Linear response for macroscopic observables in high-dimensional systems

Caroline Wormell

The University of Sydney

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Joint work with Georg Gottwald

Linear response theory

Consider a smooth family of deterministic dynamical systems $x_n = T^\varepsilon(x_{n-1})$, which are mixing with physical invariant measures μ^ε.:

$$\mathbb{E}^\varepsilon[\Psi] := \int \Psi(x)\,\mathrm{d}\mu^\varepsilon(x)$$

Linear response theory (LRT): *What is* $\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mu^\varepsilon\mathbb{E}^\varepsilon[\Psi]$*?*
(e.g. for Taylor approximations)

...supposing $\mathbb{E}^\varepsilon[\Psi]$ is differentiable

LRT in practice

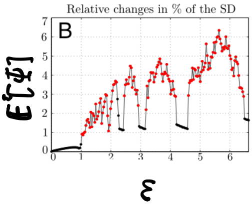
The application of linear response theory to climate systems has met with some success:

- Toy models: Majda et al '07, '10, Lucarini & Sarno '11
- Barotropic models: Bell '80, Gritsun & Dymnikov '99, Abramov & Majda '09
- Quasi-geostrophic models: Dymnikov & Gritsun '01
- Atmospheric models: North et al '04, Cionni et al '04, work of Gritsun and others '02, '07, '10, Ring & Plumb '08
- Coupled climate models: Langen & Alexeev '05, Kirk & Davidoff '09, Fuchs et al '14, Ragone et al '15

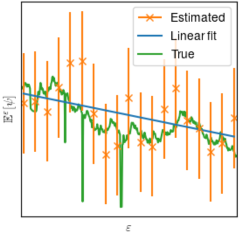
LRT in practice

However:

- Rough responses are known in atmospheric and ocean dynamics (e.g. Chekroun et al. '14)
- The failure of linear response needs very long time series to be visible (Gottwald, W. & Wouters '17)



Chekroun et al., 2014

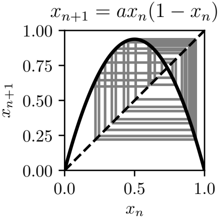


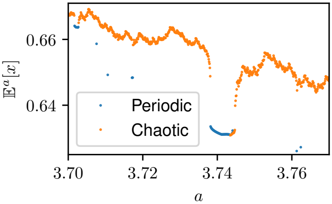
LRT in theory

Analytically, we know LRT works in

- Statistical mechanics: Kubo '66
- Stochastic dynamical systems: Hänggi '78, Hairer & Majda '10
- Axiom A (uniformly hyperbolic dissipative chaos): Ruelle '97-8
- Other dissipative systems...?

Baladi and others ('08, '10, '14, '15) proved there is no **linear response for quadratic maps, even Whitney differentiability**.

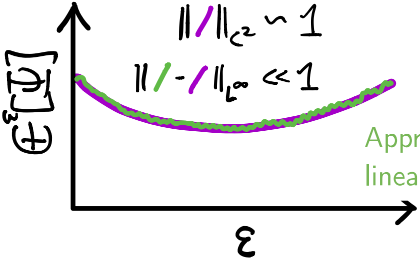




The question

In this talk we will address the following question:

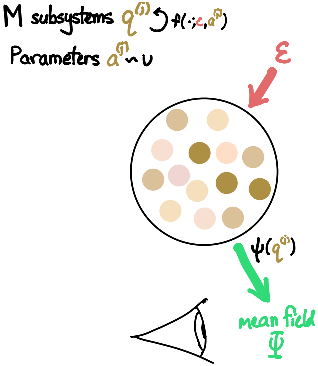
> *When and why does linear response occur (for all practical purposes) at macroscopic scales in high-dimensional systems?*



Approximate linear response

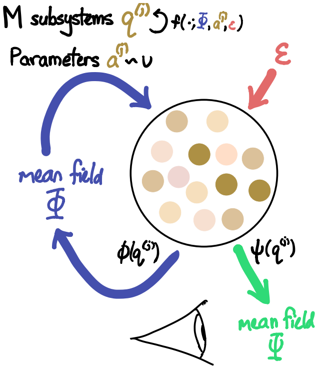
The model

We study simple complex systems:



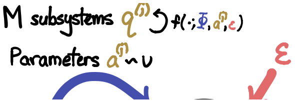
The model

We study slightly more complex complex systems:

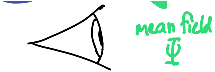


The model

We study slightly more complex complex systems:



		macroscopic observables	
microscopic subsystem		uncoupled	coupled
f satisfies LRT	finite M	✓	✓
	$M \to \infty$	✓	✯
f violates LRT with smooth $\frac{\mathrm{d}\nu}{\mathrm{d}a}$	finite M	(✓)	(✓)
	$M \to \infty$	✓	✯
f violates LRT with non-smooth $\frac{\mathrm{d}\nu}{\mathrm{d}a}$	finite M	✗	(✓)
	$M \to \infty$	✗	✗



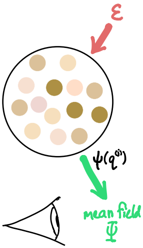
We will derive reductions for mean-field dynamics and discuss (very rich) LRT properties.

Uncoupled case

System parameters: $a^{(j)}$, $j = 1, \dots, M$ sampled from measure ν

Dynamics:

$$q_n^{(j)} = f(q_{n-1}^{(j)}; a^{(j)}, \varepsilon),\ j = 1, \dots, M$$



Observable:

$$\Psi_n = \frac{1}{M} \sum_{j=1}^{M} \psi(q_n^{(j)})$$

Each subsystem $q^{(j)}$ evolves independently: suppose they have physical measures $\mu^{a^{(j)},\varepsilon}$ and are mixing.

Uncoupled case: expectations

relevant for LRT

Two (nested) ways to take expectations:

- Over dynamics, i.e. initial conditions: $\mathbb{E}^{\varepsilon}[\,\cdots\,]$
- Over dynamical systems, i.e. selection of parameters $a^{(j)}$ (if relevant): $\langle\, \mathbb{E}^{\varepsilon}[\cdots]\,\rangle$

LRT of mean-field Ψ

We are interested in behaviour with respect to ε of

$$\mathbb{E}^{\varepsilon}\Psi = \frac{1}{M}\sum_{j=1}^{M}\mathbb{E}^{\varepsilon}[\psi(q^{(j)})]$$

The $q^{(j)}$ evolve independently of each other so at statistical equilibrium,

$$\mathbb{E}^{\varepsilon}[\psi(q^{(j)})] = \int \psi(q)\mathrm{d}\mu^{a^{(j)},\varepsilon}(q)$$

only depends on $a^{(j)}$

LRT of mean-field Ψ

Because the $a^{(j)}$ are randomly selected, a CLT in $\langle \cdot \rangle$ gives

$$\mathbb{E}^{\varepsilon}\Psi = \frac{1}{M}\sum_{j=1}^{M}\mathbb{E}^{\varepsilon}[\psi(q^{(j)})] = \bar{\Psi}^{\varepsilon} + \frac{1}{\sqrt{M}}\eta^{\varepsilon} + o(1/\sqrt{M})$$

where η^{ε} is a mean-zero Gaussian process in ε, and

$$\bar{\Psi}^{\varepsilon} = \langle \mathbb{E}^{\varepsilon}[\psi(q)] \rangle = \iint \psi(q)\,\mathrm{d}\mu^{a,\varepsilon}(q)\,\mathrm{d}\nu(a)$$

So response of mean-field Ψ is $\bar{\Psi}^{\varepsilon}$ plus small correction for finite ensemble size.

LRT of $\bar{\Psi}^\varepsilon$

$$\bar{\Psi}^\varepsilon = \langle \mathbb{E}^\varepsilon[\psi(q)] \rangle = \iint \psi(q) \, \mathrm{d}\mu^{a,\varepsilon}(q) \, \mathrm{d}\nu(a)$$

- Clearly if microscopic subsystems satisfy LRT then so does $\bar{\Psi}^\varepsilon$.
- On the other hand if the microscopic subsystems violate LRT and ν is discrete (e.g. $\nu = \delta_{a_0}$), then $\bar{\Psi}^\varepsilon$ will not have LRT.

LRT of $\bar{\Psi}^\varepsilon$

If ν is smooth (e.g. $\frac{\mathrm{d}\nu}{\mathrm{d}a} \in BV$), then averaging over $\mathrm{d}\nu(a)$ can give "collective" linear response of microscopic systems that may violate LRT:

- **Easy case:** If $f(\,\cdot\,; a, \varepsilon) = f(\,\cdot\,; a + K\varepsilon)$:

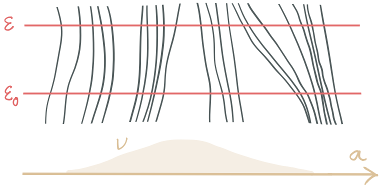
$$\begin{aligned} \frac{\mathrm{d}\bar{\Psi}^\varepsilon}{\mathrm{d}\varepsilon} &= \int \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \int \psi(q)\,\mathrm{d}\mu^{a+\varepsilon}(q)\,\mathrm{d}\nu(a) \\ &= \int \frac{\mathrm{d}}{\mathrm{d}a} \int \psi(q)\,\mathrm{d}\mu^{a+\varepsilon}(q)\,\mathrm{d}\nu(a) \\ &= -\iint \psi(q)\,\mathrm{d}\mu^{a+\varepsilon}(q)\,\mathrm{d}\left(\frac{\mathrm{d}\nu}{\mathrm{d}a}\right) \end{aligned}$$

$\implies$ LRT holds

LRT of $\bar{\Psi}^\varepsilon$

- If $f(\,\cdot\,; a, \varepsilon)$ is a family of (analytic) unimodal maps:
  - These maps obey LRT along topological conjugacy classes (Ruelle '09);
  - Avila *et al* ('03) conjectured that topological conjugacy classes of these maps have a uniformly analytic codimension-one lamination.

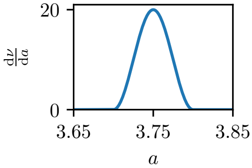
This may imply $\bar{\Psi}^\varepsilon$ has linear response.

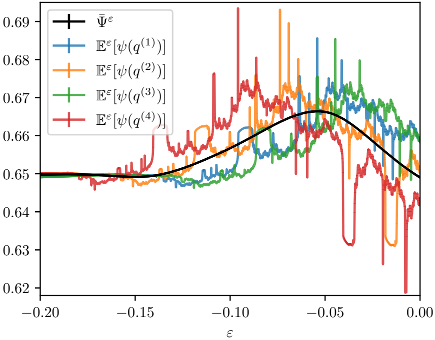


LRT of $\bar{\Psi}^\varepsilon$

Smooth family of unimodal maps:

$$f(q; a, \varepsilon) = (a + 4\varepsilon q(1-q))q(1-q),$$
$$\nu \sim \mathrm{Cosine}(3.75, 0.05)$$





LRT of η^ε

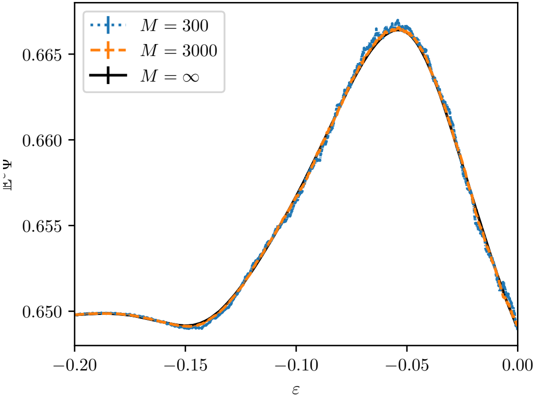
What about finite M correction η^ε?
Suppose the microscopic variables violate LRT with C^α ($\alpha < 1$) response but $\bar{\Psi}^\varepsilon$ satisfies LRT. Then

$$\left\langle (\eta^\varepsilon - \eta^{\varepsilon_0})^2 \right\rangle = \left\langle \left(\mathbb{E}^\varepsilon[\psi(q^{(j)})] - \mathbb{E}^{\varepsilon_0}[\psi(q^{(j)})]\right)^2 \right\rangle - (\bar{\Psi}^\varepsilon - \bar{\Psi}^{\varepsilon_0})^2$$
$$= \mathcal{O}(|\varepsilon - \varepsilon_0|^{2\alpha}) - \mathcal{O}(|\varepsilon - \varepsilon_0|^2) = \mathcal{O}(|\varepsilon - \varepsilon_0|^\alpha)^2.$$

Hence η^ε is C^α a.s., so violates LRT.

LRT of η^ε

Thus, for finite M we only get "approximate" LRT (when microscopic subunits do not have LRT).



Macroscopic reduction

What about the *dynamics* of Ψ_n?
The $q^{(j)}$s are independent of each other, so for any n

$$\Psi_n = \frac{1}{M} \sum_{j=1}^{M} \psi(q_n^{(j)})$$

is a sum of independent random variables.
Thus

$$\Psi_n = \mathbb{E}^{\varepsilon}\Psi + \frac{1}{\sqrt{M}}\zeta_n + o(1/\sqrt{M})$$

where $\zeta_n, n \in \mathbb{N}$ are mean-zero Gaussian random variables.

Macroscopic reduction

When $M \gg 1$, ζ *appears* to converge to a stationary Gaussian *process*.
The autocorrelation function is given by the microscopic subsystems:

$$\mathrm{Cov}[\zeta_m, \zeta_n] = \langle \mathrm{Cov}[\psi(q_m), \psi(q_n)] \rangle$$

so ζ has decay of correlations and can be approximated by e.g. an *AR* process.

Side note: as with mean-fields, variability observables such as $M(\Psi_n - \mathbb{E}^{\varepsilon}[\Psi])^2$ also have (approximate) LRT.

Non-coupling system conclusions

- Response of mean-field is at least as smooth as that of microscopic dynamics
- Possible to get LRT (for all intents and purposes) at macroscopic level with microscopic dynamics that violate LRT
- Mean-field dynamics are $\mathcal{O}(M^{-1/2})$ Gaussian fluctuations about expectation value

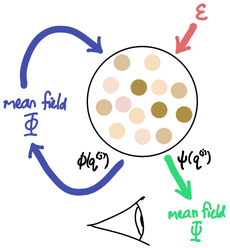
Mean-field coupled case

System parameters: $a^{(j)}$, $j = 1, \ldots, M$ sampled from measure ν

Dynamics:

$$q_n^{(j)} = f(q_{n-1}^{(j)}; \Phi_{n-1}, a^{(j)}, \varepsilon),\ \ j = 1, \ldots, M$$

$$\Phi_n = \frac{1}{M} \sum_{j=1}^{M} \phi(q_n^{(j)})$$



Observable:

$$\Psi_n = \frac{1}{M} \sum_{j=1}^{M} \psi(q_n^{(j)})$$

Externally-coupled system

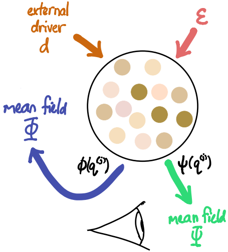
System parameters: $a^{(j)}$, $j = 1, \ldots, M$ sampled from measure ν

External driver: d_n

Dynamics:

$$q_n^{(j)} = f(q_{n-1}^{(j)}; d_{n-1}, a^{(j)}, \varepsilon),\ j = 1, \ldots, M$$

$$\Phi_n = \frac{1}{M}\sum_{j=1}^{M} \phi(q_n^{(j)})$$



Observable:

$$\Psi_n = \frac{1}{M}\sum_{j=1}^{M} \psi(q_n^{(j)})$$

Suppose $q^{(j)}$ have time-dependent physical measures $\mu_n^{d,a^{(j)},\varepsilon}$ with decay of correlations.

Externally-coupled system

We can apply the same CLT ideas, so e.g.

$$\langle \mathbb{E}^{\varepsilon}[\Phi_n | d] \rangle = \iint \phi(q) \, \mathrm{d}\mu_n^{d,a^{(j)},\varepsilon}(q) \, \mathrm{d}\nu(a)$$

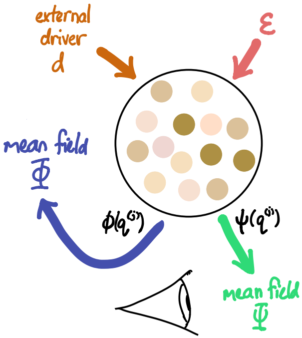
which only depends on $(d_m)_{m<n}$.
We have

$$\Phi_n = \langle \mathbb{E}^{\varepsilon}[\Phi_n | d] \rangle + \frac{1}{\sqrt{M}} \tilde{\eta}_n^{d,\varepsilon} + \frac{1}{\sqrt{M}} \tilde{\zeta}_n^{d} + o(1/\sqrt{M})$$

where the process $\tilde{\zeta}$ is now non-stationary, and $\tilde{\eta}^{\varepsilon}$ depends on time.

Macroscopic reduction of coupled system

Ansatz: if $M \gg 1$, the coupled system can be approximated by setting $d_n \equiv \Phi_n$.



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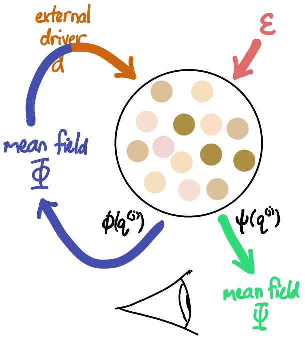

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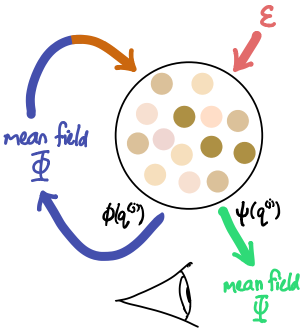


Macroscopic reduction of coupled system

This gives the macroscopic reduction:

$$\Phi_n = \langle \mathbb{E}^{\varepsilon}[\Phi_n|\Phi]\rangle + \frac{1}{\sqrt{M}}\tilde{\eta}_n^{\Phi,\varepsilon} + \frac{1}{\sqrt{M}}\tilde{\zeta}_n^{\Phi} + o(1/\sqrt{M})$$

$=: F(\Phi_{n-1}, \Phi_{n-2}, \dots; \varepsilon)$

self-generated noise

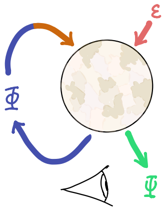
usually smaller than $\tilde{\zeta}$

LRT of coupled system: finite M

The macroscopic reduction

$$
\begin{aligned}
\Phi_n &= F(\Phi_{n-1}, \Phi_{n-2}, \ldots ; \varepsilon) + \frac{1}{\sqrt{M}} \tilde{\eta}_n^{\Phi,\varepsilon} + \frac{1}{\sqrt{M}} \tilde{\zeta}_n^{\Phi} + o(1/\sqrt{M}) \\
\Psi_n &= G(\Phi_{n-1}, \Phi_{n-2}, \ldots ; \varepsilon) + \frac{1}{\sqrt{M}} \eta_n^{\Phi,\varepsilon} + \frac{1}{\sqrt{M}} \zeta_n^{\Phi} + o(1/\sqrt{M})
\end{aligned}
$$

defines a stochastic dynamical system.



LRT of coupled system: finite M

The macroscopic reduction

$$\Phi_n = F(\Phi_{n-1}, \Phi_{n-2}, \dots; \varepsilon) + \frac{1}{\sqrt{M}}\tilde{\eta}_n^{\Phi,\varepsilon} + \frac{1}{\sqrt{M}}\tilde{\zeta}_n^{\Phi} + o(1/\sqrt{M})$$

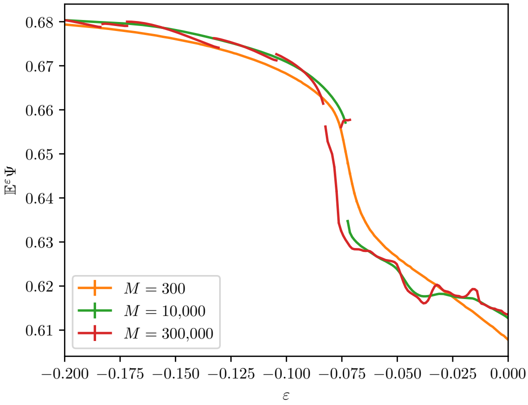
$$\Psi_n = G(\Phi_{n-1}, \Phi_{n-2}, \dots; \varepsilon) + \frac{1}{\sqrt{M}}\eta_n^{\Phi,\varepsilon} + \frac{1}{\sqrt{M}}\zeta_n^{\Phi} + o(1/\sqrt{M})$$

defines a stochastic dynamical system.
Modulo η's:

- The noise $\tilde{\zeta}^{\Psi}$ generates (annealed) LRT in the microscopic particles, so this noisy system is $\sim$smooth in Φ and ε.
- So Φ obeys LRT for finite M.
- Thus so does Ψ.

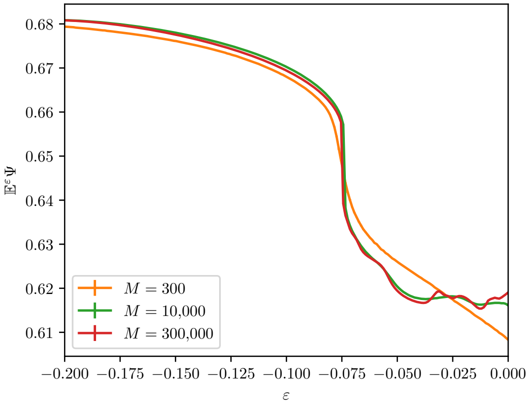
LRT of coupled system: finite M

LRT for unimodal microscopic components, $\nu = \frac{1}{3}(\delta_{a_1} + \delta_{a_2} + \delta_{a_3})$:



LRT of coupled system: finite M

LRT for unimodal microscopic components, $\frac{\mathrm{d}\nu}{\mathrm{d}x} \in C^3$:



Thermodynamic limit

As $M \to \infty$ we have macroscopic reduction

$$\Phi_n = F(\Phi_{n-1}, \Phi_{n-2}, \dots; \varepsilon)$$
$$\Psi_n = G(\Phi_{n-1}, \Phi_{n-2}, \dots; \varepsilon)$$

defines a (smooth) stochastic dynamical system.
In particular external forcing washes out over time because of microscopic mixing, so

$$\Phi_n \approx F(\Phi_{n-1}, \Phi_{n-2}, \dots, \Phi_{n-K}; \varepsilon),$$

i.e. emergent dynamics of Φ_n are low-dimensional.

Thermodynamic limit

If dynamics converges to equilibrium $\Phi_n \equiv \bar{\Phi}^\varepsilon$ we have

$$\bar{\Phi}^\varepsilon = F(\bar{\Phi}^\varepsilon, \bar{\Phi}^\varepsilon, \ldots; \varepsilon) := F_0(\bar{\Phi}^\varepsilon; \varepsilon)$$

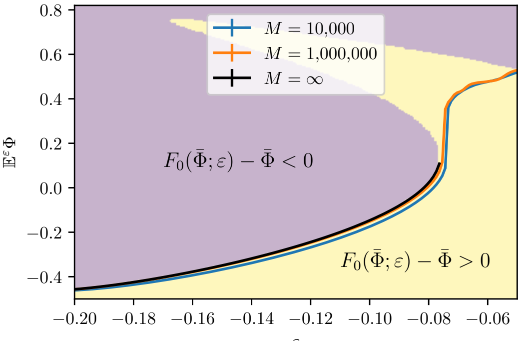
which is a smooth function if the microscopic subsystems have "collective" LRT. Then,

$$\frac{\mathrm{d}\bar{\Phi}^\varepsilon}{\mathrm{d}\varepsilon} = \left(1 - \frac{\partial F_0}{\partial \bar{\Phi}^\varepsilon}\right)^{-1} \frac{\partial F_0}{\partial \varepsilon}$$

(+ stability) and hence Φ has LRT.

Thermodynamic limit

For unimodal microscopic component example, $\frac{\mathrm{d}\nu}{\mathrm{d}x} \in C^3$, we see saddle-node bifurcation:



What are the other possible macroscopic dynamics and do they obey LRT?

Thermodynamic limit

- LRT in thermodynamic limit is difficult to study accurately using naive methods: need both long time series *and* very large microscopic ensembles.
- However, suppose $a^{(j)} \equiv a_0$. We can write system in terms of measures $\mu_n^{d,\varepsilon}$ and Perron-Frobenius operators $\mathcal{L}$:

$$\mu_n^{\Phi,\varepsilon} = \mathcal{L}_{f(\cdot;\Phi_{n-1},\varepsilon)} \mu_{n-1}^{d,\varepsilon},$$
$$\Phi_n = \int \phi(q) \, \mathrm{d}\mu_n^{\Phi,\varepsilon}(q).$$

- For uniformly expanding f these equations can be very efficiently approximated with spectral methods (W. '19).

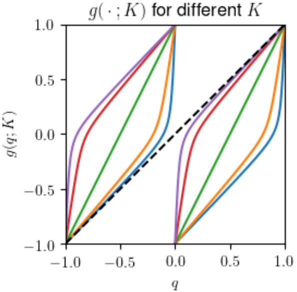
Macroscopic dynamics in thermo. limit

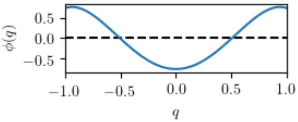
Consider a mean-field-coupled system

$$q_n^{(j)} = g(q_{n-1}^{(j)}; \varepsilon\Phi_{n-1})$$

$$\Phi_n = \frac{1}{M}\sum_{j=1}^{M} \phi(q_n^{(j)}).$$

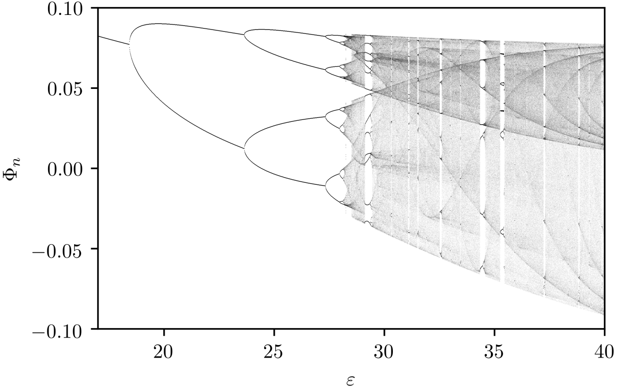
In a few lines of code, the limiting macroscopic dynamics can be simulated very accurately using `Poltergeist.jl`.





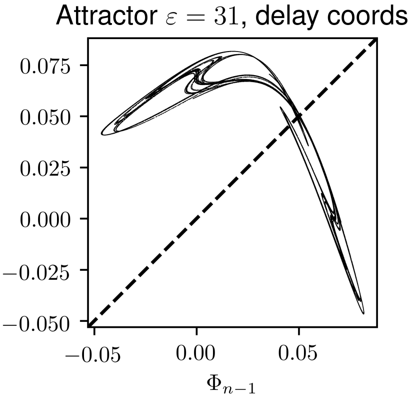
Macroscopic dynamics in thermo. limit

For large ε we see period doubling bifurcation to chaos:



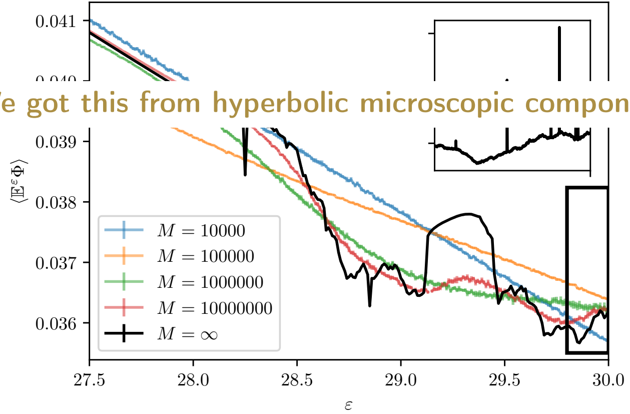
Macroscopic dynamics in thermo. limit

The attracting Φ dynamics look unimodal:



LRT in thermodynamic limit

We have breakdown of LRT in the thermodynamic limit:



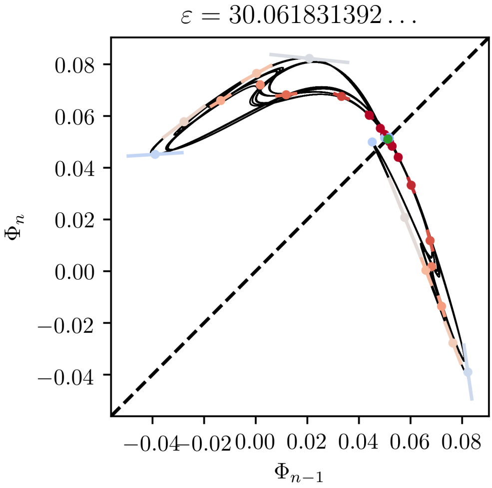
We got this from hyperbolic microscopic components!

Macroscopic dynamics in thermo. limit

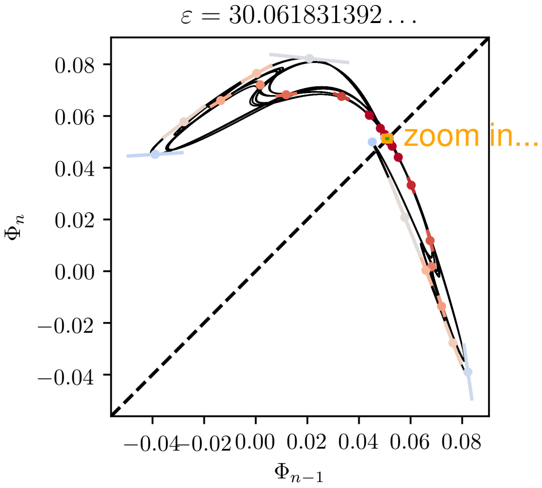
Side question: are the structure of the dynamics in the thermodynamic limit hyperbolic?
Answer: No. There are homoclinic tangencies.

How do we know? Continuation, making use of `Poltergeist.jl`.

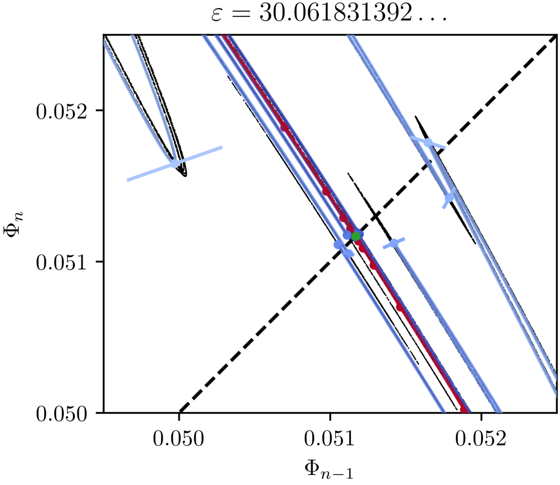
Macroscopic dynamics in thermo. limit



Macroscopic dynamics in thermo. limit



Macroscopic dynamics in thermo. limit



Conclusions

Various mechanisms by which linear response may emerge *and/or break down* in large coupled chaotic systems:

- Inhomogeneous collections of microscopic subsystems may have a differentiable average response despite individually violating LRT
- Self-generated noise can induce LRT in large but finite systems
- In thermodynamic limit LRT depends on collective microscopic LRT *and* structure of macroscopic dynamics
- Macroscopic dynamics may be non-hyperbolic chaos, violate LRT

Further directions

- Study of networks beyond big mean-field couplings
- More rigorous study of some of these phenomena would be very interesting.

Further details

Wormell, C.L. and Gottwald, G.A., 2019. Linear response for macroscopic observables in high-dimensional systems. arXiv:1907.13490.

Aside on periodic windows

Unimodal maps have periodic dynamics on a dense (but not full measure) parameter set—i.e., non-mixing.
To keep things simple, we avoid this by adding "hidden" dynamics $r_n^{(j)} \in [0,1]$:

$$f(q, r; a, \varepsilon) = \begin{cases} (\tilde{f}(q; a, \varepsilon), 2r), & r \leq 1/2 \\ (q, 2r-1), & r > 1/2. \end{cases}$$

This makes the unimodal $q^{(j)}$ dynamics mixing while retaining the same invariant measures.

(N.B. at statistical equilibrium, $\{r_n \geq 1/2\}_{n \in \mathbb{N}}$ are *i.i.d.* Bernoulli.)

"Mixing"

If dynamical system $x_n = f(x_{n-1})$ is mixing with respect to measure μ then for all $w \in L^2(\mu)$ with $\mathbb{E}[w] = 1$,

$$\mathbb{E}[\psi(x_n)w(x_0)] = \int \psi(x_n)w(x_0)\,\mathrm{d}\mu(x_0) \xrightarrow{n\to\infty} \mathbb{E}[\psi]$$

More generally, are going to assume that if $\tilde{\mu}$ is a "nice" measure,

$$\int \psi(x_n)\,\mathrm{d}\tilde{\mu}(x_0) \xrightarrow{n\to\infty} \mathbb{E}[\psi]$$