Statistical properties of deterministic dynamical systems and their applications in weather and climate forecasting

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joint work with Jason Frank, Brent Giggins, John Harlim, Ian Melbourne, Lewis Mitchell, Karsten Peters, Caroline Wormell and Jeroen Wouters



Colloquium (somewhere) 29 May 2020

Statistical limit laws for deterministic dynamical systems

I) Heuristics and a few theorems

II) Some applications

• data assimilation

- ensemble forecasting bred vectors
- sensitivity to perturbations Linear Response Theory
- numerical integration of deterministic multi-scale systems
- parametrisation of tropical convection

Motivation for stochastic parametrisation:

prediction: computational cost in running model

$$\dot{x} = f(x, y)$$
$$\dot{y} = \frac{1}{\varepsilon}g(x, y)$$
$$x \in \mathbb{R}^{n}$$
$$y \in \mathbb{R}^{m}$$

$$dX = F(X)dt + \Sigma \, dW_t$$
$$X \in \mathbb{R}^n$$

lower-dimensional stochastic problem

stiff high-dimensional deterministic multi-scale problem

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- increase of resolution necessitates stochastic approach





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convective cells



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Integrate the slow equation

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Envoking Birkhoff's Ergodic Theorem

$$X(t) = X(0) + \int_0^t F(X(s)) \, ds$$
$$F(X) = \int f(x, y) \, \mu(dy)$$

Averaged deterministic dynamics

law of large numbers

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go to long diffusive time scale

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Assuming $\int f(y)\mu(dy) = 0$ and invoking the Central Limit Theorem

$$X(t) = X(0) + W_t$$
$$dX = dW_t$$

Homogenised stochastic equation

central limit theorem

$$x_{n+1} = x_n + \varepsilon (y_n - \frac{1}{2})$$
$$y_{n+1} = 4y_n (1 - y_n)$$

strong chaos



Brownian motion

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$$\begin{aligned} x_{n+1} &= x_n + \varepsilon (y^* - y_n) \\ y_{n+1} &= \begin{cases} y_n (1 + 2^{\gamma} y_n^{\gamma}) & 0 \le y_n \le \frac{1}{2} \\ 2y_n - 1 & \frac{1}{2} \le y_n \le 1 \\ weak \ chaos \end{aligned}$$



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(GAG, & Melbourne, Proc Roy Soc A (2013))

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$$\int_{0}^{1} \int_{0}^{1} \int_{$$

n

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Homogenisation

resolved/slow:
$$dx = \frac{1}{\varepsilon} f_0(x, y) dt + f_1(x, y) dt$$

unresolved/fast: $dy = \frac{1}{\varepsilon^2} g(x, y) dt + \frac{1}{\varepsilon} \sigma(x, y) dW_t$

Assumptions:

fast y-process is ergodic with measure μ_x(mild chaoticity assumptions)
∫ f₀(x, y)dμ_x = 0

Then, in the limit of $\varepsilon \to 0$, the statistics of the slow x-dynamics is approximated by

$$dX = F(X) dt + \Sigma(X) dW_t$$

where the diffusion matrix is given by a Green-Kubo formula $\frac{1}{2}\Sigma\Sigma^T = \int_0^\infty C(s)ds$

with the auto-correlation matrix $C(t) = \mathbb{E}^{\mu_x}[f_0(x, y)f_0(x, y(t))]$ and

$$F(X) = \int f_1(x,y) \, d\mu_x + \int_0^\infty \int \nabla_x f_0(x,y(s)) \otimes f_0(x,y) \, d\mu_x \, ds$$

formally: $d\mu = \rho(x, y)dx$ $\rho(x, y) = \hat{\rho}(x)\rho_{\infty}(y|x) + \varepsilon \rho_1(x, y) + \dots$ Open problems and challenges

slow dynamics couples back into the fast dynamics

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$
$$\dot{y} = \frac{1}{\varepsilon^2} g_0(x, y)$$

What can go wrong?

If the fast invariant measure μ_x does not depend smoothly on x ("no linear response") even averaging does not "work"

$$F(X) = \int f_1(x, y) \mu_x(dy)$$

non-Lipschitz
uniqueness of solutions not guaranteed

slow dynamics couples back into the fast dynamics

finite time scale separation

Theory works in the limit $\varepsilon \to 0$ but in many physical applications ε is not so small

Where do we need the limit?

Averaging: Large deviation principle:

$$\left|\frac{1}{T}\int_0^T f_1(x, y(s))ds - F(x)\right|$$

Homogenisation: Central Limit Theorem (Weak Invariance Principle)

$$W_{\varepsilon}(t) = \varepsilon \int_{0}^{\frac{t}{\varepsilon^{2}}} f_{0}(y(s)) ds \to_{w} W(t) \text{ as } \varepsilon \to 0$$

Finite ε effects are finite size effects

The Central Limit Theorem

Assume X_i are *i.i.d.* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n \left(X_j - \mu \right) \to_d \mathcal{N}(0,1)$$

where
$$\mu = \mathbb{E}[X_i]$$
 and $\sigma^2 = \mathbb{E}[X_i^2]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0,\sigma^2}(x) \times \left(1 + \frac{1}{6\sqrt{n}} \frac{\gamma}{\sigma^3} H_3(x/\sigma)\right) + o(\frac{1}{\sqrt{n}})$$

where $H_3(x) = x^3 - 3x$ is the third Hermite polynomial and γ/σ^3 is the skewness of X_i

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The Central Limit Theorem

Assume X_i are stationary *weakly dependent* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n \left(X_j - \mu \right) \to_d \mathcal{N}(0,1)$$

where $\mu = \mathbb{E}[X_i]$ and $\sigma^2 = \mathbb{E}[X_i^2] + 2\sum_{j=1}^{\infty} \mathbb{E}[X_1 X_{j+1}]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0,\sigma^2 + \delta\sigma^2/n}(x) \times \left(1 + \frac{1}{\sqrt{n}}\delta\kappa H_3(x/\sigma)\right) + o(\frac{1}{\sqrt{n}})$$

where H_3 is the third Hermite polynomial and $\delta\sigma^2$ and $\delta\kappa$ are integrals of correlation functions of X_i (*Götze & Hipp (1983)*)

Stochastic Parametrisation using the Edgeworth expansion

Given a multi-scale dynamical system

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$
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I) determine the Edgeworth expansion coefficients $\sigma_{\rm GK}^2$, $\delta\kappa$ associated with $f_0(x, y)$

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(I) determine the Edgeworth expansion coefficients $\sigma_{\rm GK}^2$, $\delta\kappa$ associated with $f_0(x, y)$

(II) model the multi-scale system by the surrogate stochastic process

$$\begin{split} \dot{X} &= \frac{1}{\varepsilon} A(\eta) + F(X) \\ d\eta &= -\frac{1}{\varepsilon^2} \gamma \eta \, dt + \frac{1}{\sqrt{\varepsilon}} dW_t \end{split} \qquad \mbox{with} \qquad A(\eta) &= a\eta^2 + b\eta + c \\ \mbox{Id Ornstein-Uhlenbeck process} \end{split}$$

where the parameters a, b, c, γ are determined such that the Edgeworth expansion coefficients associated with $A(\eta)$ match $\sigma_{\rm GK}^2$, $\delta\kappa$

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Remark: By construction the homogenised limit system of the original and the surrogate system are the same!

The three time scales of multi-scale systems

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nontrivial fast dynamics trivial slow dynamics $x(t) = x_0$



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trivial slow dynamics $x(t) = x_0$

expect deviations of CLT on timescale $t = \varepsilon$

$$\frac{x(t) - x_0}{\sqrt{t}} \to \sigma(x_0) W_t$$

Consider $\rho_t(x(t)|x(0) = x_0) = \int dx dy \, e^{\mathcal{L}t} \delta_{x_0}(x) \mu(dy)$ for $t = \varepsilon$ $\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$ $\dot{y} = \frac{1}{\varepsilon^2} g_0(y) + \frac{1}{\varepsilon} g_1(x, y)$ $\mathcal{L}_0 \rho = -\partial_y(g_0 \rho), \, \mathcal{L}_1 \rho = -\partial_x(f_0 \rho) - \partial_y(g_1 \rho), \, \mathcal{L}_2 \rho = -\partial_x(f_1 \rho)$

Consider
$$\rho_t(x(t)|x(0) = x_0) = \int dx dy \, e^{\mathcal{L}t} \delta_{x_0}(x) \mu(dy) \quad \text{for} \quad t = \varepsilon$$

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$

$$\dot{y} = \frac{1}{\varepsilon^2} g_0(y) + \frac{1}{\varepsilon} g_1(x, y)$$

$$\mathcal{L}_0 \rho = -\partial_y (g_0 \rho), \ \mathcal{L}_1 \rho = -\partial_x (f_0 \rho) - \partial_y (g_1 \rho), \ \mathcal{L}_2 \rho = -\partial_x (f_1 \rho)$$

Calculate asymptotically, using successive applications of the Duhamel-Dyson formula, up to $\mathcal{O}(\varepsilon^n)$:

$$\frac{\mathbb{E}[x(\varepsilon) - x_0]}{\sqrt{\varepsilon}} = \sqrt{\epsilon} \,\xi = \sqrt{\epsilon} \langle f_1(x_0) \rangle$$
$$\frac{\mathbb{E}[\hat{x}^2]}{\varepsilon} = \sigma_{\mathrm{GK}}^2 - 2\varepsilon \int_0^{\frac{t}{\varepsilon^2}} ds \, (s \langle f_0 e^{\mathcal{L}_0 s} f_0 \rangle - \langle f_0 e^{\mathcal{L}_0 s} f_1 \rangle) + \cdots$$
$$\hat{x} = x - \mathbb{E}[x]$$

$$\frac{\mathbb{E}[\hat{x}^3]}{\varepsilon^{\frac{3}{2}}} = \sqrt{\varepsilon} \int_0^{\frac{t}{\varepsilon^2}} ds_1 \, ds_2 \, \langle f_0 e^{\mathcal{L}_0 s_1} f_0 e^{\mathcal{L}_0 s_2} f_0 \rangle$$

Theorem (Wouters & GAG, 2019)

The Edgeworth expansion of the transition probability $\pi_{\varepsilon}(\xi, t = \varepsilon, x_0)$ for the deterministic multi-scale system up to $\mathcal{O}(\varepsilon^{\frac{3}{2}})$ is given in the limit $t = \varepsilon \ll 1$ and $t/\varepsilon^2 \to \infty$ by

$$\pi_{\varepsilon}(\xi, t = \varepsilon, x_{0}) = \mathbf{n}_{0,\sigma^{2}}(\xi) \left(1 + \sqrt{\varepsilon} \left(\frac{c_{\frac{1}{2}}^{(1)}}{\sigma} H_{1}\left(\frac{\xi}{\sigma}\right) + \frac{c_{\frac{1}{2}}^{(3)}}{3!\sigma^{3}} H_{3}\left(\frac{\xi}{\sigma}\right) \right) + \varepsilon \left(\frac{c_{1}^{(2)} + c_{\frac{1}{2}}^{(1)^{2}}}{2\sigma^{2}} H_{2}\left(\frac{\xi}{\sigma}\right) + \frac{c_{1}^{(4)} + 4c_{\frac{1}{2}}^{(1)}c_{\frac{1}{2}}^{(3)}}{4!\sigma^{4}} H_{4}\left(\frac{\xi}{\sigma}\right) + \frac{c_{\frac{1}{2}}^{(3)^{2}}}{2(3!\sigma^{3})^{2}} H_{6}\left(\frac{\xi}{\sigma}\right) \right) \right) + \mathcal{O}(\varepsilon^{\frac{3}{2}})$$

It involves only the cumulants $c_{\varepsilon}^{(p)}$ with $p \leq 4$ with explicit expressions. These cumulants only involve the leading order measure $\mu_{x_0}^{(0)}$ and, in particular, do not involve the linear response term $\mu_{x_0}^{(1)}$.

(Wouters & GAG, Proc Roy Soc A (2019))






We have used the Edgeworth expansion to push stochastic model reduction past the limit of infinite time scale separation, going beyond the Central Limit Theorem

We have developed a machinery to calculate the Edgeworth corrections for continuous time deterministic systems

The fast dynamics are replaced by a stochastic surrogate process, the parameters of which are tuned to match the Edgeworth expansion corrections of the full multi-scale system

(Wouters & GAG, Proc Roy Soc A (2019) + SIAM MMS (2019))



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Outlook:

Use the strategy for the triad system to apply Edgeworth expansion to the barotropic vorticity equation

- ***** Use Edgeworth expansions in a data-driven approach
- ***** Prove the corrections rigorously (start with stochastic fast dynamics)

Applications of Statistical Limit Theorems

- Data assimilation Ensemble Kalman Filters
- Ensemble forecasting Stochastically perturbed bred vectors
- Linear response theory
- Numerical integration of deterministic multi-scale systems
- Parametrisation of tropical convection

I - Data Assimilation: Ensemble Kalman Filters

using the reduced stochastic model as forecast model leads to reliable ensembles via dynamics-informed inflation



(Mitchell and GAG, JAS (2012); GAG & Harlim, Proc Roy Soc A (2014))

In chaotic systems a single forecast is not meaningful





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 $p(x, 0) \approx \frac{1}{N} \sum_{j=1}^{N} S_{\chi_j} \longmapsto p(x, t) \approx \frac{1}{N} \sum_{j=1}^{N} S_{\chi_j(t)}$

Use ensemble mean and spread to estimate forecast and its uncertainty

A good ensemble should have (at least) these 4 properties (Pazó et al 2010) :



$$p(x, 0) \approx \frac{1}{N} \sum_{j=1}^{N} \delta_{X_j} \longmapsto p(x_j t) \approx \frac{1}{N} \sum_{j=1}^{N} \delta_{X_j}(t)$$



 $\boldsymbol{z}_p(t_i) = \boldsymbol{z}_c(t_i) + \delta \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}$







$$\Delta \boldsymbol{z}(t_{i+1}) = \boldsymbol{z}_p(t_{i+1}) - \boldsymbol{z}_c(t_{i+1})$$





Covariant Lyapunov Vectors \boldsymbol{l}_n $\pi_n^i(t_i) = \left| \frac{\boldsymbol{b}^i(t_j)}{\|\boldsymbol{b}^i(t_j)\|} \cdot \frac{\boldsymbol{l}_n(t_j)}{\|\boldsymbol{l}_n(t_j)\|} \right|$ collapse to a low-dimensional subspace alignment with leading Lyapunov vector bad spread

$$\rho(X,Y,t) = \hat{\rho}(X,t)\rho_{\infty}(Y|X) + \mathcal{O}(\varepsilon) \tag{X: slow}$$

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Multi-scale Lorenz 1996 model

$$\frac{dX_k}{dt} = -X_{k-1}(X_{k-2} - X_{k+1}) - X_k + F - \frac{hc}{b}\sum_{j=1}^J Y_{j,k}$$
$$\frac{dY_{j,k}}{dt} = -cbY_{j+1,k}(Y_{j+2,k} - Y_{j-1,k}) - cY_{j,k} + \frac{hc}{b}X_k$$











SPBVs

- good ensemble diversity
- reliable ensemble
- good forecast skill
- dynamically consistent
- computationally cheap

(Giggins and GAG, QJRMS (2019))

Talagrand diagram





with a unique invariant physical measure $\mu_{arepsilon}$

What is the change of the average of an observable

$$\mathbb{E}^{\varepsilon}[\Psi] = \int_{D} \Psi(x) \, d\mu_{\varepsilon}$$

upon changing the parameter from its unperturbed state with ε_0 ?



$$\mathbb{E}^{\varepsilon}[\Psi] \approx \mathbb{E}^{\varepsilon_0}[\Psi] + \delta \varepsilon \, \mathbb{E}^{\varepsilon_0}[\Psi]' \qquad \varepsilon = \varepsilon_0 + \delta \varepsilon$$

sufficient condition for linear response:

the invariant measure μ_{ε} is differentiable with respect to ε $\mu_{\varepsilon} \approx \mu_{\varepsilon_0} + \mu'_{\varepsilon}(\varepsilon_0)\delta\varepsilon$



Success stories in the Climate Sciences

Leith (1975)

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, Gritsun et al '02/'07, Gritsun & Branstator '07, Ring & Plumb '08, Gritsun '10

coupled climate models: Langen & Alexeev '05, Kirk & Davidoff '09, Fuchs et al '14, Ragone et al '15

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However, rough parameter dependency is known to exist in atmospheric and ocean dynamics



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atmospheric models: North et al '04, Cionni et al '04, Gritsun et al '02/'07, Gritsun & Branstator '07, Ring & Plumb '08, Gritsun '10

coupled climate models: Langen & Alexeev '05, Kirk & Davidoff '09, Fuchs et al '14, Ragone et al '15

However, rough parameter dependency is known to exist in atmospheric and ocean dynamics



Note: even if linear response is **not** valid, this might not be detectable in a finite time series (GAG, Wormell & Wouters '17)

(Chekroun et al '14)

statistical mechanics: Kubo '66

stochastic dynamical systems: Hänggi '78, Hairer & Majda '10

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no linear response for the logistic map

We address here the following conundrum

How can typical observables of high-dimensional systems obey linear response when their microscopic low-dimensional constituents typically do not?









Linear response holds for macroscopic observables provided

- Ψ_n is a stochastic process (diffusive limit)
- the $a^{(j)}$ are distributed according to a sufficiently smooth distribution $\nu(a)$ (heterogeneity)

IV - Numerical integration of multi-scale systems

How does the numerical time integrator affect the statistical behaviour of the simulation?







Remarks: $\hat{\sigma}^2 \Delta t \to \sigma^2$ for $\Delta t \to 0$



Remarks: $\hat{\sigma}^2 \Delta t \to \sigma^2$ for $\Delta t \to 0$ noise is neither Stratonovich nor Itô $\mathbf{E} := -\frac{1}{2} \Delta t \mathbf{h}(\mathbf{X}) \mathbf{h}'(\mathbf{X}) \mathbb{E}[\mathbf{f_0^2}]$ for *i.i.d.* fast dynamics, i.e. $\hat{\sigma}^2 = \mathbb{E}[f_0^2]$, the noise is Itô (dynamics is already rough on time scale of $\mathcal{O}(\Delta t)$) but it is never Stratonovich!
IV - Numerical integration of multi-scale systems

The only difference between the two homogenised equations is

$$\mathbf{E}:=-\frac{1}{2}\Delta t\,\mathbf{h}(\mathbf{X})\mathbf{h}'(\mathbf{X})\,\mathbb{E}[\mathbf{f_0^2}]$$

How can we interpret this extra drift term in the homogenised equation of the discretisation?

Backward error analysis:

appears in first-order schemes, but not in higher order schemes

(Frank & GAG, SIAM MMS (2018))

Can the extra term be significant? It is only $\mathcal{O}(\Delta t)$



15.6% error in mean!

V - The problem of parametrising small-scale convection

The inadequate representation of atmospheric convection in GCMs leads to

- considerable uncertainty in estimating climate sensitivity
- ambiguities in the numerical simulation of the Earth's climate, for example when comparing the inter-model mean and spread of hydrological-cycle related variables of the CMIP5 ensemble to observations.

Deterministic convective parametrisation:

- assumes single possible response of the small-scale convective state for given large-scale atmosphere-ocean state
- capable of only representing a mean effect of convective processes
- lack of variability at small scales (can propagate upscale)
- increase in spatial resolution does not allow for sufficient number of convective events to justify an average



Observational Data

Two data sets at Darwin and Kwajalein

- large scale vertical velocity ω small scale convective activity (convective area fraction)
- 6-hourly time resolution
- I90 x I90 km²(typical size of GCM grid box)
- Darwin has 1890 and Kwajalein has 1095 data points
- At Darwin observations from consecutive wet seasons (2004/2005, 2005/2006, 2006/2007), with a total of 1890 6-hour means. Over Kwajalein, the analysis is applied to the time period of May 2008 Jan 2009 yielding 1095 6-hour means





The Differences



Darwin features land-sea breeze induced convection (diurnal cycles)



The Similarities

 $p^{\text{Kwajalein}}(\text{CAF}(t)|\omega_{500}(t)) \approx p^{\text{Darwin}}(\text{CAF}(t)|\omega_{500}(t) - \Delta_{\omega})$

or analogously

 $p^{\text{Darwin}}(\text{CAF}(t)|\omega_{500}(t)) \approx p^{\text{Kwajalein}}(\text{CAF}(t)|\omega_{500}(t) + \dot{\Delta}_{\omega})$





second-order median regression



Despite the different prevalent atmospheric and oceanic regimes at the two locations, the empirical measure for the convective variables conditioned on large-scale mid-level vertical velocities for the two locations are close

linear shift

This allows us to train the stochastic models at one location and then apply it to the other!

Instantaneous Random Variables







- similarly good results for conditioning on ω_{715} or on rain rates
- cannot resolve periods of sustained non-convection near t=900

(GAG, Peters and Davies, QJRMS (2016))

How can these stochastic parametrizations be used?



The convection scheme

- receives large-scale atmospheric state per grid box (temperature, velocities, humidity,...)
- computes vertical transport of heat, moisture
- provides tendencies to update large-scale fields

The highly challenging problem of triggering convection is performed by the convection scheme



Mass-flux parametrizations

 $M_{\rm cb} = \rho_{\rm air} \ \omega_{\rm cb} \times {\rm CAF}$

proper estimation paramount to determine overall strength of convection Deterministic: assume fixed CAF at 3% Stochastic: CAF conditioned on large-scale ω_{500}

(Wohltmann, Lehmann, GAG et al, GMD (2019))