Computable characterisations of uncertainty in geophysical models

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Acknowledgements

Dedication

Abstract

Chapter ?? introduces

Chapter 1

Introduction

Chapter 2

Background

2.1 Notation

The norm symbol $\|\cdot\|$ without any additional qualifiers denotes the standard Euclidean norm for a vector, and the spectral (operator) norm induced by the Euclidean norm, i.e. for an $n \times n$ matrix A

$$\|A\| = \sup \left\{ \frac{\|Av\|}{\|v\|} \,\middle|\, v \in \mathbb{R}^n, \|v\| \neq 0 \right\}.$$

For example, we say that a random variable A is equal to another random variable B almost surely (a.s.) if $P\left(A = B\right) = 1$.

2.2 Results from dynamical systems

$$\frac{\mathrm{d}w_t}{\mathrm{d}t} = u\left(w_t, t\right), \qquad w_0 = x \in \Omega, \tag{2.1}$$

where $u : \Omega \times [0, T] \to \mathbb{R}^n$ describes the velocity at a point in space and time.

In the mathematical treatment of Lagrangian dynamics, and in particular Lagrangian coherent structures [5], trajectories solving (2.1) are summarised by the flow map. The flow map is an operator mapping

The flow map can be defined formally as follows.

Definition 2.2.1 (Flow map) *Suppose $t_1, t_2 \in [0, T]$. The* ***flow map*** $F_{t_1}^{t_2} : \mathbb{R}^n \to \mathbb{R}^n$ *from time t_1 to t_2 associated with (2.1) is the unique solution to*

$$\frac{\partial F_{t_1}^{\tau}(x)}{\partial \tau} = u\left(F_{t_1}^{\tau}(x), \tau\right), \qquad F_{t_1}^{t_1}(x) = x, \tag{2.2}$$

solved up to time $\tau = t_2$. Equivalently,

$$F_{t_1}^{t_2}(x) = x + \int_{t_1}^{t_2} u\left(F_{t_1}^{\tau}(x), \tau\right) \mathrm{d}\tau.$$

The flow map satisfies the following properties

The gradient of the flow map satisfies a useful property; the equation of variations.

Theorem 2.2.1 *Let $F_{t_1}^t$ be the flow map corresponding to (2.1). Then, the spatial gradient $\nabla F_{t_0}^t(x)$ satisfies the equation of variations*

$$\frac{\partial \nabla F_{t_1}^t(x)}{\partial t} = \nabla u\left(F_{t_1}^t(x), t\right) \nabla F_{t_1}^t(x). \tag{2.3}$$

Proof. Taking the gradient on both sides of (2.2) and using the chain rule gives

$$\nabla\left(\frac{\partial F_{t_1}^{t_2}(x)}{\partial t}\right) = \nabla u\left(F_{t_1}^t(x), t\right) \nabla F_{t_1}^t(x).$$

SMOOTHNESS □

An important inequality

Theorem 2.2.2 (Grönwall's inequality) *Let $\alpha, \beta, u : [a, b] \to \mathbb{R}$ be functions such that β and u are continuous and that the negative part of α is integrable on every closed and bounded subset of $[a, b]$. Then, if β is non-negative and for all $t \in [a, b]$,*

$$u(t) \leq \alpha(t) + \int_a^t \beta(\tau) u(\tau) \, \mathrm{d}\tau$$

then

$$u(t) \leq \alpha(t) + \int_a^t \alpha(\tau)\beta(\tau) \exp\left(\int_\tau^t \beta(s) \, \mathrm{d}s\right) \mathrm{d}\tau.$$

Additionally, if α is non-decreasing, then

$$u(t) \leq \alpha(t) \exp\left(\int_a^t \beta(\tau) \, \mathrm{d}\tau\right)$$

2.3 Stochastic differential equations

$$\mathrm{d}y_t = u\left(y_t, t\right) \mathrm{d}t + \sigma\left(y_t, t\right) \mathrm{d}W_t. \tag{2.4}$$

A solution to the stochastic differential equation can be defined rigorously [10].

Definition 2.3.1 *A stochastic process $\{y_t\}_{t\in[0,T]}$ taking values in R^n is said to be a* ***strong solution*** *of (2.4) with initial condition $y_0 = \xi$ if the following holds:*

1. *For each t,*
2. $$\int_0^T \left(\left\|u\left(y_t,t\right)\right\| + \left\|\sigma\left(y_t,t\right)\right\|^2\right) \mathrm{d}t < \infty \text{ a.s.}$$
3. *For each $t \in [0,T]$,*
$$y_t = \xi + \int_0^t u\left(y_\tau,\tau\right) \mathrm{d}\tau + \int_0^t \sigma\left(y_\tau,\tau\right) \mathrm{d}W_\tau \quad \text{a.s.}$$

Theorem 2.3.1 *Then, (2.4) has a unique strong solution.*

Proof. See Theorem 6.2.1 of [10], for instance. □

2.3.1 Analytical tools for Itô calculus

There are several tools available for the analytic treatment of Itô integrals and solutions to stochastic differential equations, which we make use of throughout. The first is Itô's Lemma (or the Itô Formula), which is a change-of-variables formula in stochastic calculus and can be thought of as a generalisation of the chain rule from deterministic calculus. We state and use the multidimensional form of the Lemma for solutions to Itô stochastic differential equations, although more general forms exist (e.g. see Theorem 5.4.1 of [7]).

Theorem 2.3.2 (Itô's Lemma) *Let X_t be the strong solution to the stochastic differential equation*

$$\mathrm{d}X_t = a\left(X_t,t\right)\mathrm{d}t + b\left(X_t,t\right)\mathrm{d}W_t,$$

where $a : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}^n$, $b : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}^{n\times p}$ and W_t is the canonical p-dimensional Wiener process. If $f : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}^m$ is twice continuously-differentiable, then the stochastic process $Y_t := f\left(X_t,t\right)$ is a strong solution to the stochastic differential equation

$$\begin{aligned}\mathrm{d}Y_t = &\left(\frac{\partial f}{\partial t}\left(X_t,t\right) + \nabla f\left(X_t,t\right)a\left(X_t,t\right) + \frac{1}{2}\mathrm{tr}\left[b\left(X_t,t\right)^\intercal \nabla\nabla f\left(X_t,t\right)b\left(X_t,t\right)\right]\right)\mathrm{d}t \\ &+ \nabla f\left(X_t,t\right)b\left(X_t,t\right)\mathrm{d}W_t.\end{aligned}$$

Proof.

□

Theorem 2.3.3 (Burkholder-Davis-Gundy Inequality) *Let M_t be an Itô-integrable stochastic process taking values in $\mathbb{R}^n$. Then, for any $p > 0$ there exists constants $c_p, C_p > 0$ independent of the stochastic process M_t such that*

$$c_p \mathbb{E}\left[\left(\int_0^t \left\|M_\tau\right\|^2 \mathrm{d}\tau\right)^p\right] \leq \mathbb{E}\left[\sup_{\tau\in[0,t]}\left\|\int_0^\tau M_s \,\mathrm{d}W_s\right\|^{2p}\right] \leq C_p \mathbb{E}\left[\left(\int_0^t \left\|M_\tau\right\|^2 \mathrm{d}\tau\right)^p\right].$$

Proof.

□

2.4 Aspects of stochastic parameterisation

When using deterministic systems to model real-world phenomena, there are many ways in which uncertainty can arise. For instance,

Stochastic parameterisation is a These unresolved subgrid effects are accounted for by introducing stochastic noise into the otherwise deterministic model.

Berner et al. [6]

Leutbecher et al. [11]

2.4.1 Additive versus multiplicative noise

When $\sigma = \sigma(t)$ depends only on t, then noise is considered *additive*. If there is spatial dependence in σ, i.e. $\sigma = \sigma(x, t)$, then the noise considered *multiplicative*.

For instance, Sura et al. [12] shows that the non-Gaussian statistics observed in atmospheric regimes can arise from linear models with multiplicative noise.

2.5 Stochastic sensitivity

In most practical situations, the Eulerian velocity data driving ocean and atmospheric models relies upon measurements of estimates obtained on a low resolution spatial discretisation.

There are limited tools within the LCS context that explcitly characterise the impact of these uncertainties As such, there is recent interest in addressing this deficiency [? 2] . Balasuriya [3] introduces stochastic sensitivity as a new tool for directly quantifying the impact of Eulerian uncertainty on Lagrangian trajectories. The evolution of Lagrangian trajectories is modelled as solution to a Itô stochastic ordinary differential equation.

need some eeva cita- e

TODO: Deterministic

The SDE model is

$$\mathrm{d}y_t = u\left(y_t, t\right)\mathrm{d}t + \epsilon\sigma\left(y_t, t\right)\mathrm{d}W_t, , \tag{2.5}$$

where $0 < \epsilon \ll 1$ is a parameter quantifying the scale of the noise, $\sigma : \mathbb{R}^2 \times [0, T] \to \mathbb{R}^{2\times 2}$ is the 2×2 diffusion matrix, and W_t is the canonical two-dimensional Wiener process. Since σ can vary by both space and time, the noise is multiplicative.

To quantify uncertainty in a way that is independent of the noise scale ϵ, [3] defined the random variable $z_\epsilon(x, t)$ on $\mathbb{R}^2 \times [0, T]$ as

$$z_\epsilon(x, t) := \frac{y_t - F_0^t(x)}{\epsilon}.$$

The main aim is to compute statistics of z_ϵ at the final time T, so that of $z_\epsilon(x, T)$. Balasuriya [3] then considers the signed projection of $z_\epsilon(x, T)$ onto a ray emanating from the deterministic position $F_0^T(x)$ in a given direction, defining

$$P_\epsilon(x, \theta) := \hat{n}^\intercal z_\epsilon(x, T),$$

where $\theta \in \left[-\pi/2, \pi/2\right)$ and

$$\hat{n}(\theta) = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}.$$

The statistics of $z_\epsilon(x, T)$ and $P_\epsilon(x, \theta)$ are considered in the limit as $\epsilon \downarrow 0$, which

TODO: something

.

The first result established by [3] is that the expected location is deterministic, in the following sense.

Theorem 2.5.1 **([3])** *For all $x \in \mathbb{R}^2$,*

$$\lim_{\epsilon\downarrow 0} \mathbb{E}\left[z_\epsilon(x, T)\right] = 0.$$

The variance of $P_\epsilon(x, \theta)$ is used to assign a computable scalar measure of uncertainty to the trajectory.

Definition 2.5.1 **([3])** *a) The **anisotropic uncertainty** is a scalar field $A : \mathbb{R}^2 \times \left[-\pi/2, \pi/2\right) \to [0, \infty)$ defined by*

$$A(x, \theta) := \sqrt{\lim_{\epsilon\downarrow 0} \mathbb{V}\left[P_\epsilon(x, \theta)\right]}.$$

*b) The **stochastic sensitivity** is a scalar field $S : \mathbb{R}^2 \to [0, \infty)$ defined by*

$$S^2(x) := \lim_{\epsilon\downarrow 0} \sup_\theta \mathbb{V}\left[P_\epsilon(x, \theta)\right].$$

By employing techniques from both deterministic and stochastic calculus (i.e. Grönwall's inequality, the Burkholder-Davis-Gundy inequality, Itô's Lemma), Balasuriya further established expressions for both the anisotropic uncertainty and the stochastic sensitivity that are computable given only the flow map and velocity data.

Theorem 2.5.2 ([3]) *For $x \in \mathbb{R}^2$, set $w := F_0^t(x)$. Then, for any $\theta \in \left[-\pi/2, \pi/2\right)$,*

$$A(x,\theta) = \left(\int_0^T \left\|\Lambda\left(x,t,T\right) J\hat{n}(\theta)\right\| \mathrm{d}t\right)^{1/2},$$

where

$$\Lambda\left(x,t,T\right) := e^{\int_t^T \left[\nabla\cdot u\right]\left(F_0^\xi(x),\xi\right)\mathrm{d}\xi} \sigma\left(F_0^t(x),t\right)^\intercal J\nabla_w F_T^t\left(w\right),$$

with the gradients ∇_w of the flow map taken with respect to the mapped position w, and

$$J := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Additionally, stochastic sensitivity is computed as

$$S^2(x) = P(x) + N(x),$$

with

$$\begin{aligned}
L(x) &:= \frac{1}{2}\sum_{i=1}^{2}\int_0^T \left[\Lambda_{i2}\left(x,t,T\right)^2 - \Lambda_{i1}\left(x,t,T\right)^2\right]\mathrm{d}t \\
M(x) &:= \sum_{i=1}^{2}\int_0^T \Lambda_{i1}\left(x,t,T\right)\Lambda_{i2}\left(x,t,T\right)\mathrm{d}t \\
N(x) &:= \sqrt{L^2(x) + M^2(x)} \\
P(x) &:= \left|\frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\int_0^T \Lambda_{ij}\left(x,t,T\right)^2\mathrm{d}t\right|,
\end{aligned}$$

where Λ_{ij} is the (i,j)-element of Λ.

2.5.1 Current applications & shortcomings

Since stochastic sensitivity is only a recent development, it has only been applied in a limited number of places so far. Here, we briefly review the literature in which the original formulation stochastic sensitivity by [3] has been applied.

- Balasuriya [4] uses stochastic sensitivity to compute an error bound for the finite-time Lyapunov computation.
- Fang et al. [8]
- Badza et al. [1] investigate the impact of velocity uncertainty on Lagrangian coherent structures (e.g. see the reviews by Balasuriya et al. [5] and Hadjighasem et al. [9]) extracted as robust sets with stochastic sensitivity.

Although

1. The tools are restricted to two-dimensional models, and the constructions using projections have no obvious extension to n-dimensions. Extending stochastic sensitivity to n-dimensions will enable application to a much broader class of models beyond the fluid flow context, including high-dimensional climate and ??? models.
2. Balasuriya [3] only computes the expectation and variance of the projections $P_\epsilon(x, \theta)$, which does not give us the distribution under the limit as ϵ approaches 0.
3. The computational formula for the anisotropic uncertainty and stochastic sensitivity require knowledge of the divergence $\nabla \cdot u$ of the velocity field.

Chapter 3

Extending stochastic sensitivity

There are several shortcomings of [3] that warrant further extension, namely:

Chapter 4

The Gaussian Limit

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