Implicit equation-free methods applied on noisy slow-fast systems

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Slow-fast systems

- systems with
  - many degrees of freedom
  - dynamics on multiple scales
- e. g. molecular dynamics, neural networks, traffic flows, ...
- assumption: there exists an attractive slow manifold
  - evolution in long terms is on slow manifold
  - massive reduction of dimensions is possible

Analysis of macroscopic dynamics

Given

- equations on a microscopic scale
- too complex or non-existing macroscopic equations

Goal

analyze macroscopic dynamics:

- equilibria
- stability
- ...

Reminder: stability of dynamical systems

Dynamical system

$$f(x(t)) = \dot{x}(t), \quad x \in \mathbb{R}^d, t \in \mathbb{R}$$

Equilibrium

x^* is an equilibrium if and only if $f(x^*) = 0$.

Stability

Let $Jf(x^*)$ be the Jacobian of f at the equilibrium x^*.
If all real parts of the eigenvalues of $Jf(x^*)$ are < 0, then x^* is **asymptotically stable**.
If the real part of an eigenvalue of $Jf(x^*)$ is > 0, then x^* is **unstable**.

Reminder II: bifurcation of a dynamical system

Dynamical system

$$f(\mu, x(t)) = \dot{x}(t), \quad x \in \mathbb{R}^d, \; \mu \in \mathbb{R}$$

Bifurcation point

Let (μ^*, x^*) be an equilibrium of f, i. e. $f(\mu^*, x^*) = 0$.
If the real part of one eigenvalue is 0, then (μ^*, x^*) is a **bifurcation point**.

Explicit equation-free scheme

I.G. Kevrekidis, C.W. Gear, J.M. Hyman, P.G. Kevrekidis, O. Runborg & C. Theodoropoulos (2003) *Commun. Math. Sci.* **1**(4)

Given

Microscopic equations
$\dot{u}(t) = f(u(t)),\ u \in \mathbb{R}^D,\ f : \mathbb{R}^D \to \mathbb{R}^D$
with microscopic time-stepper

$$M(t; u(t_0)) = u(t_0 + t)$$

Unknown

Macroscopic dynamics, $d \ll D$,
$\dot{x}(t) = F(x(t)),\ x \in \mathbb{R}^d,\ F : \mathbb{R}^d \to \mathbb{R}^d$
with macroscopic time-stepper

$$\Phi(t; x(t_0)) = x(t_0 + t)$$

Construct operators

$$\begin{array}{rll} \text{Lifting operator} & \mathcal{L} : \mathbb{R}^d \to \mathbb{R}^D, & x(t) \mapsto \mathcal{L}(x(t)) = u(t) \\ \text{Restriction operator} & \mathcal{R} : \mathbb{R}^D \to \mathbb{R}^d, & u(t) \mapsto \mathcal{R}(u(t)) = x(t) \end{array}$$

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Macroscopic time-stepper

C. Marschler, J. Sieber, R. Berkemer, A. Kawamoto & J. Starke (2014) *SIAM J. Appl. Dyn. Sys.* **13**(3)

- actually computing dynamics **off** the slow manifold C
- interesting macroscopic dynamics **on** C

Macroscopic time-stepper

$$\Phi(t; y) = \mathcal{R}(M(t; \mathcal{L}(y)))$$

The normalform example

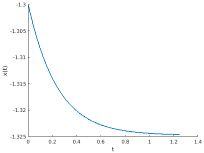
Microscopic equation

Microscopic equation

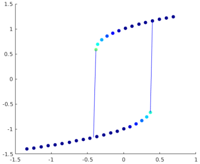
$$f(\mu, x(t)) = \dot{x}(t) = \mu - x + x^3$$

Search

equilibria x^*, i. e. $f(x^*) = 0$, and their stability for each μ without any knowledge about microscopic behaviour



Time series for $\mu = -1$ and $x(t_0) = -1.3$.



Stable equilibria by direct simulation

What and where is the olfactory bulb?

- neural structure of the vertebrale forebrain
- relatively easy to access for imaging methods
- is responsible for odor recognition
- clear input and output
- its neural network can be seen as a model for the whole brain

The Spike and Response Model (SRM)

C. Fohlmeister, W. Gerstner, R. Ritz & J.L. van Hemmen (1995)
Neural Computation **7** (5)

- a spike width has the length Δt
- a cell i fires at time $t + \Delta t$ if the membrane potential h_i reaches a certain threshold θ:

$$S_i(t + \Delta t) = \begin{cases} 1, & \text{if } h_i(t) \geq \theta, \ \frac{dh_i(t)}{dt} > 0 \\ 0, & \text{else} \end{cases},$$

- membrane potential consists of four different components:

$$h_i(t) = h_i^{syn}(t) + h_i^{s-inh}(t) + h_i^{ref}(t) + h_i^{ext}(t)$$

The membrane potential

C. R. Ellsässer. *Simulations of a Neuron Network Model in the Olfactory System* (2008)

$$h_i(t) = h_i^{syn}(t) + h_i^{s-inh}(t) + h_i^{ref}(t) + h_i^{ext}(t)$$

The components are:

- synaptic input:

$$h_i^{syn}(t) = \sum_{j=1}^{N} J_{ij} \sum_{\tau=0}^{\infty} \epsilon(\tau) S_j\left(t - \tau - \Delta_{ij}^{den}\right), \quad \text{with } \epsilon(\tau) = \frac{\tau}{\tau_\epsilon^2} \exp\left(-\frac{\tau}{\tau_\epsilon}\right),$$

- self-inhibitory input:

$$h_i^{s-inh}(t) = \sum_{\tau=0}^{\infty} \eta(\tau) S_i\left(t - \tau - \Delta_i^{s-inh}\right), \quad \text{with } \eta(\tau) = \eta_{inh} \exp\left(-\frac{\tau}{\tau_\eta}\right),$$

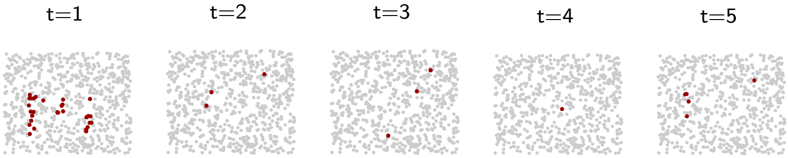
- refractoriness of the neuron $h_i^{ref}(t) = -R, R \gg 1$, if $t_i^f \leq t \leq t_i^f + \tau_{ref}$, and
- external input $h_i^{ext}(t)$

The cells in the neural network

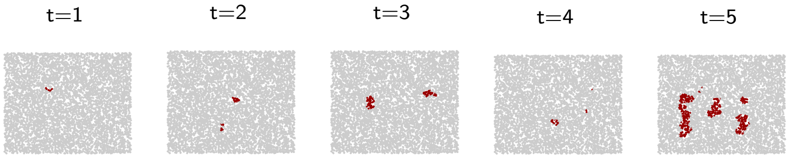
- mitral and granular cells have reciprocal connectivity
- mitral cells excite granular cells, granular cells inhibit the activities of mitral cells
- coupling J_{ij} depends on the distance d_{ij} between the cells i and j:

$$J_{ij} = \begin{cases} J_{exc} & \text{, for MC } i \text{ and GC } j, \quad d_{ij} < r_{exc} \\ -J_{inh} \exp\left(\frac{-10 d_{ij}}{r_{inh}}\right) & \text{, for GC } i \text{ and MC } j, \quad d_{ij} < r_{exc} \\ 0 & \text{, otherwise.} \end{cases}$$

Time delay of the synaptic input



Mitral cells



Granular cells

Macro-variable: the fire rate difference

- consider the case of two different odors
- interested in the macroscopic variable $\Delta_s = F_1 - F_2$, the difference between the fire rates F_1 and F_2
- it holds for the concentrations $c_1 + c_2 = 1$

What happens if we change the odor concentrations?

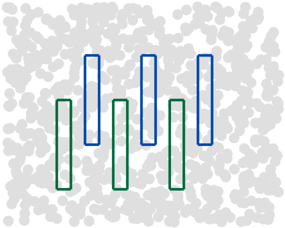
- direct simulation of interaction between single cells is the microscopic time-stepper
- Restriction operator is taking the average over e. g. 1000 time steps of both centres

Natural anatomy for two different odors

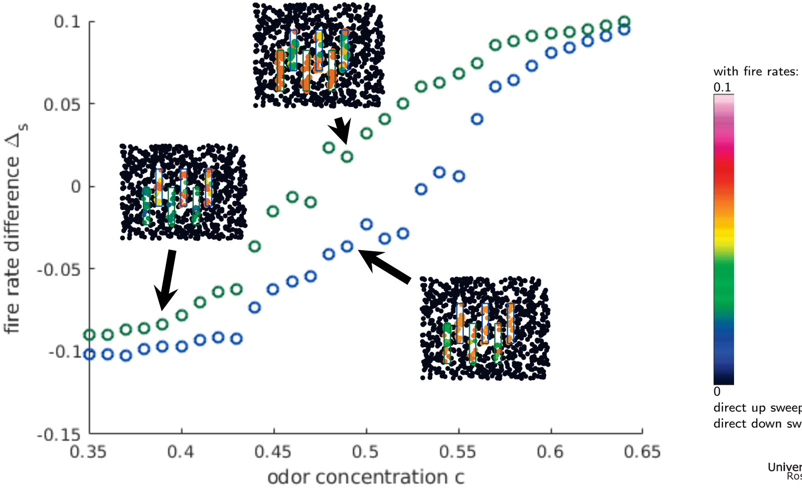
figures adapted to N.M. Abraham, H. Spors, A. Carleton, T. W. Margrie, T. Kuner & A.T. Schaefer (2004) *Neuron*, **44** (5)

Academic implementation

- no overlay of areas due to 2D-picture of a 3D-network
- both areas have exactly the same size
- cells uniformly distributed to avoid artificial effects
- two “layers” for mitral and granular cells with no physical distance

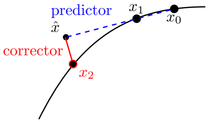


Hysteresis of neural network



direct up sweep: o,
direct down sweep: o

Pseudo-arclength continuation



E. Doedel, H.B. Keller & J.-P. Kernévez (1991) *International Journal of Bifurcation and Chaos*, **1** (3)

Goal

Find next macroscopic equilibrium x_2, i. e. $F(x_2) = 0$.

Pseudo-arclength continuation

Fulfill two conditions:

- predictor:

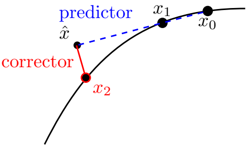
$$\hat{x} = x_1 + s \cdot \frac{w}{\|w\|}\,, \quad \text{with } w = (x_1^{(1)} - x_0^{(1)}, x_1^{(2)} - x_0^{(2)})$$

- corrector:

$$F(x_2) = 0\,, \qquad w^{(1)}(x_2^{(1)} - \hat{x}^{(1)}) + w^{(2)}(x_2^{(2)} - \hat{x}^{(2)}) = 0$$

Can be solved with a Newton-method.

Pseudo-arclength continuation



Reminder

$$\begin{aligned}\Phi(t; x(t_0)) &= x(t_0 + t)\\ &= \mathcal{R}(M(t_{skip}; \mathcal{L}(x(t_0))))\end{aligned}$$

Task

Compute

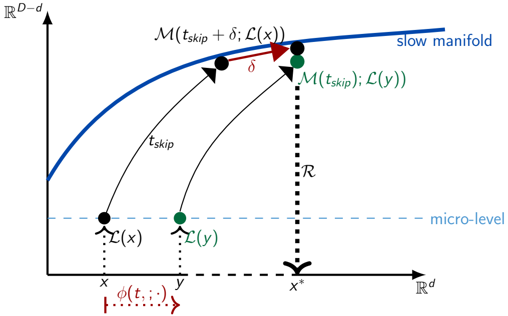
$$0 = F(\sigma) = \frac{d}{dt}\mathcal{R}(M(t_{skip}, \mathcal{L}(\sigma))) = \frac{\partial}{\partial\delta}\mathcal{R}(M(t_{skip} + \delta, \mathcal{L}(\sigma)))\Big|_{\delta=0},$$

with approximated right-hand side

$$F(\sigma) = \frac{\mathcal{R}(M(t_{skip} + \delta, \mathcal{L}(\sigma))) - \mathcal{R}(M(t_{skip}, \mathcal{L}(\sigma)))}{\delta}.$$

Implicit equation-free scheme

I. G. Kevrekidis & G. Samaey (2009) *Annual Review of Physical Chemistry* **60**



- introducing healing time t_{skip}
- consider macroscopic time-δ map $y = \Phi(\delta; x)$
- lifting error can be reduced significantly
- the state y is defined implicitely

Macroscopic time-stepper

$$\mathcal{R}(M(t_{skip};\mathcal{L}(y))) = \mathcal{R}(M(t_{skip}+\delta;\mathcal{L}(x)))$$

idea for figure: C. Marschler, J. Sieber, P. G. Hjorth, and J. Starke (2015) *Traffic and Granular Flow'13*: 423-439, *Springer*

Difficulties for chosing δ

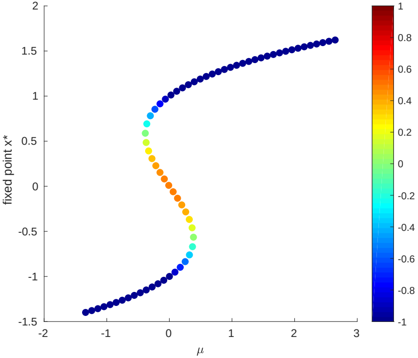
$$F(\sigma) = \frac{\mathcal{R}(M(t_{skip} + \delta, \mathcal{L}(\sigma))) - \mathcal{R}(M(t_{skip}, \mathcal{L}(\sigma)))}{\delta}$$

- if δ too small:
  - numerically not accessible
  - might catch only noise
- if δ too big:
  - already on the slow manifold or close to it
  - no information about unstable dynamics

PAC for normalform

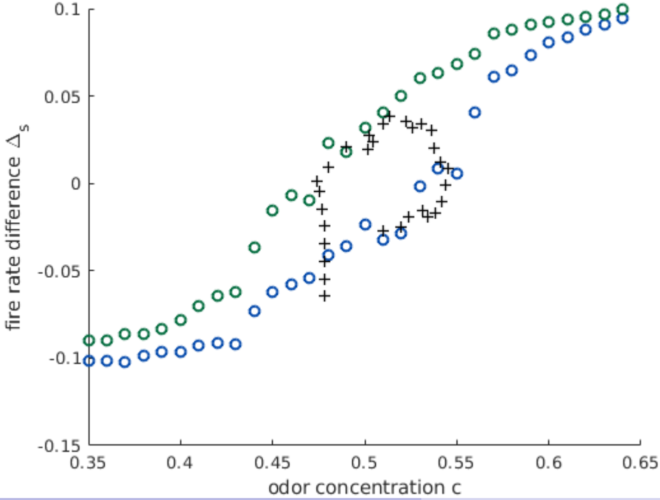
Normalform

Microscopic equation: $\dot{x}(t) = \mu - x + x^3$



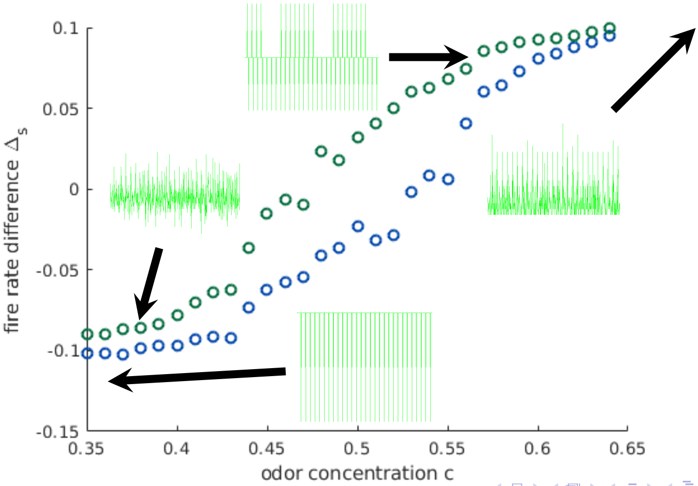
with eigenvalues of the Jacobian (here derivative) for stability information

PAC for neural network



direct up sweep: o,
direct down sweep: o,
equation-free continuation (work in progress): +

Chaotic dynamics in the neural network



PAC für Normalform with noise term

Normalform with noise

$$dX_t = (\mu - X_t + {X_t}^3)dt + \sigma dW_t$$

for the Ensemble Kalman Filter with the model

$$dX_t = \sigma dW_t \,,$$

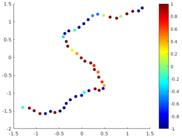
1000 ensembles, and observation model

$$dY_t = X_t + \sigma dV_t \,.$$

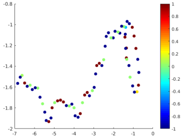
PAC für Normalform with noise term

PAC without any filtering

$\sigma^2 = 0.01$

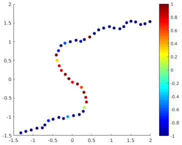


$\sigma^2 = 0.1$

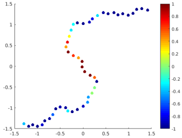


PAC with EnKF for simple model with 1000 ensembles

$\sigma^2 = 0.01$



$\sigma^2 = 0.1$



Difficulties

- computational effort for evolve operator is high (~ 0.5 seconds for one time step):
  - long time series are hard to get
  - taking the mean of many realizations is expensive
- noise is not known
- no model given
- How to chose the right time window for the derivatives?

Outlook

- noise estimation like Mehra (1970, 1972) and Bélanger (1972, 1974)
- model estimation like Berry & Sauer (2013, 2018) and Hamilton, Berry & Sauer (2016)
- automatic time window estimation for implicit equation-free method once the noise is estimated/known

Literature

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