Neural Fields, Finite-Dimensional Approximation, Large Deviations, and SDE Continuation

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Outline

Part 1: Neural Fields
(joint work with **Martin Riedler**, Linz/Vienna):

1. Neural Fields - Amari-type
2. Galerkin Approximation
3. Large Deviation Principle(s)

Part 2: SDE Continuation

1. Numerical Continuation
2. Extension to SODEs
3. Calculating Kramers' Law
4. Extension to SPDEs

Neural Fields

Amari-type neural field model:

$$\mathrm{d}U_t(x) = \left[-\alpha U_t(x) + \int_{\mathcal{B}} w(x,y) f(U_t(y))\, \mathrm{d}y\right] \mathrm{d}t + \varepsilon\, \mathrm{d}W_t(x).$$

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- $\mathcal{B} \subset \mathbb{R}^d$ bounded closed domain. Hilbert space $X = L^2(\mathcal{B})$.
- $(x,t) \in \mathcal{B} \times [0,T]$, $u = u(x,t) \in \mathbb{R}$, $\alpha > 0$, $0 < \varepsilon \ll 1$.

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- $f : \mathbb{R} \to (0, +\infty)$ gain function, modelling neural input.
- $Q : X \to X$ trace-class, non-negative symmetric operator: eigenvalues $\lambda_i^2 \in \mathbb{R}$, eigenfunctions v_i.
- $W_t(x) := \sum_{i=1}^{\infty} \lambda_i \beta_t^i v_i(x)$, β_t^i iid Brownian motions.

Existence and Regularity

Assumptions:

- $Kg(x) := \int_{\mathcal{B}} w(x,y)g(y)\,\mathrm{d}y$ is a compact self-adjoint operator on $L^2(\mathcal{B})$.
- $F(g)(x) := f(g(x))$ is a Lipschitz continuous Nemytzkii operator on $L^2(\mathcal{B})$.

Neural field as evolution equation

$$\mathrm{d}U_t = [-\alpha U_t + KF(U_t)]\,\mathrm{d}t + \varepsilon\,\mathrm{d}W_t.$$

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(daPrato-Zabczyk92) $\Rightarrow$ Mild solution $u \in C([0,T], L^2(\mathcal{B}))$

$$U_t = \mathrm{e}^{-\alpha t} U_0 + \int_0^t \mathrm{e}^{-\alpha(t-s)} KF(U_s)\, \mathrm{d}s + \varepsilon \int_0^t \mathrm{e}^{-\alpha(t-s)}\, \mathrm{d}W_s.$$

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Lemma (K./Riedler, 2013)

v_i Lipschitz with constants L_i and for some $\rho \in (0,1)$

$$\sup_{x\in\mathcal{B}} \left| \sum_{i=1}^{\infty} \lambda_i^2\, v_i(x)^2 \right| < \infty\,, \qquad \sup_{x\in\mathcal{B}} \left| \sum_{i=1}^{\infty} \lambda_i^2 L_i^{2\rho} |v_i(x)|^{2(1-\rho)} \right| < \infty$$

$\Rightarrow u \in C([0,T], C(\mathcal{B}))$.

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where

$$(KF)^i (u_t^1, u_t^2, \ldots) := \int_{\mathcal{B}} f \left(\sum_{j=1}^{\infty} u_t^j \; v_j(x) \right) \left(\int_{\mathcal{B}} w(x,y) v_i(y) dy \right) \, \mathrm{d}x$$

Approximation Accuracy

Theorem (K./Riedler, 2013)

For all $T > 0$

$$\lim_{N\to\infty} \sup_{t\in[0,T]} \|U_t - U_t^N\|_{L^2(\mathcal{B})} = 0 \quad a.s.$$

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If "regularity-lemma" conditions hold and

$$U_0 \in C(\mathcal{B}) \quad \textit{such that} \lim_{N\to\infty} \|U_0 - P^N U_0\|_{C(\mathcal{B})} = 0$$

then

$$\lim_{N\to\infty} \sup_{t\in[0,T]} \|U_t - U_t^N\|_{C(\mathcal{B})} = 0 \quad a.s.$$

Proof.

Lengthy calculation using a technique by Blömker/Jentzen (SINUM 2013). □

Large Deviations Principle (LDP)

Example: Stochastic ordinary differential equation

$$\mathrm{d}u_t = g(u_t)\,\mathrm{d}t + \varepsilon G(u_t)\,\mathrm{d}\beta_t.$$

where

- $u_t \in \mathbb{R}^N$, $g : \mathbb{R}^N \to \mathbb{R}^N$, $G : \mathbb{R}^N \to \mathbb{R}^{N\times k}$,
- $\beta_t = (\beta_t^1, \ldots, \beta_t^k)^T$ vector of k iid Brownian motions,
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Goal: Estimate first-exit time

$$\tau_{\mathcal{D}}^{\varepsilon} := \inf\{t > 0 : u_t = u_t^{\varepsilon} \notin \mathcal{D}\}.$$

An Abstract Theorem

- $\mathcal{X} := C_0([0,T],\mathbb{R}^N) = \{\phi \in C([0,T],\mathbb{R}^N) : \phi(0) = u_0\}$.
- $H_1^N := \{\phi : [0,T] \to \mathbb{R}^N : \phi$ absolutely continuous, $\phi' \in L^2$, $\phi(0) = 0\}$.
- Diffusion matrix $\mathfrak{D}(u) := G(u)^T G(u) \in \mathbb{R}^{N\times N}$ positive definite.

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Theorem (Freidlin, Wentzell)

The SODE satisfies an LDP

$$
\begin{aligned}
-\inf_{\Gamma^o} I \quad &\le \quad \liminf_{\varepsilon\to 0} \varepsilon^2 \ln \mathbb{P}((u_t^\varepsilon)_{t\in[0,T]} \in \Gamma) \le \\
&\le \quad \limsup_{\varepsilon\to 0} \varepsilon^2 \ln \mathbb{P}((u_t^\varepsilon)_{t\in[0,T]} \in \Gamma) \quad \le \quad -\inf_{\bar{\Gamma}} I.
\end{aligned}
$$

for any measurable set of paths $\Gamma \subset \mathcal{X}$ with rate function

$$
I(\phi) = \begin{cases} \frac{1}{2}\int_0^T (\phi_t' - g(\phi_t))^T \mathfrak{D}(\phi_t)^{-1} (\phi_t' - g(\phi_t))dt, & \phi \in u_0 + H_1^N, \\ +\infty & \textit{otherwise.} \end{cases}
$$

Arhennius-Eyring-**Kramers' Formula**

- Gradient structure and additive noise

$$\mathrm{d}u_t = -\nabla V(u_t)\,\mathrm{d}t + \varepsilon \mathrm{Id}\,\mathrm{d}\beta_t.$$

- V has precisely two local minima $u^*_\pm$, single saddle point u^*_s.
- Hessian $\nabla^2 V(u^*_s)$ at saddle has eigenvalues

$$\rho_1(u^*_s) < 0 < \rho_2(u^*_s) < \cdots < \rho_N(u^*_s).$$

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Theorem (Kramers' Formula)

Mean first-passage u^*_- to u^*_+ obeys:

$$\mathbb{E}[\tau_{u^*_- \to u^*_+}\}] \sim \frac{2\pi}{|\rho_1(u^*_s)|}\sqrt{\frac{|\det(\nabla^2 V(u^*_s))|}{\det(\nabla^2 V(u^*_-))}}\, e^{2(V(u^*_s)-V(u^*_-))/\varepsilon^2}.$$

Back to Neural Fields... Kramers' Formula and LDP

Observations (K./Riedler, 2013)

- *From [Laing/Troy03,Enulescu/Bestehorn07]* $\varepsilon = 0 \Rightarrow$ *neural field has energy-structure. Let* $g := f^{-1}$, $P(x,t) = f(U(x,t))$.

$$\partial_t P(x,t) = -\frac{1}{g'(P(x,t))} \nabla E[P(x,t)].$$

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- *Change-of-variable* $\Rightarrow$ *multiplicative noise.*
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  - *Space-time dependent factor* $1/g'(P(x,t))$.
  - *Trace-class noise.*
- *LDP follows from evolution equation [daPratoZabczyk92].*
- *LDP can be approximated using Galerkin method.*

Part 2 SDE Continuation: Motivation

Consider the general differential equation

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$F(u; \lambda)$ could lead to ODE, DDE, PDE, SDE, SPDE, etc.

Problem: Forward simulation is usually very restrictive!

1. Simulate over initial values u_0.
2. Simulate over parameter space $\mu \in \mathbb{R}^p$.
3. Simulate over noise realizations $\omega \in \Omega$.

Do you really understand the nonlinear dynamics from averages?

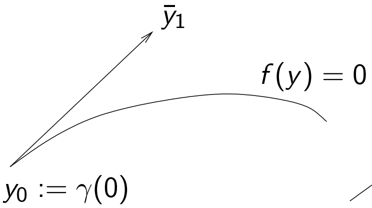
Deterministic DEs Standard Method: Continuation

Consider the ODE

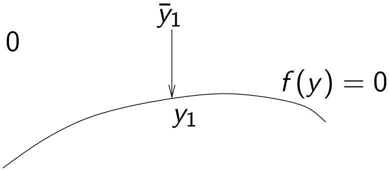
$$x' = f(x;\mu), \qquad f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n.$$

Let $(x;\mu) =: y$. A curve $y = \gamma(s)$ of equilibria satisfies

$$f(\gamma(s)) = 0. \qquad \text{(note: } Df(\gamma(0))\gamma'(0) = 0\text{)}$$



(a) Prediction Step



(b) Correction Step

Important: Excellent guess from (a) for Newton's Method in (b).

Numerical Bifurcation Analysis for Stochastic Systems?

Consider the stochastic (ordinary) differential equation (SDE)

$$dx_t = g(x_t;\mu)\,dt + \varepsilon G(x_t;\mu)\,dW_t, \quad x_t \in \mathbb{R}^n,$$

$W_t = (W_{1,t}, W_{2,t}, \ldots, W_{k,t})^T$ Brownian motion, $F(x_t;\mu) \in \mathbb{R}^{n\times k}$;
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- **Appproach 1:** Forward Monte-Carlo simulation.
- **Problems:** Sampling often prohibitive.

- **Appproach 2:** Use probability density $p = p(x,t)$. Requires Fokker-Planck solution

$$\frac{\partial p}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}(g(x;\mu)p) + \frac{\varepsilon^2}{2}\sum_{i,j=1}^{n} \frac{\partial}{\partial x_i \partial x_j}(\mathfrak{D}_{ij}(x;\mu)p).$$

- **Problems:** High-dimensional PDE; not even $\varepsilon = 0$ is good!

Strategy - Generalization to SDEs

Step 1: Recall

$$\mathrm{d}x_t = g(x_t;\mu)\,\mathrm{d}t + \varepsilon G(x_t;\mu)\,\mathrm{d}W_t.$$

Step 2: Expand near (locally stable) deterministic equilibrium x^*

$$\mathrm{d}X_t = A(x^*;\mu)X_t\,\mathrm{d}t + \varepsilon F(x^*;\mu)\,\mathrm{d}W_t$$

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Step 3: The covariance matrix $C_t := \mathrm{Cov}(X_t)$ solves

$$\begin{aligned} C_t' &= A(x^*;\mu)C_t + C_t A(x^*;\mu)^T + \varepsilon^2 G(x^*;\mu)G(x^*;\mu)^T \\ \text{equil.} \Rightarrow 0 &= A(x^*;\mu)C + CA(x^*;\mu)^T + \varepsilon^2 G(x^*;\mu)G(x^*;\mu)^T \end{aligned}$$

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Step 4: Define the covariance ellipsoid

$$\mathcal{B}(h) := \left\{x \in \mathbb{R}^n : (x-x^*)^T C^{-1}(x-x^*) \le h^2\right\}.$$

Covariance Ellipsoids via Continuation

Important observations:

- Continue the equilibrium $x^* = x^*(\mu)$ as usual.
- For covariance ellipsoid one has to solve a Lyapunov equation

$$AC + CA^T + B = 0$$

- During continuation the matrix

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  is available as a submatrix of $\mathrm{D}g(x^*;\mu)$.
- Efficient iterative methods for Lyapunov equations exist.
- A simple initial guess for $C(\mu_2)$ at $(x^*(\mu_2), \mu_2)$ is

$$C(x^*(\mu_1);\mu_1).$$

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$$\mathcal{E} := \left\{ x \in \mathbb{R}^n : v^T x \leq v^T x^* + (v^T Q v)^{1/2} \quad \forall v \in \mathbb{R}^n \right\}.$$

defines an ellipsoid centered at x^*.

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Fact: May solve an optimization problem

$$\begin{aligned} \delta &= \delta(\mathcal{E}(x_1^*, Q_1), \mathcal{E}(x_2^*, Q_2)) \\ &= \max_{\|v\|=1} \left(v^T x_1^* - (v^T Q_1 v)^{1/2} - v^T x_2^* - (v^T Q_2 v)^{1/2} \right). \end{aligned}$$

Idea: Use iterative method (e.g. SQP) & initial guess from continuation to compute δ.

Neural Competition

Consider two neural populations

$$\begin{aligned} x_1' &= -x_1 + S(I_c - \beta x_2 - g y_1), \\ x_2' &= -x_2 + S(I_c - \beta x_1 - g y_2), \\ y_1' &= \epsilon(x_1 - y_1), \\ y_2' &= \epsilon(x_2 - y_2), \end{aligned}$$

where

- $x_{1,2}$ = averaged firing rates,
- $y_{1,2}$ = fatigue/reset variables,
- $S(u) := \frac{1}{1+\exp(-r(u-\theta))}$.

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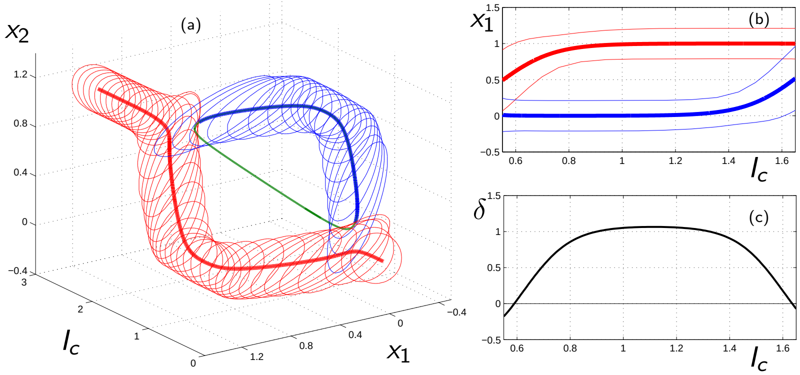
Look at noisy fast subsystem $\epsilon = 0$

$$\begin{pmatrix} dx_1 \\ dx_2 \end{pmatrix} = \begin{pmatrix} -x_1 + S(I_c - \beta x_2 - g y_1) \\ -x_2 + S(I_c - \beta x_1 - g y_2) \end{pmatrix} dt + \varepsilon^2 G(x)\, dW_t$$

Numerical Continuation...



For parameter values

$$y_1 = 0.7, \quad y_2 = 0.75, \quad \beta = 1.1, \quad g = 0.5, \quad r = 10, \quad \theta = 0.2.$$

and

$$\varepsilon^2 G(x^*) G(x^*)^T = \varepsilon^2 \begin{pmatrix} 1 & 0.4 \\ 0.4 & 1 \end{pmatrix} \qquad \text{for } \varepsilon^2 = 0.3.$$

Metastability and Noise-Induced Switching

Consider a gradient system

$$\mathrm{d}x_t = -\nabla V_\mu(x_t)\,\mathrm{d}t + \varepsilon\,\mathrm{d}W_t, \qquad V_\mu : \mathbb{R}^n \to \mathbb{R}. \qquad (1)$$

Assume

- two stable equilibria x^* and y^*
- saddle z^*, one unstable direction eigenvalue $\lambda(z^*;\mu) > 0$

Kramers' Law

$$\mathbb{E}[\tau_{x^*\to y^*}] = \frac{2\pi}{|\lambda(z^*;\mu)|}\sqrt{\frac{|\det(A(z^*;\mu))|}{\det(A(x^*;\mu))}}\, e^{2[V_\mu(z^*)-V_\mu(x^*)]/\varepsilon^2}$$

where $A(x^*;\mu) = \mathrm{D}^2 U_\mu(x^*;\mu) \in \mathbb{R}^{n\times n}$.

Continuation and Kramers' Law

Kramers' Law

$$\mathbb{E}[\tau_{x^* \to y^*}] = \frac{2\pi}{|\lambda(z^*;\mu)|}\sqrt{\frac{|\det(A(z^*;\mu))|}{\det(A(x^*;\mu))}}e^{2[V_\mu(z^*)-V_\mu(x^*)]/\varepsilon^2}$$

Observations:

- Just continue the equilibria x^*, y^*, z^* as usual.
- Jacobian $A(z^*;\mu)$ is available.
- Compute $\det(A(x^*;\mu))$ via LU decomposition.
- Leading eigenvalue $\lambda(z^*;\mu)$ may use Rayleigh iteration.

Extension to SPDEs

Starting point: (cubic-quintic) Allen-Cahn PDE

$$\frac{\partial u}{\partial t} = \Delta u - 4(\mu u + u^3 - u^5).$$

$u = u(x, t)$, $x \in \Omega \subset \mathbb{R}^2$, given boundary conditions.

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Extension to SPDEs

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$$\frac{\partial u}{\partial t} = \Delta u - 4(\mu u + u^3 - u^5) + g(u)\xi.$$

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Main Steps:

1. Compute bifurcation for PDE (e.g. $\rightarrow$ `pde2path`).
2. Consider the SPDE version (e.g. $\rightarrow$ trace-class noise).
3. Discretize in space (e.g. $\rightarrow$ FDM, FEM, Galerkin).

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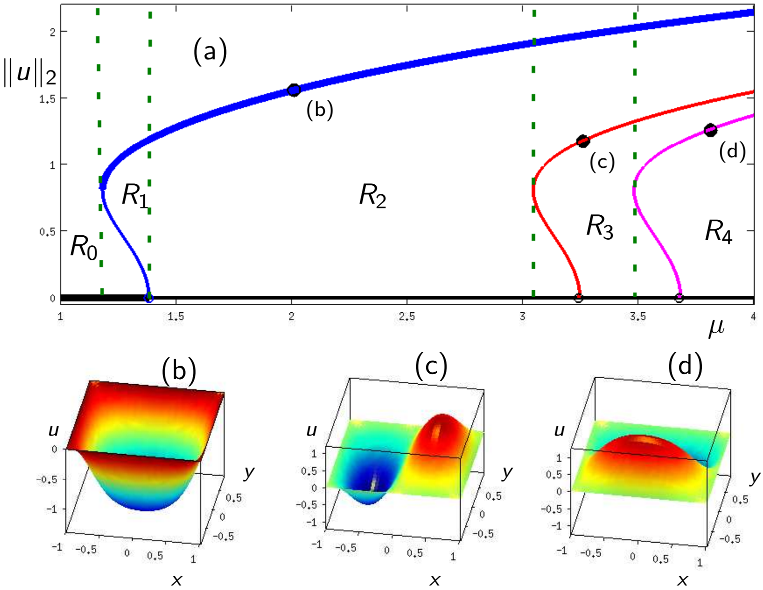
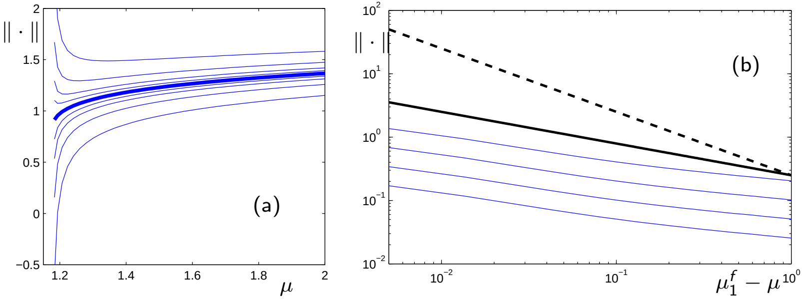
4. Apply numerical continuation for SDEs.

PDE: Deterministic Numerical Continuation



SPDE: Stochastic Numerical Continuation



- scaling law of the variance near bifurcation point
- link to early-warning signs
- Computation on standard desktop computer for SPDEs

Overview

- Infinite-dimensional neural fields
- Numerical continuation methods for SODEs
- Numerics extends to SPDEs and SPIDEs

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A general strategy:

1. Abstract stochastic analysis
2. Conversion into numerical deterministic problem
3. Continuation and iterative methods

- see also: **www.asc.tuwien.ac.at/∼ckuehn** and **arXiv**

Remark: Multiscale Dynamics (almost) everywhere!

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Thank you for your attention.