Precise large deviations for statistical field theories with weak noise

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- 1. Motivation and introduction
- 2. Technical results and details
- 3. Applications of the theory

(about 15 minutes & 10 slides each)

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Precise LDT for weak noise theories

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Motivation and introduction

Extreme events: rare, but high impact...



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... or maybe not so rare on a different timescale



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Extreme events in statistical physics: Intermittency in fluids

Incompressible 3D Navier–Stokes turbulence at high Re dominated by intense localized events of vortex stretching and energy dissipation



⁽Buaria, Pumir, Bodenschatz, Yeung 2019)

Goal: Use these structures to calculate tail statistics in turbulence Began with: Gurarie, Migdal, Falkovich, Kolokolov, Lebedev, Chernykh, Stepanov, ...in 1990s

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Extreme events in statistical physics: interface growth

Task: Find detailed height statistics for Kardar-Parisi-Zhang (KPZ) eq.



Question: How do non-Gaussian statistics start to arise at small times t?

Studied by: Kolokolov, Korshunov, Meerson, Katzav, Vilenkin, Kamenev, Sasorov, Smith, Krajenbrink, Le Doussal, ... since 2010s

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Extreme events in fluid dynamics: oil spill events



Thunder Horse PDQ offshore oil platform



After Hurricane Dennis 2005



- pollutant diffuses & advected by currents
- limited measurements \Rightarrow add randomness
- what is ℙ[pollutant concentration ≥ z]?

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Extreme events in fluid dynamics: oil spill events

2d advection-diffusion equation for pollutant concentration c(x, t)



with v given, w Gaussian random vector field (white-in-time, smooth in space)



 \Rightarrow want to estimate tail probability $P(z) := \mathbb{P}[c(target, T) \ge z] \ll 1$

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Estimating rare event probabilities $\mathbb{P}[F(\eta) \ge z] \ll 1$





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2. asymptotic approximations



large deviation theory (LDT), instanton calculus

⇒ systematic; provides insights into physics of rare events

LDT: how it works in finite dimensions



Setup:

- $\eta \sim \mathcal{N}(0, \mathsf{Id})$ random vector in \mathbb{R}^N
- want to calculate $\mathbb{P}[F(\eta) \ge z] \ll 1$
- approximate event set by most likely point

Requires:

1. most likely point η_z

Optimize $\eta_z = \arg \min \frac{1}{2} ||\eta||^2$ s.t. $F(\eta) = z$, then approximate

$$P(z) \asymp \exp(-I(z))$$

log-asymptotic estimate with rate function $I(z) = \frac{1}{2} \|\eta_z\|^2$

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Precise LDT: how it works in finite dimensions



Setup:

- $\eta \sim \mathcal{N}(0, \mathsf{Id})$ random vector in \mathbb{R}^N
- want to calculate $\mathbb{P}[F(\eta) \ge z] \ll 1$
- approximate event set by paraboloid Requires:
 - 1. most likely point η_z
 - 2. curvatures at η_z via $\nabla^2 F(\eta_z)$

First optimize $\eta_z = \arg \min \frac{1}{2} ||\eta||^2$ s.t. $F(\eta) = z$, **then**:

$$P(z) \sim (2\pi)^{-1/2} C(z) \exp(-I(z))$$

$$I(z) = \frac{1}{2} \|\eta_z\|^2 \quad \& \quad C(z) = \left[2I(z) \det\left(\mathsf{Id} - \lambda_z \mathsf{pr}_{\eta_z^{\perp}} \nabla^2 F(\eta_z) \mathsf{pr}_{\eta_z^{\perp}}\right)\right]^{-1/2}$$

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Can we calculate the same kind of **precise LDT estimates** in infinite dimensions, so for Langevin equations/field theories?

 \Rightarrow develop robust&general methods i.p. for prefactor computation

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Technical results and details

Setup: Extreme events for Langevin equations via LDT

Consider the Langevin equation

$$\begin{cases} \dot{\phi} &= b(\phi) + \sqrt{\varepsilon}\sigma(\phi)\eta(t) \,, \\ \phi(0) &= \phi_0 \in \mathbb{R}^n \,, \end{cases}$$

with small ε and final-time observable $f(\phi(T)) \in \mathbb{R}$. Our goal:

• Precise estimate for tail probability

$$P(z) \stackrel{\varepsilon\downarrow 0}{\sim} (\varepsilon/2\pi)^{1/2} C(z) \exp\left(-S[\phi_z]/\varepsilon\right)$$

of $f(\phi(T))$ with leading **pre-exponential** term C(z)

- Closed-form result for C(z), can evaluate for field theories $n \to \infty$
- For non-gradient system $b \neq -\nabla V$, finite times $T < \infty$



Setup: Extreme events for Langevin equations via LDT



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Setup: Extreme events for Langevin equations via LDT



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Semiclass. expansion of path integral for PDF $\rho(z) = \mathbb{E}[\delta(f(\phi(T)) - z)]$

$$\rho(z) = \int_{\phi(0)=\phi_0} \mathscr{D}\phi \ \delta(f(\phi(T)) - z) J[\phi] \exp\left(-S[\phi]/\varepsilon\right)$$





Expand path integral to second order around ϕ_z $\Rightarrow \rho(z) \sim \mathcal{N}J[\phi_z]e^{-\frac{S}{\varepsilon}}/\sqrt{\text{Det}(\delta^2 S)}$

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Our contributions: optimization algorithms and determinants



Formulated minimization as optimal control problem

$$\begin{split} \min_{\eta} \left\{ S[\eta] - \lambda(f(\phi[\eta](\mathcal{T})) - z) \right. \\ \left. + \frac{\mu}{2}(f(\phi[\eta](\mathcal{T})) - z)^2 \right\} \end{split}$$

to automate, apply to non-convex settings, and scale to large n





Derived 2 strategies to **compute prefactor** C(z) in practice:

- (i) solve n × n matrix Riccati
 diff. eq. initial value problem
- (ii) iteratively find largest eigenvalues for Fredholm det.

Extended results to zero modes

 \Rightarrow instanton calc. more robust, prefactor calc. now possible at all

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Details on the prefactor: (i) Riccati approach

Idea: Derive diff. eq. for covariance matrix of fluctuations around ϕ_z

Riccati equation for $Q: [0, T] \rightarrow \mathbb{R}^{n \times n}$ with Q(0) = 0 and

$$\dot{Q} = \sigma \sigma^{\top} + Q \nabla b(\phi_z)^{\top} + \nabla b(\phi_z) Q + Q \left\langle \nabla^2 b(\phi_z), \theta_z \right\rangle Q$$

(for additive noise $\sigma = \text{const.}$, generalization to multiplicative noise straightforward) S.t.

$$C(z) = |\lambda_z|^{-1} \exp\left\{\frac{1}{2} \int_0^T \operatorname{tr}\left[\langle \nabla^2 b(\phi_z), \theta_z \rangle Q\right] \mathrm{d}t\right\} \times \\ \times \left[\det\left(U_z\right) \langle \nabla f(\phi_z(T)), Q(T) U_z^{-1} \nabla f(\phi_z(T)) \rangle\right]^{-1/2}$$

Many roads to Rome: WKB analysis for KBE, Feynman–Kac, path integral discretization, Gel'fand–Yaglom method, Forman's theorem

See: Maier, Stein 1996; Lehmann, Reimann, Hänggi 2003; TS, Grafke, Grauer 2021; Bouchet, Reygner 2022; TS, Grafke, Grauer 2023; Grafke, Schäfer, Vanden-Eijnden 2024; Rosinberg, Tarjus, Munakata 2024

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Properties:

- $n \times n$ symmetric matrix diff. eq. for Langevin eq. in \mathbb{R}^n
- initial-value problem, solve once
- nonlinear, but can linearize by Radon transformation $Q = \gamma \zeta^{-1}$

Advantages :)

- can (always formally) solve exactly via time-ordered exponential
- can solve exactly for simple enough instanton
- can use perturbation theory in additional small parameters

Disadvantages :(

- numerical time integration can be tricky (pseudo-singularities)
- very hard to use in high dimensions $n \gg 1$, i.e. beyond (1+1) dim. field theories $\Rightarrow n \times n$ too large, and γ, ζ blow up

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Details on the prefactor: (ii) Fredholm determinant

Analogous to finite dim. for additive noise

$$\begin{cases} \dot{\phi} &= b(\phi) + \sigma \eta, \\ \phi(0) &= \phi_0 \in \mathbb{R}^n, \end{cases}$$

with e.g. final-time observable $f(\phi(T)) \in \mathbb{R}$. Then with $F: \eta \mapsto f(\phi(T))$ for $\eta = dW/dt$:



• keep noise variable as main object of interest:

$$P(z)\approx (2\pi)^{-1/2}C(z)\exp(-I(z))$$

with $I(z) = \frac{1}{2} \|\eta_z\|_{L^2}^2$; where $\eta_z = \arg \min \frac{1}{2} \|\eta\|_{L^2}^2$ s.t. $F(\eta) = z$

• prefactor with Fredholm determinant of trace-class operator

$$C(z) = \left[2I(z) \det \left(\mathsf{Id} - \lambda_z \mathsf{pr}_{\eta_z^{\perp}} \left. \frac{\delta^2 F}{\delta \eta^2} \right|_{\eta_z} \mathsf{pr}_{\eta_z^{\perp}} \right) \right]^{-1/2}$$

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Details on the prefactor: (ii) Fredholm determinant

This prefactor is easy to evaluate numerically, even for very large *n*!!!

$$C(z) = \left[2I(z) \det \left(\left| \mathsf{Id} - \lambda_z \mathsf{pr} \left| \frac{\delta^2 F}{\delta \eta^2} \right|_{\eta_z} \mathsf{pr} \right) \right]^{-1/2} \approx \left[2I(z) \prod_{i=1}^M (1 - \mu_i) \right]^{-1/2}$$

Need to find largest eigenvalues μ_i of (projected) second variation of noise-to-observable map F, can do that **iteratively**.

with
$$\begin{cases} \dot{\gamma} = \nabla b(\phi_z)\gamma + \sigma\delta\eta, \\ \dot{\zeta} = -\langle \nabla^2 b(\phi_z), \theta_z \rangle \gamma - \nabla b^\top(\phi_z)\zeta, \end{cases} & \& \begin{cases} \gamma(0) = 0, \\ \zeta(T) = \lambda_z \nabla^2 f(\phi_z(T))\gamma(T). \end{cases}$$

see also: Bureković, Schäfer, Grauer 2024, for an application to stochastic NLS

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What about multiplicative noise? arXiv:2502.20114 (2025)

Now consider

$$egin{array}{lll} \dot{\phi} &= b\left(\phi
ight) + \sigma(\phi)\eta\,, \ \phi(0) &= \phi_0 \in \mathbb{R}^n\,, \end{array}$$

- still have $P(z) \approx (2\pi)^{-1/2} C(z) \exp(-I(z))$ with same I(z)
- BUT: Hessian $A = \delta^2 F / \delta \eta^2$ no longer guaranteed to be trace-class!

A is still *Hilbert–Schmidt*; then natural replacement of Fredholm determinant is **Carleman–Fredholm determinant**

$$\mathsf{det}_2(\mathsf{Id}-A) := \mathsf{det}\left((\mathsf{Id}-A)\exp(A)\right)$$

 $[\mathsf{think} \, \det_2(\mathsf{Id} - A) \approx \det\left((\mathsf{Id} - A)(\mathsf{Id} + A)\right) = \det\left(\mathsf{Id} - A^2\right)]$

 \Rightarrow generalize C(z) w/ det₂ (cf. Ben Arous (1988)), idea: \pm tr A counter term

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Instantons and fluctuations can be observed in practice



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Precise LDT for weak noise theories

Applications of the theory

Burgers eq. for $u \colon [0, L] \times [0, T] \to \mathbb{R}$ with stochastic large-scale forcing

$$\begin{cases} \partial_t u + u \partial_x u - \partial_{xx} u = \sqrt{\varepsilon} \sigma * \eta, \\ u(\cdot, 0) = 0 \end{cases}$$



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Gradient statistics in 1D Burgers: instanton computation

$$\min_{\eta,u} \frac{1}{2} \int_0^T \mathrm{d}t \int_0^L \mathrm{d}x \ \eta(x,t)^2 \quad \text{s.t.}$$

$$\begin{cases} \partial_t u + u \partial_x u - \partial_{xx} u = \sigma * \eta, \\ u(\cdot, 0) = 0, \\ \partial_x u(0, T) = z \end{cases}$$

PDF of $\partial_x u(0, T)$ Instanton fields $z = \partial_{-}u(0, 1) = -255$ $z = \partial_{-}u(0, 1) = -12$ $z = \partial_{-}u(0, 1) = 11$ $\varepsilon = 0.1$ 10^{0} $\varepsilon = 1.0$ $\varepsilon = 10.0$ 10^{-2} $\epsilon = 100.0$ $\overset{(z)}{\overset{n_{v_{Q}}}{\overset{n_{v_{Q}}}{\overset{n=0}}}} 10^{-4}$ 10^{-6} 10^{-1} - 7 $-\frac{\pi}{2}$ $-\pi$ -5 ÷. -5-5 -10Ó

 \Rightarrow log-asymptotic PDF estimate $\propto \exp\{-S[u_z]/\varepsilon\}$, fit constant prefactor

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Gradient statistics in 1D Burgers: prefactor computation



Application: Extreme average growth events in 1D KPZ eq.

Consider KPZ eq. $\partial_t h = \nu \partial_{xx} h + \frac{\lambda}{2} (\partial_x h)^2 + \sqrt{\mathcal{D}\eta}$ on ring of length L with h(x, 0) = 0, and analyze tail statistics of $\frac{1}{L} \int_0^L h(x, T) dx$ at small T.

Instantons (with multiple DPTs here, depending on *L*):



(Joint work with P. Sasorov and B. Meerson; further analysis of DPT with O. Shpielberg)

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Rate function at small L (2nd order dynamical phase transition to slight modulation):



Interesting L-z phase diagram in system, but no time to talk about it

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Gaussian fluctuations at small *L* after Cole–Hopf transform

(analytical result below DPT, numerical result including zero mode w/ Riccati afterwards):



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First: optimization, finding the instanton



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Precise LDT for weak noise theories



Use dominant eigenvalues μ_i

$${\sf det}_2({\sf Id}-{\cal A})pprox \prod_{i=1}^M (1-\mu_i) e^{\mu_i}$$

found iteratively and matrix-free with 2nd order adjoints in JAX

scaling $\mu_i \propto 1/i$, indeed not trace-class but Hilbert–Schmidt

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Resulting estimates compared to direct sampling



at different noise strengths ε of the random advecting field

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Application: Extreme strain events in 3D Navier–Stokes eq.





 \Rightarrow correct prediction $\mathbb{P}[\partial_3 u_3(0, T) \leq -25] \approx 1.5 \cdot 10^{-5}$ at $\text{Re}_{\lambda} = 6.4$

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Conclusion

Conclusion & Outlook

Results:

- Robust numerical optimization to find instantons
- Gaussian fluctuations computed by Riccati eq. or Fredholm det.
- $\bullet\,$ Also for non-unique instantons w/ zero modes
- For non-eq. statistical field theories such as Navier–Stokes and KPZ, good agreement to Monte Carlo

What's next?

- Asymptotic analytical predictions/scaling of prefactor
- Higher-order fluctuations around instanton: loop expansion or FRG
- Extend to more general stochastic and dynamical systems
- Spectrum of Hessians: spectral gaps & asymptotic density of states?
- Incorporating renormalization of field theory into prefactor

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Thank you for your attention!



Read more e.g. in: T. Schorlepp and T. Grafke (2025) "Scalability of the second-order reliability method for stochastic differential equations with multiplicative noise" (arXiv:2502.20114)