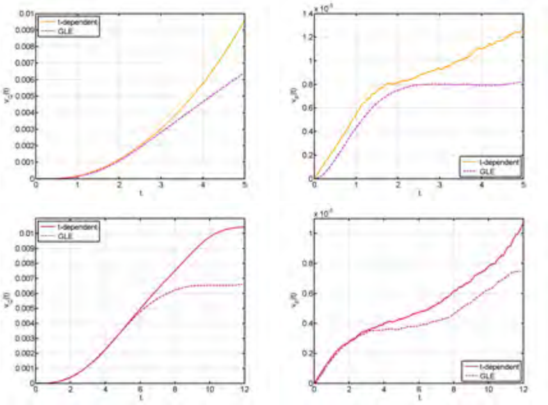

Figure: Same as in Figure 6 for the variances. A longer interval of the transient state of the GLE system dynamics is well approximated by the Langevin equation for smaller correlation time.

Overdamped GLE

- We propose to model the overdamped equation governing the evolution of Q using a RDE with colored noise excitation.
- Given the data for Q obtained by the GLE we will learn the parameters of a linear RDE with colored noise excitation Y_t

$$\begin{cases} d\hat{Q}_t = -A\,\hat{Q}_t dt + B\,Y_t \\ \hat{Q}_{t=0} = q_0 \end{cases}$$

- We consider the long-time limit where the system has reached the steady state.
- We learn the system parameters and the parameters of the colored noise using the MLE RE Gaussian approximation.

RE Inference of the overdamped GLE

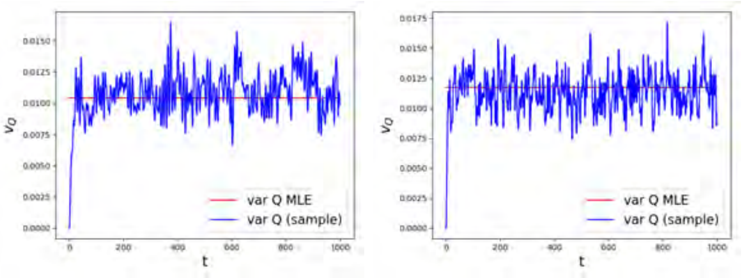

Figure: a. Comparison of the variance of Q(t) for $\tau = 0.1$ (left) and $\tau = 0.5$ (right) with the long time variance of $\hat{Q}$ obtained by the the MLE RE Gaussian Approximation. The parameter of the linear model for $\hat{Q}_t$ and of the shifted OU process Y_t are $(A, B, \alpha, \omega_0, \sigma) = (0.21, 0.361, 0.05, 0.34, 0.12)$ and $(A, B, \alpha, \omega_0, \sigma) = (0.241, 0.509, 0.406, 0.402, 0.1)$, all the parameters were learned from 100 paths of 100 data points of observation each obtained by the GLE.

Summary and directions for future work

- We presented a MLE Gaussian approximation scheme that uses the two-time response excitation moments of colored RDEs.
- We presented some benchmark examples for linear systems and different correlations of the excitation for which analytic solutions of the two-time moment system exist.
- We discussed a model that approximates the GLE with a Langevin equation having a time-dependent potential instead.
- We discussed a model that could use instead a colored noise linear RDE to model the overdamped limit of the position Q.
- We shall use the MLE RE Gaussian approximation scheme to infer the parameters of non-Markovian systems in the transient state.
- For non-linear RDEs, some closure parameters could be learned by data during the solution of the MLE RE Gaussian approximation scheme.

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Thank you!

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