A. Large Deviations Theory

A large deviation principle (LDP): Let P^{ϵ} be a family of probability measures on a suitable measurable

space (\mathcal{X}, Σ) , then it satisfies an LDP with a rate function $I: \mathcal{X} \to \mathbb{R}$ if for all subsets $\Omega \subset \Sigma$,

we have [4, 5],

$$P^{\epsilon}\left(\Omega\right) \asymp \exp\left(-\epsilon^{-1} \inf_{z \in \Omega} I\left(z\right)\right),$$
 (1)

where \asymp denotes log-asymptotic equivalence in the limit $\epsilon \to 0$.

The Gärtner-Ellis theorem: If the limiting behavior of a scaled CGF,

$$G(\lambda) \equiv \lim_{\epsilon \to 0} \epsilon \log \mathbb{E}[e^{\epsilon^{-1}\langle \lambda, z^{\epsilon} \rangle}]. \tag{2}$$

exists for each λ , then its Legendre-Fenchel (LF) transform

is the rate function of the LDP of the process z^{ϵ} , i.e.

$$I(z) = \sup_{\lambda \in \mathbb{R}^n} (\langle \lambda, z \rangle - G(\lambda)), \quad z = \lim_{\epsilon \to 0} z^{\epsilon},$$

A geometric interpretation of the LF transform (2)

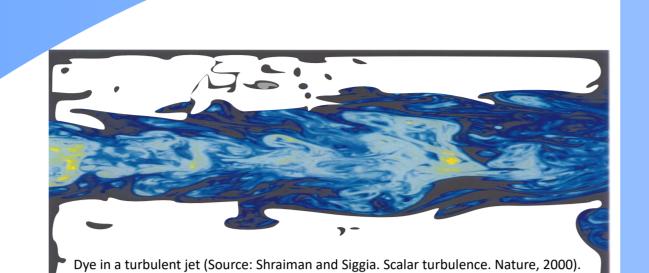
is that the argument of one of $G(\lambda)$ and I(z) is

the slope of the other [7], i.e.,

 $\nabla I(z) = \lambda, \quad \nabla G(\lambda) = z,$

when $G(\lambda)$ is a **finite** and a **differentiable** function, and the rate function I(z) is

strictly convex.



I. Motivation \ Introduction

- *) In turbulence theory, one often Studies statistical and probabilistic properties in fluid dynamics.
- *) In this poster, we investigate the probability of extreme gradients of a passive scalar in medium with a variety of Reynolds numbers R_e , using LDT (section A).
- *) The numerical algorithm for finding rare events is based on changing probability measures, and instanton equations (sections B & C).
- *) For a turbulent flow with heavy-tailed distributions, the standard method fails (section C). Therefore, here we use a **nonlinear** reparametrization (section D) which is a newly proposed in [1] (or you can scan the QR code).

II. Recent Fluid Deformation (RFD) Model of Passive Scalar Turbulence

This statistical model of the gradient of a passive scalar, $\psi = \nabla \theta \in \mathbb{R}^3$, is given by [2,3]:

 $d\psi(t) = b(\psi, \mathbf{A}) dt + \sqrt{\epsilon} dM(t),$

 $d\mathbf{A}(t) = V(\mathbf{A}) dt + \sqrt{\epsilon} d\mathbf{W}(t),$

where the drift terms are:

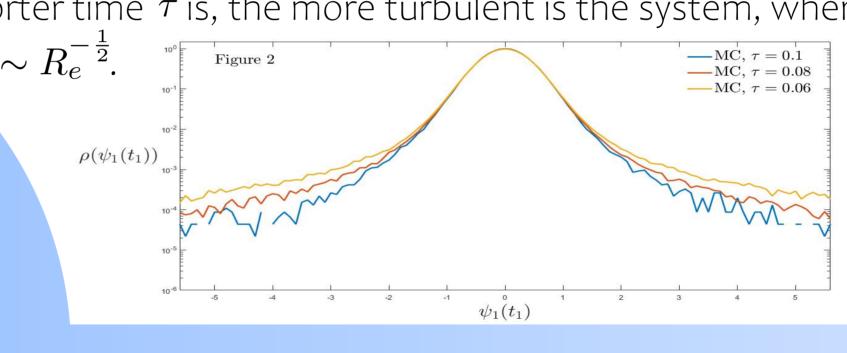
$$b(\psi, \mathbf{A}) = -\mathbf{A}^T(t) \psi(t) - \frac{\operatorname{tr}(\mathbf{C}_{\tau}^{-1})}{3 T_{\theta}} \psi(t),$$
 $V(\mathbf{A}) = \mathbf{A}^2 + \frac{\operatorname{tr}(\mathbf{A}^2)}{\operatorname{tr}(\mathbf{C}_{\tau}^{-1})} \mathbf{C}_{\tau}^{-1} \frac{\operatorname{tr}(\mathbf{C}_{\tau}^{-1})}{3 T_{A}} \mathbf{A}.$

And ${f C}_{ au}(t)pprox e^{ au{f A}}~e^{ au{f A}^T}$ is a stationary Cauchy-Green tensor, and $\mathbf{A}(t) \in \mathbb{R}^{3 \times 3}$ is the **velocity gradient**. The small parameter of the system is $\,\epsilon.$ Setting the integral times $\,T_A$ and $\,T_{ heta}$ to unity, the only remaining temporal scale is au, which is the **decorrelation time scale** after which any correlation of ${f A}$ is neglected. **Figure (2)** shows that

the shorter time au is, the more turbulent is the system, where $au \sim R_e^{-\frac{\pi}{2}}$



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$P(\psi_1(t_1))$

Scalar Turbulence via Large Deviation Theory Mnerh Algahtani and Tobias Grafke

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D. Instantons of Nonlinear Reparameterizations

Every situation where the tails of p(z) are fat correspond with non-convex rate functions,

and will break the above assumption of the mapping $z \to \lambda(z)$ being a bijection.

The **main contribution** of [1] is the realization that the introduction of a nonlinear map $F: \mathbb{R}^n \to \mathbb{R}^n$ allows us to loosen the restriction of the convexity of

I(z). In analogy to (4) and the description in section B,

we can now define the **nonlinearly tilted measure**;

$$p_{\lambda}^{F}(z) = \frac{\exp(\epsilon^{-1}\langle \lambda, F(z) \rangle)}{\mathbb{E}_{p}[\exp(\epsilon^{-1}\langle \lambda, F(z) \rangle)]} p(z)$$
$$= \exp(\epsilon^{-1}\langle \lambda, F(z) \rangle - G_{F}(\lambda))) p(z),$$

where the **nonlinearly tilted CGF** is given by

$$G_F(\lambda) = \sup_{F^{-1}(y) \in \mathbb{R}^n} \left(\langle \lambda, y \rangle - I \circ F^{-1}(y) \right), \quad y = F(z),$$

and is being bounded and differentiable. At the same time, the effective rate function $I \circ F^{-1}(y)$ is strictly convex. The **conditions** of the nonlinear reparametrization are;

1- F is a diffeomorphism, and

2- $I \circ F^{-1}(y)$ is strictly convex, i.e. $\langle v \operatorname{Hess}(I \circ F^{-1})(y) v \rangle > 0 \ \forall \ v \in \mathbb{R}^n$.

IV. Modification: Nonlinearly Tilted Instantons

 $P(\psi_1(t_1))$

Optimizations algorithm is now done via instanton equations with nonlinear final time tilting, $F(z) = \operatorname{sign}(z) \log \log |z|$,

 $z \in \mathbb{R} \setminus [-1,1]$, for which the reparametrized expectation remains bounded. Other choices of F would be possible. Figure (4) compares the nonlinearly tilted instantons

> (dashed lines), with MC results (solid lines). It shows that the nonlinear instantons correctly predicts the far tail probilities, since reparametrizing the observable

> > function.

via F convexifies its rate

III. Instantons of Extreme Gradients of a Passive Scalar

Finding the maximum likelihood pathways, instantons, of achieving **extreme final configurations** $z:=\psi_i(t_1)$ can be done via instanton equations (8), (section C). Figure (3) shows the distribution of end points of instantonic trajectories (dashed lines) against MC results (solid lines), for a range of au that exhibits **heavy**tailed distributions. It displays an excellent agreement between the two. However, instantons are limited to small values of z due to the **nonconvexity** of the rate function (see section B), which has been overcome using the nonlinear reparameterizations (section D).

C. Instanton Equations

In order to use the described **methodology**

to find the instanton (minimizer) for a rare

outcome z, we must demand that the

the mapping $z \to \lambda(z)$ is a bijection:

For every outcome $\,z\,$ there must be a

unique tilt λ , which holds only when

the rate function I is **strictly convex.**

Consider a stochastic system,

$$dX_t^{\epsilon} = b(X_t^{\epsilon}) dt + \sqrt{\epsilon} \sigma dW_t, X_{t_0}^{\epsilon} = x_0.(5)$$

The noise covariance $\chi = \sigma \sigma^T \in \mathbb{R}^{n \times n}$ is

assumed to be invertible. We are interested in the chance of trajectories X_t^{ϵ} departing

from an asymptotically stable fixed point \bar{x} ,

and eventually leaving $D \subset \mathbb{R}^n$ that is attracted to \bar{x} . These trajectories belong to the set:

 $A_z := \overline{\{\varphi \in \mathbf{C}_{t_0 t_1}(\mathbb{R}^n) | \varphi(t_0) = \bar{x}, \varphi(t_1) = z \notin D\}}. (6)$

From LDP, we have,

B. Lagrange Multiplier and Exponentially Tilted Measures

The problem of finding the rare event probability is now reduced to an optimization problem, i.e.

 $\inf_{z \in \mathbb{R}} I(z)$, where the minimizer is called **instanton**. This constrained optimization problem

can be transformed into an unconstrained one using a Lagrange multiplier [8], i.e.,

 $\inf_{z \in \Omega} I(z) \Leftrightarrow \inf_{z \in \mathbb{R}^n} \left(I(z) - \langle \lambda, z \rangle \right).$

of the **exponentially tilted measure** [9]. If

A probabilistic interpretation of Lagrange multiplier $\,\lambda\,$ is in the form

 $\mathbb{E}_p\left[\exp\left(\epsilon^{-1}\left\langle\lambda,\,z\right\rangle\right)\right] < \infty$

then the exponentially tilted measure is defined as,

$$\lim_{\epsilon \to 0} \epsilon \log p(z) = -\inf_{z \in A_z} I(z) = -S(\varphi^*), \qquad (7)$$

where φ^* is the minimizer (instanton), and

$$S(arphi)=rac{1}{2}\int_{t_0}^{t_1}\|\dot{arphi}_t-b(arphi(t))\|_\chi^2\,dt$$
 is Freidlin-Wentzell rate function

of system (5). The integrand of S can be understood as a **Lagrangian**.

In Hamiltonian formulation, $H\left(\varphi,\vartheta\right)=\sup\left(\langle\vartheta,\dot{\varphi}\rangle-L\left(\varphi,\dot{\varphi}
ight)
ight)$, where $\vartheta=\partial L/\partial\dot{\varphi}$

is the conjugate momentum of φ [10]. Now, the minimizer φ^* can also be expressed as

the solution of Hamilton's equations,
$$\dot{\varphi}=\partial_{\vartheta}H(\varphi,\vartheta)=b\left(\varphi\right)+\chi\ \vartheta,$$

$$\dot{\vartheta} = -\partial_{\varphi} H(\varphi, \vartheta) = -\left(\nabla_{\varphi} b\left(\varphi\right)\right)^{T} \vartheta,$$

with boundary conditions, $\varphi(t_0) = \bar{x}, \ \vartheta(t_1) = \lambda$. These quations are often termed **instanton equations**.