Identification of Order Parameters and invariant Manifolds for Stochastic Systems from Data

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Abstract

The slaving principle allows for a dramatic reduction of the degrees of freedom of complex systems close to instabilities [1, 2]. The macroscopic behavior is then governed by a low number of collective modes, whose amplitudes are called order parameters. An up to now unsolved problem is the identification of order parameters for stochastic systems from data. We present two promising approaches on how to tackle this problem.

The Slaving Principle

Any system of Langevin equations

$$\dot{q}_i = f_i(\{q_j\}) + \xi_i(t)\,, \quad i = 1,\ldots,m$$

can be transformed into

$$\begin{aligned}\dot{\boldsymbol{u}}(t) &= \boldsymbol{\Lambda}_u \boldsymbol{u}(t) + \boldsymbol{N}_u(\boldsymbol{u}(t),\boldsymbol{s}(t)) + \boldsymbol{\xi}_u(t)\\ \dot{\boldsymbol{s}}(t) &= \boldsymbol{\Lambda}_s \boldsymbol{s}(t) + \boldsymbol{N}_s(\boldsymbol{u}(t),\boldsymbol{s}(t)) + \boldsymbol{\xi}_s(t)\\ \boldsymbol{\Lambda}_u &= \mathrm{diag}(\lambda_1,\ldots,\lambda_\ell)\\ \boldsymbol{\Lambda}_s &= \mathrm{diag}(\lambda_{\ell+1},\ldots,\lambda_m)\,,\end{aligned}$$

where

$$\mathrm{Re}\{\lambda_1\},\ldots,\mathrm{Re}\{\lambda_\ell\} > 0 \geq \mathrm{Re}\{\lambda_{\ell+1}\},\ldots,\mathrm{Re}\{\lambda_m\}\,.$$

Close to instabilities, due to separation of time scales, the slaving principle [1, 2] allows to express the stable mode amplitudes s_i as explicit functions of the order parameters u_j:

$$s_i = h_i[\{u_j\}, t]$$

⇒ Closed set of order parameter equations:

$$\dot{\boldsymbol{u}} = \boldsymbol{\Lambda}_u \boldsymbol{u} + \boldsymbol{N}_u(\boldsymbol{u},\boldsymbol{s}(\boldsymbol{u})) + \tilde{\boldsymbol{\xi}}_u(t) \qquad (1)$$

Consequence for stationary jpdf (cf. [3]):

$$\begin{aligned}p(\boldsymbol{u},\boldsymbol{s}) &= p(\boldsymbol{s}|\boldsymbol{u})f(\boldsymbol{u})\\ p(\boldsymbol{s}|\boldsymbol{u}) &= \prod_{i=\ell+1}^{m} p(s_i|\boldsymbol{u})\\ p(s_i|\boldsymbol{u}) &= N\exp\left\{-(s_i - h_i[\{u_j\}])^2/Q\right\}\end{aligned}$$

The Problem

Let $\boldsymbol{q}(t)$ be a time series of m components assumed to be governed by an unknown system of Langevin equations. Order parameters are assumed to be obtained by the linear transformation

$$u_i = \sum_{j=1}^{m} = \alpha_{ij} q_j\,.$$

- find a numerical algorithm that extracts the coefficients α_{ij} from the given time series
- find manifolds $s_i = h_i[\{u_j\}]$
- estimate order parameter dynamics (1)

Test System: Haken-Zwanzig

As a test system for algorithms we start with the simple Haken-Zwanzig system with one order parameter and one enslaved mode amplitude [1, 2]:

$$\begin{aligned}\dot{u} &= \epsilon u - us + \xi_u(t) &(2a)\\ \dot{s} &= -\gamma s + u^2 + \xi_s(t) &(2b)\\ &\epsilon,\gamma > 0\,,\ \epsilon \ll \gamma\end{aligned}$$

- two stable nodes $(\pm\sqrt{\gamma\epsilon}, \epsilon)$
- one saddle point $(0, 0)$
- invariant manifold $s(u) = (1/\gamma)u^2 + \mathcal{O}(u^4)$

The drift method

Enslaved mode amplitude s is faster than order parameter u. Hence, the corresponding drift coefficients obey

$$\left\langle \left|D_u^{(1)}\right|\right\rangle \ll \left\langle \left|D_s^{(1)}\right|\right\rangle\,.$$

- estimate drift vector field from time series (s. [4] for a description of the method)
- search for projection direction with minimal, respectively maximal, absolute value of the drift, averaged over the phase space

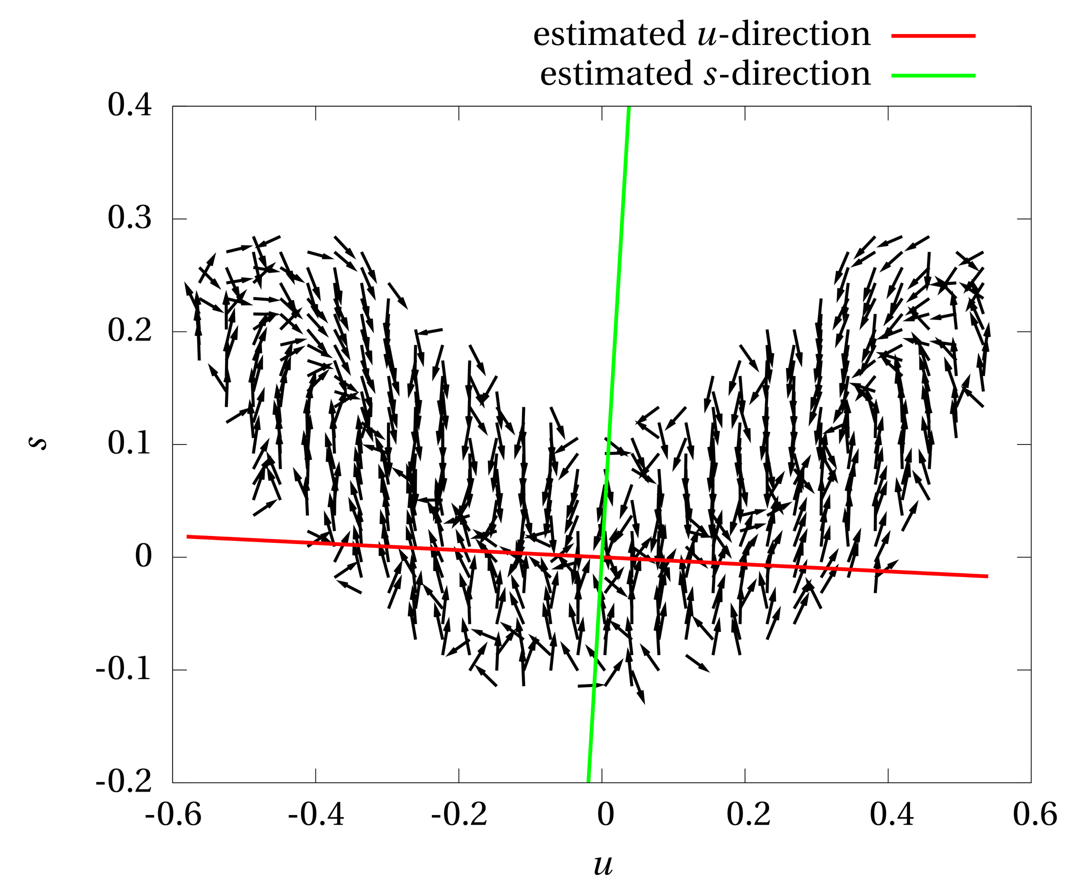

Figure 1: Estimated u- and s-direction obtained by the drift method. The arrows show the estimated drift vector field. Each vector is set to unit length.

The method of information

Information entropy of a stochastic process $X(t)$ (cf. [3]):

$$i(X) = -\int p_X(x)\ln p_X(x)\mathrm{d}x$$

- assumption: $i(u) > i(s)$
- therefore, under the constraint $\alpha_1^2 + \alpha_2^2 = 1$:

$$i(\alpha_1 u + \alpha_2 s) = \begin{cases}\text{maximal for} & (\alpha_1,\alpha_2) = (1,0)\\ \text{minimal for} & (\alpha_1,\alpha_2) = (0,1)\end{cases}$$

- maximize information with respect to $\boldsymbol{\alpha}$ ⇒ u-direction
- minimize information with respect to $\boldsymbol{\alpha}$ ⇒ s-direction

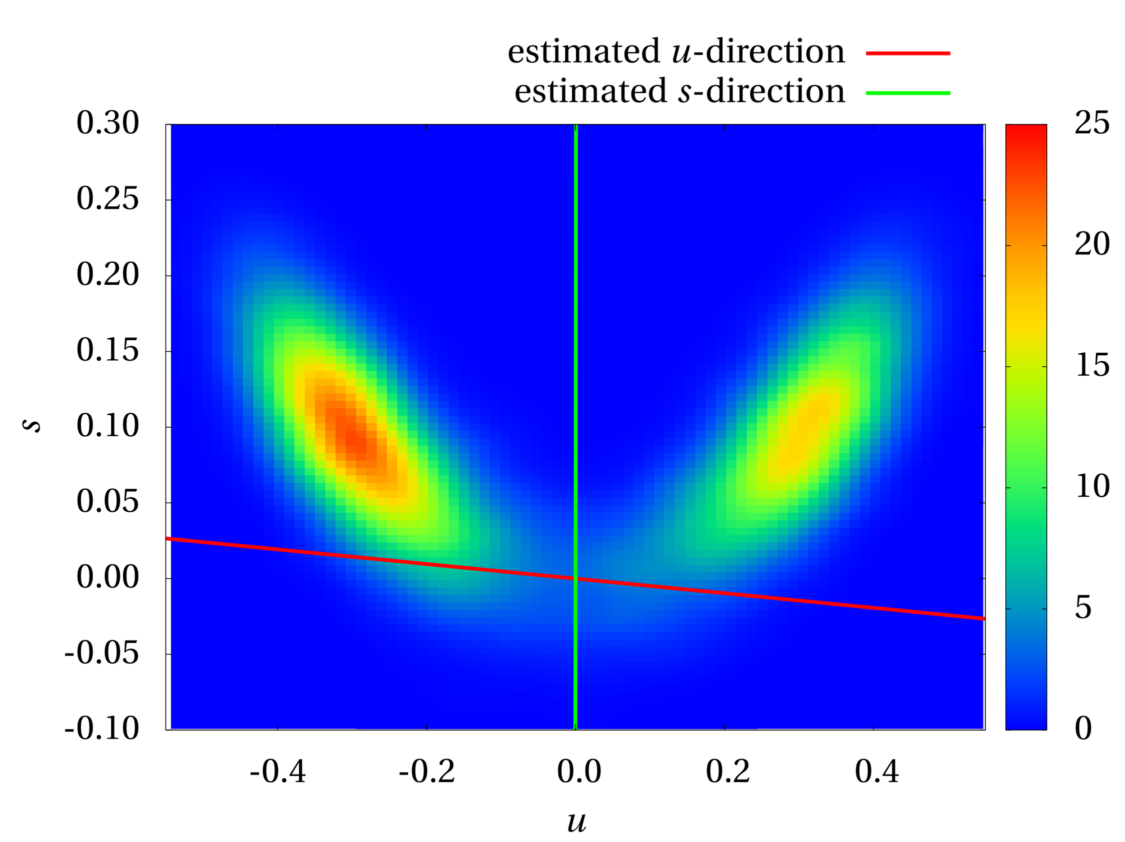

Figure 2: Estimated u- and s-directions obtained by the method of maximizing, respectively minimizing, the information entropy. The figure shows color-coded the jpdf $p(u, s)$. The red line corresponds to the estimated u-direction, the green one to the estimated s-direction. Note that the symmetry is broken because of the finite size of the data set.

Estimation of order parameter dynamics

Order parameter dynamics:

$$\begin{aligned}\dot{u} &= D^{(1)}(u) + \sqrt{2D^{(2)}(u)}\Gamma(t)\\ \langle\Gamma(t)\Gamma(t')\rangle &= \delta(t-t')\end{aligned}$$

Kramers-Moyal coefficients:

$$D^{(n)}(x) = \frac{1}{n!}\lim_{\tau\to 0}\frac{1}{\tau}\left\langle [X(t+\tau) - X(t)]^n\right\rangle\Big|_{X(t)=x} \qquad (3)$$

According to the slaving principle in lowest order approximation:

$$D^{(1)}(u) = \epsilon u - \frac{1}{\gamma}u^3 \qquad (4)$$

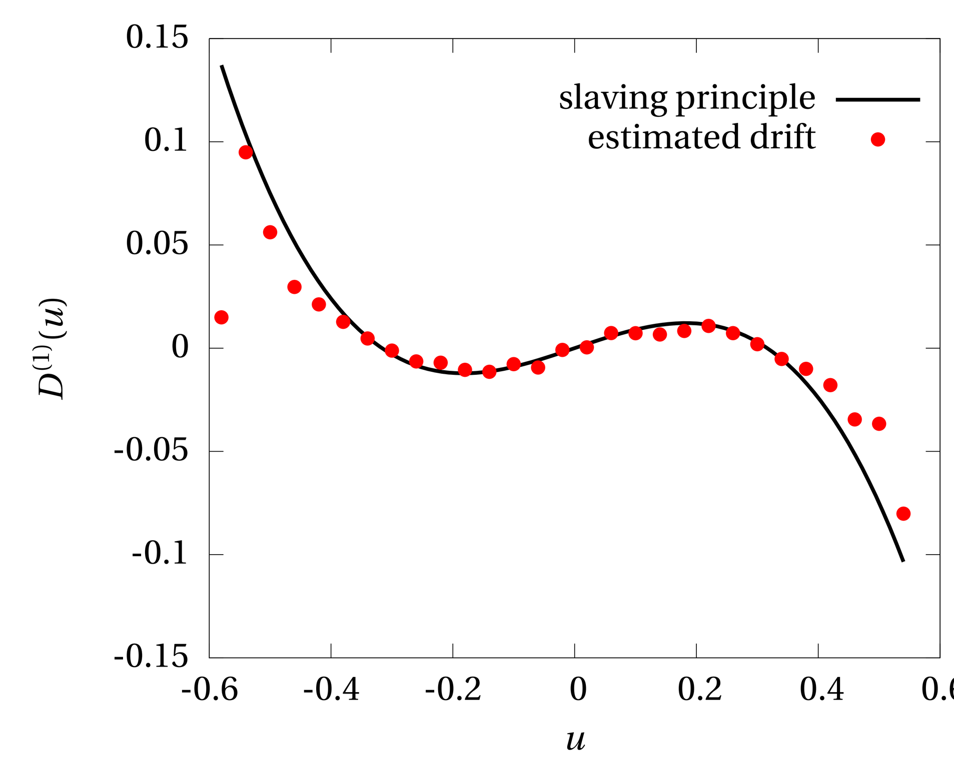

Figure 3: The drift coefficient for the order parameter. The red dots are the result of numerically evaluating Eq. (3) for $n = 1$ with a method described in [4]. The black curve corresponds to the expected result according to the slaving principle, Eq. (4).

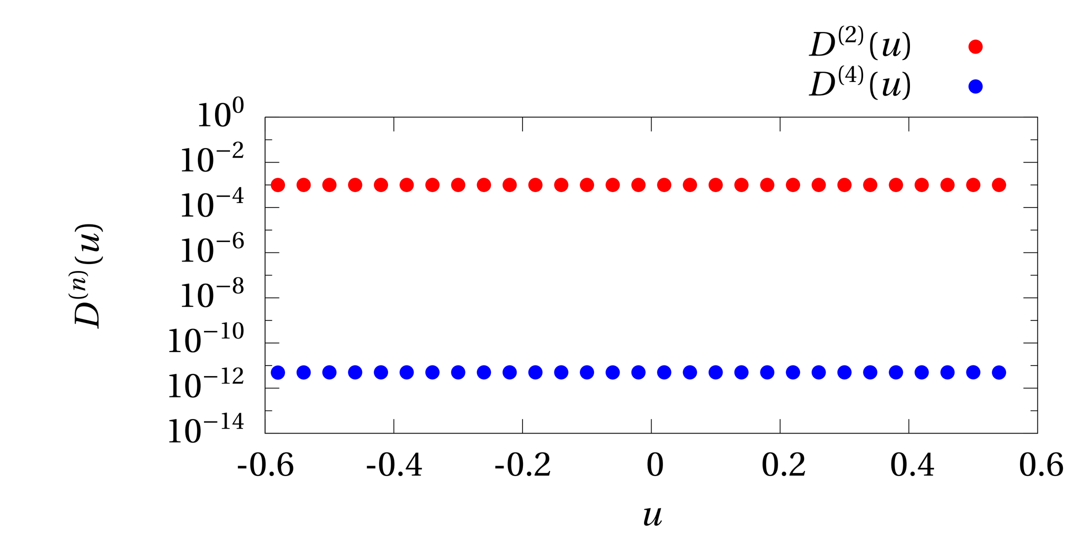

Figure 4: Second and fourth Kramers-Moyal coefficient for the order parameter obtained by numerically evaluating Eq. (3) with a method described in [4]. Obviously $D^{(4)}$ is practically zero, so according to the Pawula theorem all coefficients $D^{(n)}$ with $n \geq 3$ vanish too.

Conclusion & References

- The drift vector field and the information entropy seem to be promising quantities to identify order parameters.
- Order parameter dynamics can be described by effective Langevin dynamics.
- Methods have to be tested for higher dimensional systems.

References

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