Computable characterisations of uncertainty in geophysical models

Liam Blake

March 7, 2023

Thesis submitted for the degree of
Master of Philosophy
in
Applied Mathematics
at The University of Adelaide
Faculty of Sciences, Engineering and Technology
School of Computer and Mathematical Sciences

THE UNIVERSITY
of ADELAIDE

Contents

List of Tables

List of Figures

Signed Statement

I certify that this work contains no material which has been accepted for the award of any other degree or diploma in my name in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission in my name for any other degree or diploma in any university or other tertiary institution without the prior approval of the University of Adelaide and where applicable, any partner institution responsible for the joint award of this degree.

I give consent to this copy of my thesis, when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968.

I also give permission for the digital version of my thesis to be made available on the web, via the University's digital research repository, the Library Search and also through web search engines, unless permission has been granted by the University to restrict access for a period of time.

Signed: ..... Date: .....

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 $P(A = B) = 1$.

2.2 Results from dynamical systems

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

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 [6], 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, under ASSUMPTIONS? For any $r, s, t \in [0, T]$ and points $x, w \in \mathbb{R}^n$,

1. F_s^t is invertible with inverse

$$\left[F_s^t\right]^{-1}(w) = F_t^s(w).$$

2. $F_s^t\left(F_r^s(x)\right) = F_r^t(x)$

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

For an introduction to stochastic differential equations, see Øksendal [30] or Kallianpur and Sundar [22].

Definition 2.3.1 (Canonical Wiener process)

The differential form of an n-dimensional Itô stochastic differential equation is

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

where the solution y_t is a stochastic process taking values in $\mathbb{R}^n$, $u : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is the drift and $\sigma : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^{n\times n}$ is the diffusivity. The driving process W_t is the canonical, n-dimensional Wiener process as defined in Definition 2.3.1. For a (possibly random) initial condition y_0, the solution y_t to (2.4) satisfies

$$y_t = y_0 + \int_0^t u\left(y_\tau, \tau\right)\mathrm{d}\tau + \int_0^t \sigma\left(y_\tau, \tau\right)\mathrm{d}W_\tau. \tag{2.5}$$

In the most general case, the drift u and diffusivity σ are permitted to themselves be random functions [22], but in this thesis we assumed that both are deterministic.

As with deterministic differential equations, we are interested in knowing precisely when solutions to (2.4) exist, and whether these solutions are unique.

A solution to the stochastic differential equation can be defined rigorously [22].

Definition 2.3.2 *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. $$\int_0^T \left(\left\|u\left(y_t, t\right)\right\| + \left\|\sigma\left(y_t, t\right)\right\|^2\right)\mathrm{d}t < \infty \ a.s.$$
3. *For each $t \in [0, T]$,*
$$y_t = \xi + \int_0^t u\left(y_\tau, \tau\right)\mathrm{d}\tau + \int_0^t \sigma\left(y_\tau, \tau\right)\mathrm{d}W_\tau \quad a.s.$$

Solutions are known as *strongly unique* if, for any two strong solutions x_t and y_t to (2.4) defined on the same measure space,

$$P\left(x_t = y_t, \quad \forall t \in [0, T]\right) = 1$$

That is, x_t and y_t are equal almost surely.

We can now state the requirements for (2.4) to have unique solutions.

Theorem 2.3.1 (Kallianpur and Sundar [22]) *Let u_i be the ith component of u and σ_{ij} the (i,j)th component of σ, for $i,j = 1,\dots,n$. Suppose that for each $i,j = 1,\dots,n$,*

(i) u_i is Borel-measurable, and

(ii) σ_{ij} is Borel-measurable.

Suppose further that for all $t \in [0,T]$ and $x,y \in \mathbb{R}^n$, there is a positive constant K independent of t and x,y such that

(iii) $\left\|u(x,t)\right\|^2 + \left\|\sigma(x,t)\right\|^2 \leq K\left(1 + \|x\|^2\right)$ *a.s.*

(iv) $\left\|u(x,t) - u(y,t)\right\|^2 + \left\|\sigma(x,t) - \sigma(y,t)\right\|^2 \leq K\|x-y\|$ *a.s.*

Then, (2.4) has a strongly unique strong solution.

Proof. See Theorem 6.2.1 of [22], 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 [22]).

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

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

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 $Y_t \coloneqq f(X_t,t)$ is a strong solution to the stochastic differential equation

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

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*

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

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. [7]

Leutbecher et al. [27]

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. [38] 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 [**?** 3] . Balasuriya [4] 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.

Probably ne some non-Sa citations her

TODO: Deterministic

The SDE model is

$$\mathrm{d}y_t = u\left(y_t, t\right)\mathrm{d}t + \varepsilon\sigma\left(y_t, t\right)\mathrm{d}W_t, , \tag{2.6}$$

where $0 < \varepsilon \ll 1$ 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, [4] defined the random variable $z_\varepsilon(x, t)$ on $\mathbb{R}^2 \times [0, T]$ as

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

The main aim is to compute statistics of z_ε at the final time T, so that of $z_\varepsilon(x, T)$. Balasuriya [4] then considers the signed projection of $z_\varepsilon(x, T)$ onto a ray emanating from the deterministic position $F_0^T(x)$ in a given direction, defining

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

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

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

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

TODO: something

.

The first result established by [4] is that the expected location is deterministic, in the following sense.

Theorem 2.5.1 ([4]) *For all $x \in \mathbb{R}^2$,*

$$\lim_{\varepsilon\downarrow 0} \mathbb{E}\big[z_\varepsilon(x, T)\big] = 0.$$

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

Definition 2.5.1 ([4]) *a) The **anisotropic uncertainty** is a scalar field $A : \mathbb{R}^2 \times \big[-\pi/2, \pi/2\big) \to [0, \infty)$ defined by*

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

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

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

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 ([4]) *For $x \in \mathbb{R}^2$, set $w \coloneqq F_0^t(x)$. 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

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

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

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

Additionally, stochastic sensitivity is computed as

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

with

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

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 [4] has been applied.

- Balasuriya [5] uses stochastic sensitivity to compute an error bound for the finite-time Lyapunov computation.
- Fang et al. [17]
- Badza et al. [2] investigate the impact of velocity uncertainty on Lagrangian coherent structures (e.g. see the reviews by Balasuriya et al. [6] and Hadjighasem et al. [19]) 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 [4] only computes the expectation and variance of the projections $P_\varepsilon(x, \theta)$, 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

Publication: Gaussian characterisation of model uncertainty

The following is a copy of the published article by Blake et al. [10].

3.1 Statement of Authorship

3.2 Introduction

Many phenomena across geophysical, biological and socio-economic applications can be modelled using a continuous-time dynamical system, i.e., an ordinary differential equation [11, 39, 40, e.g.]. Given initial values of a multi-dimensional state variable, such equations can be solved numerically to predict the state at future times. The governing dynamics may be specified using existing phenomenological models, but in modern applications these are usually supplemented or driven by observed data. Standard examples include the modelling of weather using available data [25, 33], and predicting concentrations of, for instance, temperature, pollutants or phytoplankton in the ocean using observed current velocity data [1, 16].

All methods using this approach have uncertainties in the model specification arising from a variety of sources [17]: the model not capturing all phenomena because of the inevitable lack of a complete understanding of all processes involved, errors in measured data, information only available on spatio-temporal grids (resolution error), etc. In the absence of any other understanding of these multitudinous issues, a well-established way of tackling such uncertainties in the model is to think of these as stochastic [7, 30]. Running many realisations of stochastic perturbations to the deterministic model can generate statistics to improve predictions and estimate their associated uncertainties [2, 13, e.g.]. However, in practice a very large number of simulations is necessary to generate convergent statistics [18, 26]. Thus, numerically solving such stochastic systems – potentially with

data-based terms – is often computationally expensive, and does not necessarily provide conceptual insight into how the model uncertainties affect predictions.

Clearly, possessing a broader theoretical understanding of how stochastic terms impact continuous dynamical systems would be valuable. Stochastic differential equations (SDEs) provide a natural framework for introducing uncertainty, as a noise process, into the continuous time evolution of a variable. Generally, in modelling situations the dynamics are highly nonlinear and one expects the noise to be multiplicative (i.e. vary with both state and time), e.g. in atmospheric [37, 38] and oceanic [23] systems and from experimental and observational considerations. Such SDEs are intractable to solve analytically [30] and computationally expensive to simulate accurately [29]. Having a data-based model—that is, possessing terms in the equations which are driven by data rather than by explicitly specified functions—renders additional problems in obtaining a theoretical understanding of the prediction error.

A common intuitive approach to characterising the uncertainty arising from an otherwise analytically intractable nonlinear SDE is via a multivariate Gaussian approximation, which is used across a diversity of literature. For instance, one can formally "linearise" the SDE in some sense to obtain a Gaussian density, and this approach is used in filtering theory [20]. Other approaches first assume a Gaussian distribution and obtain formal computations for its mean and covariance [36]. However, both approaches lack rigorous justification and a precise understanding of *how* the Gaussian distribution arises from the nonlinear SDE. This is particularly the case when the noise is multiplicative, which is a situation that is often ignored but necessary in practice. Sanz-Alonso and Stuart [35] partially addressed these issues, by showing that the Kullback-Leibler (KL) divergence between the solutions of autonomous SDEs with additive noise and a linearised equivalent can be bounded by the scale of the noise. In this manuscript, we relax the hypotheses of [35] to cater for time-dependent coefficients and for multiplicative noise. Furthermore, our result explicitly establishes the convergence rate of all moments of the deviation considered in [35], which cannot be inferred from the KL divergence alone.

In this paper, we remedy this deficiency by proving rigorously that the noise-scaled deviation between the SDE solution and a reference deterministic solution converges towards a multivariate Gaussian distribution, in the limit of small noise. We consider a general class of SDEs with fully non-autonomous terms and multiplicative noise. The Gaussian distribution arises as the solution to a formal linearisation of the SDE about a deterministic trajectory (in the absence of noise). By bounding all raw moments of the difference between the SDE and the linearised solutions by the noise scale (see Theorem 3.3.1), we show that the stochastic deviation converges in distribution to a multivariate Gaussian random variable (see Theorem 3.3.2). The covariance matrix characterising this Gaussian can be explicitly written in terms of the flow map of the underlying deterministic system and the (potentially spatio-temporally varying) diffusion matrix, and is available even if the deterministic model is only available via data. The

Gaussian distribution is consistent with that seen in other literature [20, 35, 36], while we additionally show convergence of *all* the moments of the deviation distribution. The results hold independently of the initial condition and for all finite times; the uncertainty evolution of any deterministic trajectory with time is therefore encapsulated in our results.

The quantification of prediction uncertainty that we present here was originally motivated by the "stochastic sensitivity" approach of Balasuriya [4]. In the context of two-dimensional, unsteady fluid flow, stochastic sensitivity works with Eulerian velocity data as the underlying deterministic model, and seeks to quantify the uncertainty in an eventual Lagrangian trajectory location. This methodology was developed as a tool for determining Lagrangian coherent structures (LCS) [6, 19] in fluid flows, in that clusters of trajectories which have small uncertainty may be thought of as more "coherent" than others. In particular, [4] derived the limiting mean and variance of the noise-scaled deviation, and provided computable expressions in terms of the deterministic flow map and velocity field. However, this was restricted to two-dimensional systems and did not characterise the limiting distribution itself.

The contributions of this work are:

- In Section 3.3, we prove rigorously that all moments of the noise-scaled solution to a multidimensional stochastic differential equation with non-autonomous coefficients and multiplicative noise converges towards those of a linearised SDE, in the limit of small noise. The Gaussian distribution solving the linearised SDE appears in other literature and applications but often lacks justification [20, 36]. On the other hand, when the linearisation is justified, this is disregarding time-dependence in the coefficients and multiplicative noise [35].

- We present characterisations of the limiting Gaussian distribution in terms of gradients of *either* the velocity field (as an ODE consistent with that arising elsewhere [20, 35, 36]) or the deterministic flow map. The latter is an alternative characterisation that allows the Gaussian distribution to be computed *entirely from the solution dynamics* of a determinstic model and specification of any multiplicative noise effects known prior.

- In Section 3.4, we generalise the two-dimensional stochastic sensitivity approach of [4] to arbitrary dimensions. Our expressions enable the computation of stochastic sensitivity in any dimension, as a scalar measure of uncertainty about any solution trajectory of the deterministic model. This also extends stochastic sensitivity as a means of Lagrangian coherent structure extraction to fluid flows of arbitrary dimension.

- In Section 3.5, we validate the results of Section 3.3 using stochastic simulations from a 2-dimensional model. In particular, we demonstrate that the first four moments of the distance between the realisations and the Gaussian limit follow the predicted

bound. We also illustrate a key prediction from Section 3.4; that the computable covariance matrix of the Gaussian limit captures the time-evolution of uncertainty, even when the noise is multiplicative.

This work is relevant to the well-known "stochastic parameterisation" approach in weather and climate modelling, in which stochastic components are introduced to account for unresolved subgrid effects [7, 27, 31]. Since this work is fundamental, in establishing a convergence result for a general class stochastic differential equations, we do not explicitly describe how to construct an appropriate stochastic parameterisation (e.g. specification of the coefficients of the SDE). Instead, we expect that this result will be useful in the analysis of stochastic parameterisations, and to convert otherwise computationally expensive schemes into an efficient approximations, a goal explicitly identified in [27]. We also expect that this work will find application in data assimilation [12, 20, 25, 33], as a means of characterising forecast uncertainty. The original stochastic sensitivity tools have been applied to identify Lagrangian coherent structures (LCSs) in 2-dimensional fluid flow [2, 4]. By extending the theory of these tools into arbitrary dimensions, our results can also be used to extract coherent structures in n-dimensional flows. These potential applications are discussed in Section 3.6.

3.3 The Gaussian limit

Suppose we are interested in the evolution of a $\mathbb{R}^n$-valued state variable y_t over a finite time interval $[0, T]$. Our model, accounting for uncertainties arising from a range of sources, for the evolution of this variable is the Itô stochastic differential equation

$$\mathrm{d}y_t^{(\varepsilon)} = u\left(y_t^{(\varepsilon)}, t\right)\mathrm{d}t + \varepsilon\,\sigma\left(y_t^{(\varepsilon)}, t\right)\mathrm{d}W_t, \tag{3.1}$$

where $u : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n$ is the governing reference vector field, and can be inferred from underlying physics or available data, for instance. The canonical n-dimensional Wiener process W_t is a continuous white-noise stochastic process with independent Gaussian increments. The scale of the noise is parameterised as $0 < \varepsilon \ll 1$ and $\sigma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^{n\times n}$ is a deterministic diffusion matrix. The noise in (3.1) is multiplicative, in that the diffusion matrix σ can vary with both state and time. We assume that σ is specified *a priori*, or if no such information is known, then $\sigma \equiv I_n$, the $n \times n$ identity matrix, is a default choice. We assume certain generic smoothness and boundedness conditions on the various functions outlined; these are stated explicitly in **??** in **??** and ensure the existence of unique solutions to (3.1). The stochastic solution $y_t^{(\varepsilon)}$ to (3.1) describes the evolution of the state variable through time, accounting for ongoing uncertainty with noise-scale ε.

In the absence of any uncertainty (i.e. $\varepsilon = 0$), (3.1) reduces to the ordinary differential equation

$$\frac{\mathrm{d}w_t}{\mathrm{d}t} = u\left(w_t, t\right). \tag{3.2}$$

Let the flow map $F_0^t : \mathbb{R}^n \to \mathbb{R}^n$ be the function which evolves an initial condition from time 0 to time t according to the flow of (3.2). We refer to (3.2) as the *reference* deterministic model associated with (3.1) in that it either demonstrates the dominant physics (as would be the case if we think of the noise in (3.1) as capturing stochastic parameterisation) or is the best-available model (for example if u is available from data, and (3.1) represents the uncertainty of such data). Solutions to the reference deterministic model are more readily available, e.g. in terms of computational efficiency when solving numerically, than those of the stochastic model, but do not account for inevitable uncertainty. Here, we establish a Gaussian characterisation and approximation of the solution to (3.1) constructed from the deterministic flow map, thereby taking advantage of the easily available solutions to (3.1) and avoiding the need for computationally expensive stochastic simulation.

To characterise the uncertainty, we fix the *identical* initial condition $x \in \mathbb{R}^n$ to *both* the stochastic model (3.1) and the reference deterministic model (3.2), and consider their evolution in time. We will show that the stochastic deviation between solutions of these can be characterised exactly in terms of a Gaussian in the limit of small noise, i.e. $\varepsilon \to 0$. This quantifies the time-evolving uncertainty of predictions from the deterministic model (3.2). We provide explicit analytical expressions for the limiting distribution, written in terms of the flow map of the deterministic system and σ, thereby providing strong theoretical insight while nullifying the need to perform expensive SDE simulations in approximating such a distribution.

To express our results, we define the noise-scaled deviation

$$z_t^{(\varepsilon)}(x) := \frac{y_t^{(\varepsilon)} - F_0^t(x)}{\varepsilon}, \quad z_0^{(\varepsilon)}(x) = 0, \tag{3.3}$$

where $x \in \mathbb{R}^n$ is fixed and certain, and satisfies $y_0^{(\varepsilon)} = x$. We wish to understand the limiting behaviour of $z_t^{(\varepsilon)}(x)$ as ε approaches zero.

Theorem 3.3.1 (All moments are bounded) *Fix $x \in \mathbb{R}^n$ and let $z_t(x)$ be the solution to the linearised SDE*

$$\mathrm{d}z_t(x) = \nabla u\left(F_0^t(x), t\right) z_t(x)\,\mathrm{d}t + \sigma\left(F_0^t(x), t\right)\mathrm{d}W_t, \quad z_0(x) = 0, \tag{3.4}$$

where W_t is the same *Wiener process driving (3.1). Then for any $r \geq 1$ and $t \in [0, T]$, there exists a $D_r(t) \in [0, \infty)$ independent of x such that for all $\varepsilon > 0$,*

$$\mathbb{E}\left[\left\|z_t^{(\varepsilon)}(x) - z_t(x)\right\|^r\right] \leq D_r(t)\,\varepsilon^r, \tag{3.5}$$

where $\|\cdot\|$ is the Euclidean norm.

Proof. See **??**. Showing the result employs the Burkholder-Davis-Gundy inequality, Grönwall's inequality, Taylor's theorem and the bounds placed on the SDE coefficients, to explicitly construct the bounding coefficient $D_r(t)$. □

Taking the limit as ε approaches 0 in (3.5) shows that $z_t^{(\varepsilon)}(x)$ converges in rth moment to $z_t(x)$, which in turn implies convergence in probability and convergence in distribution (or weak convergence). It is important to note that the stochastic differential equation (3.1) and the linearised equation (3.4) must be defined with the *same* Wiener process W_t for Theorem 3.3.1 to hold as stated. However, by weakening the convergence we can think of $z_t^{(\varepsilon)}(x)$ as converging to a Gaussian distribution (the distribution of the linearised solution) with no reference to the driving Wiener process.

Theorem 3.3.2 (Explicit Gaussian limit) *For any $x \in \mathbb{R}^n$ and $t \in [0, T]$,*

$$z_t^{(\varepsilon)}(x) \xrightarrow{d} \mathcal{N}\left(0, \Sigma(x,t)\right) \quad \text{as} \quad \varepsilon \to 0,$$

where the covariance matrix Σ is given by

$$\Sigma(x,t) = \int_0^t L\left(x,t,\tau\right) L\left(x,t,\tau\right)^\intercal \, \mathrm{d}\tau, \tag{3.6}$$

with

$$L\left(x,t,\tau\right) \coloneqq \nabla F_0^t(x) \left[\nabla F_0^\tau(x)\right]^{-1} \sigma\left(F_0^\tau(x), \tau\right). \tag{3.7}$$

Moreover, the covariance matrix Σ is the matrix solution to the ordinary differential equation

$$\frac{\mathrm{d}\Sigma}{\mathrm{d}t} = \left[\nabla u\left(F_0^t(x), t\right)\right] \Sigma + \Sigma \left[\nabla u\left(F_0^t(x), t\right)\right]^\intercal + \sigma\left(F_0^t(x), t\right) \sigma\left(F_0^t(x), t\right)^\intercal, \tag{3.8}$$

subject to $\Sigma(x, 0) = O$, the $n \times n$ zero matrix.

Proof. See **??**. The Gaussianity of the limiting process $z_t(x)$, and therefore the limit in distribution of $z_t^{(\varepsilon)}(x)$, is first established, and then the explicit expression for the covariance matrix Σ is derived by employing Itô's isometry and properties of the flow map. □

The covariance matrix Σ uniquely characterises the limiting Gaussian distribution in Theorem 3.3.2, and captures the impact of both the deterministic dynamics of the model (through the flow map gradients) and multiplicative noise (by evaluating the diffusion matrix σ along the deterministic trajectory). Through (3.6) and (3.7), the Gaussian distribution can be computed entirely from flow map data and specification of σ, without any reference to the governing vector field u in (3.2). Alternatively, if the velocity gradients ∇u are available, then Σ can be computed as the solution to (3.8). Solving (3.2) and (3.8) jointly describes the scheme for computing the Gaussian approximation seen elsewhere,

e.g. Algorithm 9.4 of [36] or Equations (1.2) and (1.3) of [35]. Moreover, for a fixed time $t \in [0, T]$, Theorem 3.3.2 justifies the approximation

$$y_t^{(\varepsilon)} \dot{\sim} \mathcal{N}\left(F_0^t(x), \varepsilon^2 \Sigma(x,t)\right), \tag{3.9}$$

for small values of ε.

The theoretical results in this section, and the computability of the limiting distribution will be verified with numerical simulation of an example in Section 3.5. This theory has many applications and extensions which are discussed in Section 3.6.

3.4 Extending stochastic sensitivity

The covariance matrix Σ provides a direct extension of the stochastic sensitivity tools first introduced by Balasuriya [4] for the fluid flow context. Here, the deterministic model (3.2) is seen as a "best-available" model for the evolution of trajectories, and the driving vector field u is the Eulerian velocity of the fluid. Stochastic sensitivity ascribes a scalar value to each deterministic trajectory by computing the maximum variance of the scaled deviations, when projected onto rays emanating from the origin [4]. The natural restating of this original definition of stochastic sensitivity [4] in the n-dimensional setting is as follows:

Definition 3.4.1 (Stochastic sensitivity in $\mathbb{R}^n$) *The* stochastic sensitivity *is a scalar field* $S^2 : \mathbb{R}^n \times [0,T] \to [0,\infty)$ *given by*

$$S^2(x,t) := \limsup_{\varepsilon \downarrow 0} \left\{ \mathbb{V}\left[p^\intercal z_t^{(\varepsilon)}(x)\right] \ : \ p \in \mathbb{R}^n, \|p\| = 1 \right\}.$$

Definition 3.4.1 is in the spirit of principal components analysis [21], performing a dimension reduction by projecting onto the direction in which the variance is maximised, thus capturing the most uncertainty in the data with a scalar value.

The anisotropic uncertainty in two-dimensions [4] is the direction-dependent projection (prior to optimising over all directions in Definition 3.4.1). Explicit theoretical expressions for both the stochastic sensitivity and the anisotropic sensitivity in two dimensions were obtained by Balasuriya [4]; these allowed for quantifying certainty in eventual trajectory locations without having to perform stochastic simulations. We show here that our results in n-dimensions are a generalisation of the two-dimensional ones in [4], which moreover establish Gaussianity as well as an explicit expression for the uncertainty measure. A theoretically pleasing and computable expression for the stochastic sensitivity is obtainable:

Theorem 3.4.1 (Computation of S^2) *For any $x \in \mathbb{R}^n$ and $t \in [0,T]$,*

$$S^2(x,t) = \left\|\Sigma(x,t)\right\|, \tag{3.10}$$

where the covariance matrix Σ *is defined in* (3.6) *and* $\|\cdot\|$ *denotes here the spectral norm induced by the Euclidean norm. Equivalently,* $S^2(x,t)$ *is given by the maximum eigenvalue of* $\Sigma(x,t)$*.*

Proof. See **??**. This result uses Theorem 3.3.1 to establish the convergence of the covariance matrices, and then the properties of the spectral norm to establish (3.10). □
The stochastic sensitivity field can be calculated given any velocity data u, and through the explicit expression (3.6) for Σ can even be computed from only flow map data. Computation does not require knowledge of the noise scale ε, so the S^2 field is intrinsic in capturing the impact of the model dynamics on uncertainty, and any specified non-uniform diffusivity.

It has already been shown that, in the fluid flow context, stochastic sensitivity can identify coherent regions in two-dimensions [2, 4]. A simple approach is to define robust sets, which are those initial conditions for which the corresponding S^2 value, i.e., the uncertainty in eventual location, are below some specified threshold. This threshold can be defined precisely in terms of a spatial lengthscale of interest and the advective and diffusive characteristics of the flow, as Definition 2.9 of [4]. Such a definition extends to the n-dimensional case as presented here, moreover establishing an easily computable method for determining coherent sets by using the covariance matrix Σ.

Independent of the fluid mechanics context, Theorem 3.4.1 indicates that even for general systems, the matrix norm of $\Sigma(x,t)$, i.e., the stochastic sensitivity $S^2(x,t)$, can be used as *one* number which encapsulates the uncertainty of an initial state x after t time units.

3.5 Numerical validation and applications

This section will validate the theory presented in Section 3.3. Following the example in Chapter 5 of [34], we consider an unsteady meandering jet in two dimensions, which may serve as an idealised model of geophysical Rossby waves. The velocity field for $y \equiv (y_1, y_2)$ is given by [34]

$$u\,(y,t) = \begin{bmatrix} c - A\sin\left(Ky_1\right)\cos\left(y_2\right) + \epsilon_{\mathrm{mj}} l_1 \sin\left(k_1\left(y_1 - c_1 t\right)\right)\cos\left(l_1 y_2\right) \\ AK\cos\left(Ky_1\right)\sin\left(y_2\right) + \epsilon_{\mathrm{mj}} k_1 \cos\left(k_1\left(y_1 - c_1 t\right)\right)\sin\left(l_1 y_2\right) \end{bmatrix}. \tag{3.11}$$

The velocity field describes a kinematic travelling wave with deterministic oscillatory perturbations in a co-moving frame. Here, A is the amplitude and c is the phase speed of the primary wave, and K is the wavenumber in the y_1-direction. The oscillatory perturbation has amplitude ϵ_{mj}, phase speed c_1 (in the co-moving frame), and wavenumbers k_1 and l_1 in the y_1- and y_2-directions respectively. Throughout, we take the parameter values $c = 0.5$, $A = 1$, $K = 4$, $l_1 = 2$, $k_1 = 1$, $c_1 = \pi$, and $\epsilon_{\mathrm{mj}} = 0.3$. For these

values, the flow consists of a meandering jet with vortex structures within the meanders, and a chaotic zone which influences the fluid transfer between the jet and the vortices. All necessary flow map data is obtained by directly solving (3.2) numerically, with the standard Euler scheme. The flow map gradients required for computing the covariance matrix with (3.6) are calculated via a star-grid finite-difference approximation, using a spatial resolution of 0.001.

All simulations in this section were generated using the Julia programming language [8], with implementations of the ordinary and stochastic differential equation solvers provided by the DifferentialEquations.jl package [32]. All figures were created using the Makie.jl package [15]. The code is available as open source[1].

3.5.1 Validation of Theorem 3.3.1

This section will validate the bound in Theorem 3.3.1 directly, and illustrate the convergence of the SDE solution towards the expected Gaussian distribution described in Theorem 3.3.2. For each value of ε considered, we use the Euler-Maruyama method [24] to generate $N = 10000$ independent realisations of the solutions to (3.1) and (3.4). A step size of $\delta t = 10^{-4}$ is used to ensure that numerical error does not dominate over the theoretical predictions. These solution samples are generated with the *same* realisations of the Wiener process increments $W_{t+\delta t} - W_t \sim \mathcal{N}(0, \delta t I_n)$. We consider the initial condition $x = (0, 1)$ and the prediction of the model at time $t = 1$. For each realisation of $y_t^{(\varepsilon)}$, a corresponding realisation of the scaled deviation $z_t^{(\varepsilon)}(x)$ is computed. In the following, let $\hat{z}_1^{(\varepsilon)}, \ldots, \hat{z}_N^{(\varepsilon)}$ and $\hat{z}_1, \ldots, \hat{z}_N$ denote the N realisations of $z_t^{(\varepsilon)}(x)$ and $z_t(x)$ respectively.

Figure 3.1 shows the resulting simulations of $y_t^{(\varepsilon)}$ for four different values of ε. The realisations are binned as a histogram and bin counts are normalised, to provide an empirical estimate of the probability density function of $y_t^{(\varepsilon)}$. Superimposed (in solid black) are the first, second and third standard-deviation contours of the probability density function of the Gaussian approximation (3.9). The first three standard-deviation levels of the 2×2 sample covariance matrix of the realisations, are also overlaid (in dashed blue). As ε decreases towards 0, the samples increasingly resemble a Gaussian distribution, and both the mean and covariance coincide with the corresponding limits.

To directly validate Theorem 3.3.1 for $r \geq 1$, define the error metric

$$\Gamma_z^{(r)}(\varepsilon) \coloneqq \frac{1}{N} \sum_{i=1}^{N} \left\| \hat{z}_i^{(\varepsilon)} - \hat{z}_i \right\|^r,$$

which is an estimator of the right-hand side of (3.5). For $r = 1, 2, 3, 4$, $\Gamma_z^{(r)}(\varepsilon)$ is shown (in a logarithmic scale) for decreasing values of ε in Figure 3.2. Theorem 3.3.1 predicts

[1] at https://github.com/liamblake/explicit-gaussian-characterisation-uncertainty.

that $\log_{10}\left(\Gamma_z^{(r)}(\varepsilon)\right)$ should decay linearly with a slope greater than r as ε decreases to zero. The lines of best fit for each value of r in Figure 3.2 show this behaviour, and are therefore consistent with Theorem 3.3.1.

3.5.2 The evolution of $\Sigma(x,t)$ through time

Here we shall illustrate that the limiting covariance matrix Σ captures the time-evolution of model uncertainty. Consider the same meandering jet model in (3.11), with the parameter values used in the previous subsection. We fix the noise scale parameter at $\varepsilon = 0.03$ and consider the evolution of the stochastic solution to (3.1) and the limiting Gaussian distribution (3.9) for times t in the interval $[0,1]$. We also consider two different choices of the diffusion matrix σ: the identity as before, and

$$\sigma_M(x) := \begin{bmatrix} x_1 & 0.5 \\ x_1 & 0.5\,(x_1 + x_2) \end{bmatrix}, \tag{3.12}$$

to include both multiplicative and non-diagonal noise which grow for larger values of the coordinates.

Figure 3.3 plots histograms of realisations of the solution to (3.1) at several different times, evolving from the same initial condition $x = (0,1)$, and the time-evolution of the corresponding deterministic trajectory solving (3.2). Overlaid on each histogram are the contours of the limiting Gaussian distributions, computed entirely from covariance matrix (3.6). Although each distribution is non-Gaussian, the evolution of the uncertainty distribution through time is captured by Σ. For examples, features of the error distributions, such as stretching and rotation, are reflected in Σ. This remains the case even when the noise is multiplicative with $\sigma = \sigma_M$. The computation of Σ circumvents the need for expensive Monte-Carlo simulation to draw conclusions about such evolution of uncertainty.

3.6 Discussion

This paper has contributed a rigorous justification, in terms of error bounds and a small-noise limit, for an easily computable linearisation approximation to the solution of nonlinear stochastic differential equations, as seen across diverse places in the literature [20, 35, 36, e.g.]. The theory applies to fully non-autonomous SDEs with multiplicative noise. This result extends the convergence bound on the Kullback-Leibler divergence by Sanz-Alonso and Stuart [35] to an explicit bound on the convergence of all moments of the difference between the exact SDE solution and the approximation, and further establishes the exact Gaussian distribution in the small-noise limit. While it is known that convergence of the KL divergence leads to convergence of the moments [28], this manuscript provides the exact rate of that convergence. Our bound is verified numerically

by plotting the first four raw moments of the distance between the true noise-scaled solution and the linearised solution (see Figure 3.2). The results, plotted across three orders of magnitude of the small noise parameter, match our theoretical prediction exactly.

In addition, we described a framework in which uncertainty in deterministic models can be ascribed without the need for expensive stochastic simulation, and purely from the deterministic solution dynamics. We illustrated how the Gaussian limit reflects the time-evolution of uncertainty (see Figure 3.3), even when the true uncertainty distributions are themselves non-Gaussian.

A powerful advantage of this framework is that the diffusivity matrix σ is permitted to vary spatio-temporally, allowing for multiplicative noise. Multiplicative noise is often ignored in practice, due to difficulties in working with analytically (see, for instance, the prior lack of rigourous justification of linearisations when the noise is multiplicative) and generating numerical realisations efficiently (e.g. the review in [29]). It has also been shown that multiplicative noise on linear dynamics can model departures from Gaussianity observed in climate statistics [38], as opposed to nonlinear dynamics with only additive noise. The spatio-temporal dependence of σ can also capture experimental and observational considerations that are otherwise ignored in the deterministic model, such as cloud cover when using satellite measurements or nonuniform uncertain across the field of view of a camera. We therefore present a highly flexible framework that can capture any prior knowledge of non-uniform uncertainty that arises from modelling or experimental considerations.

This paper also supplied theoretical and computational extension to the "stochastic sensitivity" tools introduced by Balasuriya [4]. Stochastic sensitivity was hitherto derived as the variance of an unknown limiting distribution and could only be computed in two spatial dimensions: we established that stochastic sensitivity, in any number of dimensions, is computable as the operator norm of the covariance matrix of our limiting SDE. We have also established that the limiting distribution in question is Gaussian, which may provide insight into properties of stochastic sensitivity as a means of uncertainty quantification in any model (not just in the fluids context) where an n-dimensional state variable evolves according to a "best available" model.

The Gaussian approximation presented here arises as the leading order term in a power series expansion of the SDE solution in terms of the noise scale parameter ε [9]. A further extension would be to explore the higher-order terms in such an expansion, which could lead to a practical framework for constructing higher-order characterisations and approximations of the stochastic solution. However, the higher-order terms are known to be individually non-Markovian, and satisfy non-linear SDEs for which the solution is not expected to be analytically available [9].

In this paper, we have assumed throughout that the initial condition x, from which both the stochastic differential equation and the deterministic flow map evolves from, is *certain* (i.e. not a random quantity). However, in practice there is uncertainty associated

with the initial state which should also be accounted for. The bound in Theorem 3.3.1 is independent of the initial condition, suggesting that the required extension of the theoretical result is straightforward. This extension will broaden our framework, allowing for uncertainties in *both* the initial state and the time-evolution of the model to be characterised at once in a precise sense.

Similarly, we assume that the reference deterministic model (3.2) for the evolution of the state variable is "correct" and known exactly, in that in the absence of any noise (i.e. $\varepsilon = 0$), the SDE model (3.1) reduces to the deterministic (3.2). The Gaussian characterisation is computed from knowledge of either the driving vector field or the solution data itself, i.e. the flow map. However, these components of the deterministic model may not be known exactly, e.g. from solving (3.2) numerically, interpolation error, etc. There is a need to extend the theory presented here to account for this case; to, for instance, establish a bound in the error between the SDE solution and the limiting Gaussian, as in Theorem 3.3.1, if the Gaussian distribution is constructed from an "incorrect" deterministic model. Both of these theoretical extensions, to uncertain initial conditions and incorrect deterministic dynamics, are currently being pursued.

3.6.1 Applications

Here, we briefly discuss some anticipated applications of this work across a wide range of fields, including climate and ocean modelling, data assimilation and Lagrangian coherent structures.

This work fits in with recent interest in stochastic parameterisation as a means to account for unresolved subgrid effects in climate modelling [7, 27, 31]. In particular, the recent review [27] concludes, "The aim of current and future developments in stochastic representations of model uncertainty is to develop schemes that are computationally highly efficient and contribute only moderately to the overall computational cost...". This paper provides one method to convert a stochastic parameterisation (formulated as a SDE) to a computationally cheaper set of coupled ODEs for the mean and variance of an approximate Gaussian, together with a convergence proof and error estimates.

To ascribe uncertainties directly onto the deterministic model, we assume that the diffusivity matrix σ is specified *a priori*, to capture any known multiplicative noise effects. There are methods for estimating σ directly from observed data, e.g. the Bayesian inference approach of [41] or via statistical estimation as in [14], which can be used in our framework. In particular, [41] relies upon computationally expensive numerical approximations to compute the likelihood of each trajectory, whereas from this paper we have a potentially more efficient computation, using the analytically available Gaussian limit. Coupling these approaches with the approximation here could provide a complete and practical framework to characterise the uncertainty in the flow by efficiently estimating the (multiplicative) diffusion from observed trajectory data.

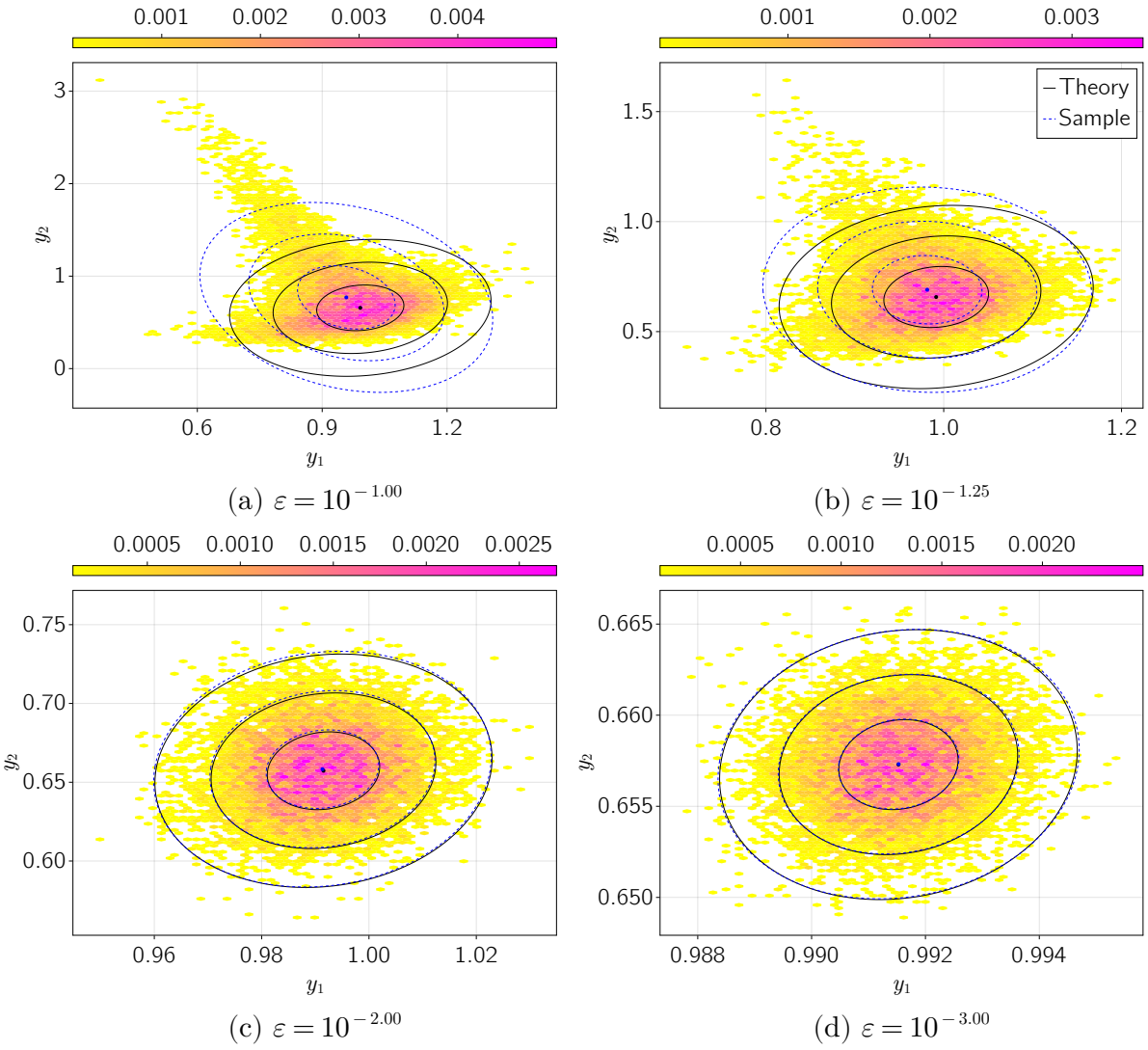
Data assimilation is a framework for improving uncertainties in predictions by combining

model forecasts with observational data, accounting for error in both, and uncertainty quantification refers to the broader goal of capturing the uncertainty inherent in prediction [12, 20, 25, 33]. The Gaussian limit here provides a characterisation of model uncertainty, and may therefore be useful in data assimilation and uncertainty quantification. The linearisation of the stochastic differential equation (3.1) used to construct the Gaussian approximation has been employed in data assimilation, e.g. in the continuous time continuous state-space extended Kalman filter [20, §9]. The convergence analysis of this paper could contribute a new term, estimating the error due to linearisation, to the *forecast uncertainty* covariance matrix employed in these extended Kalman filters.

Stochastic sensitivity provides a novel method for extracting Lagrangian coherent structures (LCSs) [6, 19] from fluid flow, by considering regions with uncertainty (as measured by the stochastic sensitivity field) below a prescribed threshold. Whereas the original formulation in [4] was restricted to two-dimensional flows, here we have an extension of the LCS extraction scheme to arbitrary dimensions.

Moreover, most traditional LCS measures are completely deterministic measures, not accounting for any uncertainty in the driving velocity field, and the sensitivity of these methods to such uncertainty has not been investigated in detail. The robustness of several LCS methods to stochastic noise has recently been explored in [2], but via stochastic simulation and summary statistics. In this paper we have presented a theoretical result for characterising Lagrangian trajectory uncertainty, which can be used to perform a purely theoretical analysis of such sensitivity in LCS computations. An initial study into the impact of uncertainty of one such method – the finite-time Lyapunov exponent – has already been performed using stochastic sensitivity [5], albeit in only two-dimensions and without knowledge that the limiting distribution is Gaussian.

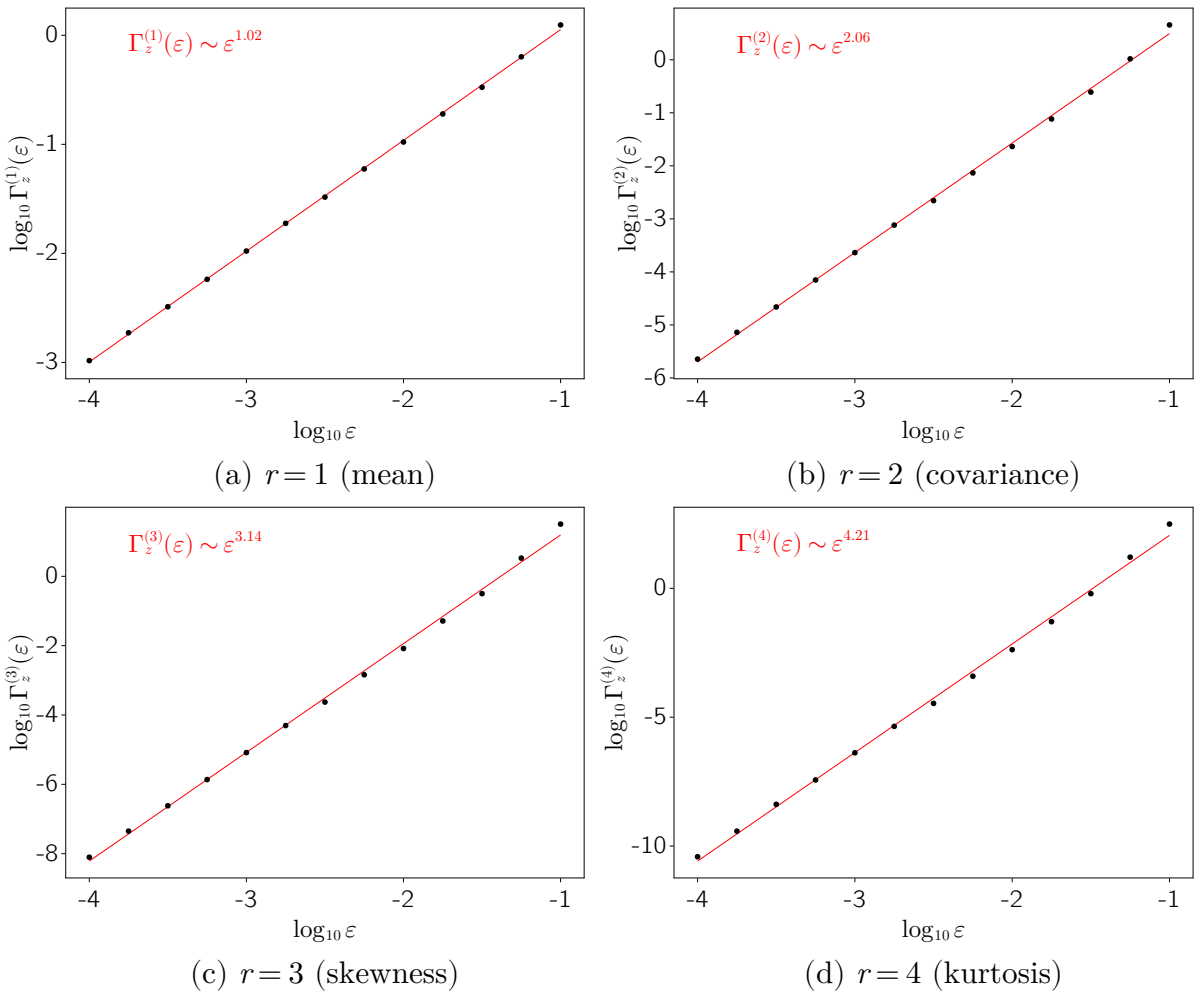
3.7 Detailed appendices



(a) $\varepsilon = 10^{-1.00}$ (b) $\varepsilon = 10^{-1.25}$

(c) $\varepsilon = 10^{-2.00}$ (d) $\varepsilon = 10^{-3.00}$

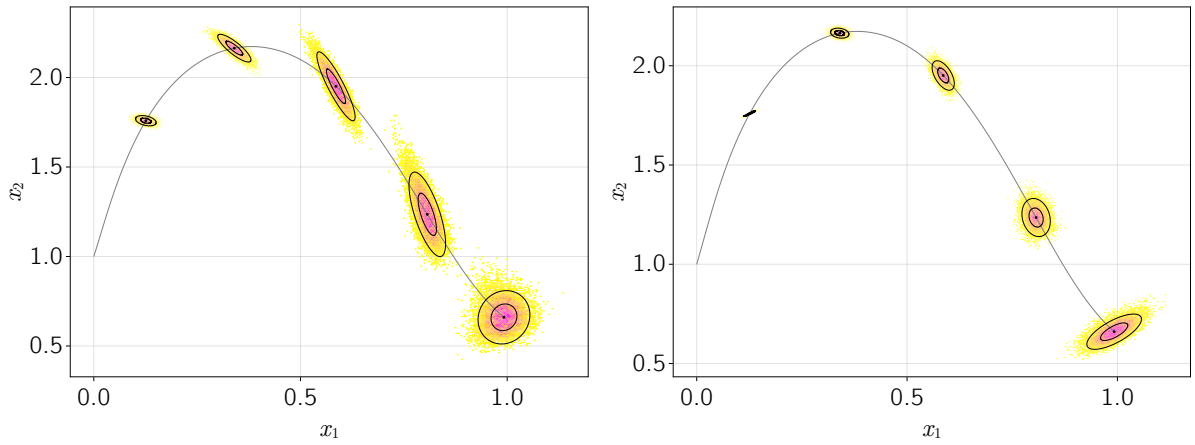
Figure 3.1: Histograms of $y_t^{(\varepsilon)}$ from direct simulation of (3.1), for four different ε values. Overlaid in black are contours of the Gaussian limit (3.9), which correspond to the first three standard deviation levels centred at the limiting mean $F_0^t(x)$. In dashed blue are corresponding contours computed from the sample covariance matrix of the realisations.



(a) $r = 1$ (mean) (b) $r = 2$ (covariance)

(c) $r = 3$ (skewness) (d) $r = 4$ (kurtosis)

Figure 3.2: Validation of Theorem 3.3.1, by plotting the sample rth raw moment distance (the error metric $\Gamma_z^{(r)}(\varepsilon)$) between 10000 realisations of $z_t^{(\varepsilon)}(x)$ and $z_t(x)$, for decreasing values of ε. A line of best fit (in red) is placed on each, and the resulting slope indicated.



(a) $\sigma(x,t) = I_2$ (b) $\sigma(x,t) = \sigma_M(x)$

Figure 3.3: Histograms of $y_t^{(0.03)}$ for (from left to right) $t = 0.2, 0.4, 0.6, 0.8, 1.0$, with the time-evolution of the deterministic trajectory in grey and contours of the limiting covariance matrix (3.6) for each time. The right figure uses the diffusion matrix $\sigma_M(x)$ as defined in (3.12).

Bibliography

[1] A. J. Abascal, S. Castanedo, R. Medina, I. J. Losada, and E. Alvarez-Fanjul. Application of HF radar currents to oil spill modelling. *Marine Pollution Bulletin*, 58(2):238–248, Feb. 2009. ISSN 0025-326X. doi: 10.1016/j.marpolbul.2008.09.020.

[2] A. Badza, T. W. Mattner, and S. Balasuriya. How sensitive are Lagrangian coherent structures to uncertainties in data? *Physica D: Nonlinear Phenomena*, 444:133580, Feb. 2023. ISSN 0167-2789. doi: 10.1016/j.physd.2022.133580.

[3] S. Balasuriya. Stochastic approaches to Lagrangian coherent structures. *The Role of Metrics in the Theory of Partial Differential Equations*, 85:95–105, Jan. 2020. doi: 10.2969/aspm/08510095.

[4] S. Balasuriya. Stochastic Sensitivity: A Computable Lagrangian Uncertainty Measure for Unsteady Flows. *SIAM Review*, 62:781–816, Nov. 2020. doi: 10.1137/18M1222922.

[5] S. Balasuriya. Uncertainty in finite-time Lyapunov exponent computations. *Journal of Computational Dynamics*, 7(2):313–337, 2020. doi: 10.3934/jcd.2020013.

[6] S. Balasuriya, N. T. Ouellette, and I. I. Rypina. Generalized Lagrangian coherent structures. *Physica D: Nonlinear Phenomena*, 372:31–51, June 2018. ISSN 0167-2789. doi: 10.1016/j.physd.2018.01.011.

[7] J. Berner, U. Achatz, L. Batté, L. Bengtsson, A. de la Cámara, H. M. Christensen, M. Colangeli, D. R. B. Coleman, D. Crommelin, S. I. Dolaptchiev, C. L. E. Franzke, P. Friederichs, P. Imkeller, H. Järvinen, S. Juricke, V. Kitsios, F. Lott, V. Lucarini, S. Mahajan, T. N. Palmer, C. Penland, M. Sakradzija, J.-S. von Storch, A. Weisheimer, M. Weniger, P. D. Williams, and J.-I. Yano. Stochastic Parameterization: Toward a New View of Weather and Climate Models. *Bulletin of the American Meteorological Society*, 98(3):565–588, Mar. 2017. ISSN 0003-0007, 1520-0477. doi: 10.1175/BAMS-D-15-00268.1.

[8] J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah. Julia: A Fresh Approach to Numerical Computing. *SIAM Review*, 59(1):65–98, Jan. 2017. ISSN 0036-1445. doi: 10.1137/141000671.

[9] Y. N. Blagoveshchenskii. Diffusion Processes Depending on a Small Parameter. *Theory of Probability and its Applications*, 7(2):17, 1962. ISSN 0040585X. doi: 10.1137/1107013.

[10] L. Blake, J. Maclean, and S. Balasuriya. Explicit Gaussian characterisation of model uncertainty in the limit of small noise. *submitted to SIAM/ASA Journal on Uncertainty Quantification*, 2023.

[11] F. Brauer and C. Castillo-Chávez. *Mathematical models in population biology and epidemiology*. Number 40 in Texts in applied mathematics. Springer, New York, 2nd ed edition, 2012. ISBN 978-1-4614-1685-2.

[12] A. Budhiraja, E. Friedlander, C. Guider, C. K. R. T. Jones, and J. Maclean. Assimilating Data into Models. In *Handbook of Environmental and Ecological Statistics*. Chapman and Hall/CRC, 1st edition edition, 2019. ISBN 978-1-315-15250-9.

[13] M. Collins. Ensembles and probabilities: a new era in the prediction of climate change. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 365(1857):1957–1970, June 2007. doi: 10.1098/rsta.2007.2068.

[14] C. J. Cotter and G. A. Pavliotis. Estimating eddy diffusivities from noisy Lagrangian observations. *Communications in Mathematical Sciences*, 7(4):805–838, Dec. 2009. ISSN 1945-0796. doi: 10.4310/CMS.2009.v7.n4.a2.

[15] S. Danisch and J. Krumbiegel. Makie.jl: Flexible high-performance data visualization for Julia. *Journal of Open Source Software*, 6(65):3349, Sept. 2021. ISSN 2475-9066. doi: 10.21105/joss.03349.

[16] F. d'Ovidio, S. De Monte, S. Alvain, Y. Dandonneau, and M. Lévy. Fluid dynamical niches of phytoplankton types. *Proceedings of the National Academy of Sciences*, 107 (43):18366–18370, Oct. 2010. doi: 10.1073/pnas.1004620107.

[17] L. Fang, S. Balasuriya, and N. T. Ouellette. Disentangling resolution, precision, and inherent stochasticity in nonlinear systems. *Physical Review Research*, 2(2):023343, June 2020. doi: 10.1103/PhysRevResearch.2.023343.

[18] F. Feppon and P. F. J. Lermusiaux. Dynamically Orthogonal Numerical Schemes for Efficient Stochastic Advection and Lagrangian Transport. *SIAM Review*, 60(3): 595–625, Jan. 2018. ISSN 0036-1445. doi: 10.1137/16M1109394.

[19] A. Hadjighasem, M. Farazmand, D. Blazevski, G. Froyland, and G. Haller. A critical comparison of Lagrangian methods for coherent structure detection. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 27(5):053104, May 2017. ISSN 1054-1500. doi: 10.1063/1.4982720.

[20] A. H. Jazwinski. *Stochastic Processes and Filtering Theory*, volume 64 of *Mathematics in Science and Engineering*. Elsevier Science, Burlington, 2014. ISBN 978-0-08-096090-6.

[21] I. T. Jolliffe. *Principal Component Analysis*. Springer Series in Statistics. Springer, New York, NY, second edition, 2002. ISBN 978-0-387-22440-4.

[22] G. Kallianpur and P. Sundar. *Stochastic analysis and diffusion processes*. Number 24 in Oxford graduate texts in mathematics. Oxford University Press, Oxford, United Kingdom, first edition edition, 2014. ISBN 978-0-19-965706-3 978-0-19-965707-0.

[23] I. Kamenkovich, I. I. Rypina, and P. Berloff. Properties and Origins of the Anisotropic Eddy-Induced Transport in the North Atlantic. *Journal of Physical Oceanography*, 45 (3):778–791, Mar. 2015. ISSN 0022-3670, 1520-0485. doi: 10.1175/JPO-D-14-0164.1.

[24] P. E. Kloeden and E. Platen. *Numerical Solution of Stochastic Differential Equations*. Applications of Mathematics. Springer, Berlin, Heidelberg, 1st edition, 1992. ISBN 978-3-540-54062-5.

[25] K. Law, A. Stuart, and K. Zygalakis. *Data assimilation: a mathematical introduction*. Number volume 62 in Texts in applied mathematics. Springer, Cham Heidelberg New York Dordrecht London, 2015. ISBN 978-3-319-20324-9 978-3-319-36687-6. doi: 10.1007/978-3-319-20325-6.

[26] M. Leutbecher. Ensemble size: How suboptimal is less than infinity? *Quarterly Journal of the Royal Meteorological Society*, 145(S1):107–128, 2019. ISSN 1477-870X. doi: 10.1002/qj.3387.

[27] M. Leutbecher, S.-J. Lock, P. Ollinaho, S. T. K. Lang, G. Balsamo, P. Bechtold, M. Bonavita, H. M. Christensen, M. Diamantakis, E. Dutra, S. English, M. Fisher, R. M. Forbes, J. Goddard, T. Haiden, R. J. Hogan, S. Juricke, H. Lawrence, D. MacLeod, L. Magnusson, S. Malardel, S. Massart, I. Sandu, P. K. Smolarkiewicz, A. Subramanian, F. Vitart, N. Wedi, and A. Weisheimer. Stochastic representations of model uncertainties at ECMWF: state of the art and future vision. *Quarterly Journal of the Royal Meteorological Society*, 143(707):2315–2339, 2017. ISSN 1477-870X. doi: 10.1002/qj.3094.

[28] Y. Lu, A. Stuart, and H. Weber. Gaussian Approximations for Probability Measures on $\mathbb{R}^d$. *SIAM/ASA Journal on Uncertainty Quantification*, 5(1):1136–1165, Jan. 2017. doi: 10.1137/16M1105384.

[29] C. M. Mora, H. A. Mardones, J. C. Jimenez, M. Selva, and R. Biscay. A Stable Numerical Scheme for Stochastic Differential Equations with Multiplicative Noise. *SIAM Journal on Numerical Analysis*, 55(4):1614–1649, Jan. 2017. ISSN 0036-1429. doi: 10.1137/140984488.

[30] B. Øksendal. *Stochastic Differential Equations*. Universitext. Springer, Berlin, Heidelberg, sixth edition, 2003. ISBN 978-3-540-04758-2 978-3-642-14394-6. doi: 10.1007/978-3-642-14394-6.

[31] T. N. Palmer. Stochastic weather and climate models. *Nature Reviews Physics*, 1 (7):463–471, July 2019. ISSN 2522-5820. doi: 10.1038/s42254-019-0062-2.

[32] C. Rackauckas and Q. Nie. DifferentialEquations.jl – A Performant and Feature-Rich Ecosystem for Solving Differential Equations in Julia. *Journal of Open Research Software*, 5(1):15, May 2017. ISSN 2049-9647. doi: 10.5334/jors.151.

[33] S. Reich and C. Cotter. *Probabilistic Forecasting and Bayesian Data Assimilation*. Cambridge University Press, Cambridge, 2015. ISBN 978-1-107-06939-8. doi: 10.1017/CBO9781107706804.

[34] R. M. Samelson and S. Wiggins. *Lagrangian Transport in Geophysical Jets and Waves: The Dynamical Systems Approach*, volume 31 of *Interdisciplinary Applied Mathematics*. Springer, New York, NY, 2006.

[35] D. Sanz-Alonso and A. M. Stuart. Gaussian Approximations of Small Noise Diffusions in Kullback-Leibler Divergence. *Communications in Mathematical Sciences*, 15(7): 2087–2097, Oct. 2017. ISSN 1539-6746. doi: https://dx.doi.org/10.4310/CMS.2017.v15.n7.a13.

[36] S. Särkkä and A. Solin. *Applied Stochastic Differential Equations*. Institute of Mathematical Statistics Textbooks. Cambridge University Press, Cambridge, 2019. ISBN 978-1-316-51008-7. doi: 10.1017/9781108186735.

[37] P. Sura. Stochastic Analysis of Southern and Pacific Ocean Sea Surface Winds. *Journal of the Atmospheric Sciences*, 60(4):654–666, Feb. 2003. ISSN 0022-4928, 1520-0469. doi: 10.1175/1520-0469(2003)060⟨0654:SAOSAP⟩2.0.CO;2.

[38] P. Sura, M. Newman, C. Penland, and P. Sardeshmukh. Multiplicative Noise and Non-Gaussianity: A Paradigm for Atmospheric Regimes? *Journal of the Atmospheric Sciences*, 62(5):1391–1409, May 2005. ISSN 0022-4928, 1520-0469. doi: 10.1175/JAS3408.1.

[39] T. Tél, A. de Moura, C. Grebogi, and G. Károlyi. Chemical and biological activity in open flows: A dynamical system approach. *Physics Reports*, 413(2):91–196, July 2005. ISSN 0370-1573. doi: 10.1016/j.physrep.2005.01.005.

[40] S. Wiggins. The Dynamical Systems Approach to Lagrangian Transport in Oceanic Flows. *Annual Review of Fluid Mechanics*, 37(1):295–328, Jan. 2005. ISSN 0066-4189, 1545-4479. doi: 10.1146/annurev.fluid.37.061903.175815.

[41] Y. K. Ying, J. R. Maddison, and J. Vanneste. Bayesian inference of ocean diffusivity from Lagrangian trajectory data. *Ocean Modelling*, 140:101401, Aug. 2019. ISSN 1463-5003. doi: 10.1016/j.ocemod.2019.101401.