

Large Deviations for Weakly Interacting Particle Systems

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- PART I: Gibbs measures on n -particle configurations
 - Problem Description and Motivation
 - Background on Large Deviations
 - Results
- PART II: Random Projections of High-dimensional measures
 - Random Projections
 - The CLT for Convex Sets
 - Large Deviations for Random Projections of Gibbs Measures

Gibbs measures on n -particle configurations

Gibbs measures on n -particle configurations

- configuration $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$ of n particles in \mathbb{R}^d
- subject to
 - a confining potential $V : \mathbb{R}^d \mapsto (-\infty, \infty]$
 - a symmetric pairwise interaction potential $W : \mathbb{R}^d \times \mathbb{R}^d \mapsto (-\infty, \infty]$
- Probability distribution on n -particle configurations

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) \doteq \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

where ℓ is a non-atomic, σ -finite measure on \mathbb{R}^d
(e.g., Lebesgue measure)
and Z_n is the normalizing constant or partition function

Gibbs measures on n -particle configurations

Recall

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where H_n is the Hamiltonian defined by

$$H_n(\mathbf{x}^n) \equiv H_n(\mathbf{x}_1, \dots, \mathbf{x}_n) =: \frac{1}{n} \sum_{i=1}^n V(\mathbf{x}_i) + \frac{1}{2n^2} \sum_{i,j=1, i \neq j}^n W(\mathbf{x}_i, \mathbf{x}_j)$$

which can be rewritten as

$$H_n(\mathbf{x}^n) = \int_{\mathbb{R}^d} V(\mathbf{x}) L_n(\mathbf{x}^n; d\mathbf{x}) + \frac{1}{2} \int_{\neq} W(\mathbf{x}, \mathbf{y}) m_{\mathbf{x}^n}^n(d\mathbf{x}) m_{\mathbf{x}^n}^n(d\mathbf{y}).$$

Gibbs measures on n -particle configurations

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where $m_{\mathbf{x}^n}^n(\cdot)$ is the empirical measure:

$$m_{\mathbf{x}^n}^n(\cdot) =: \frac{1}{n} \sum_{i=1}^n \delta_{\mathbf{x}_i}(\cdot),$$

where $\delta_{\mathbf{y}}$ denotes the Dirac delta mass at $\mathbf{y} \in \mathbb{R}^d$, and \int_{\neq} represents the integral over $\mathbb{R}^d \times \mathbb{R}^d \setminus \{(x, x) : x \in \mathbb{R}^d\}$

Motivation: where P_n arises – I

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

- Equilibrium distribution of n interacting Brownian particles at inverse temperature γ_n

If V, W are sufficiently smooth, then P_n (with ℓ as Lebesgue measure) is the invariant distribution of the Markovian (reversible) diffusion on $(\mathbb{R}^d)^n$:

$$dX_t^n = \nabla H_n(X_t^n) dt + dB_t^n$$

where $B^n = (B_1, \dots, B_n)$, with B_1, \dots, B_n are independent standard d -dimensional Brownian motions

Motivation: where P_n arises – II

Recall

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

- When $d = 1$, $V(x) = |x|^2$, and $W(x, y) = \beta \log \frac{1}{|x-y|}$ with $\beta > 0$, then P_n is the law of the β -ensemble in **Random Matrix Theory**. Specifically, for
 - $\beta = 1$, P_n is the law of the eigenvalues of the Gaussian Orthogonal Ensemble (GOE) of random symmetric matrices
 - $\beta = 2$, P_n is the law of the eigenvalues of the Gaussian Unitary Ensemble (GUE) of random Hermitian matrices

Motivation: where P_n arises – II contd.

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

- When $d = 2$, and $\mathbb{R}^d \equiv \mathbb{C}$, $\gamma_n = n^2$, $V(x) = |x|^2$ and $W(x, y) = 2 \log \frac{1}{|x-y|}$ then P_n is the law of the (complex) eigenvalues of a random $n \times n$ matrix with iid complex Gaussian entries with covariance $\mathbb{I}_2/2n$, where \mathbb{I}_2 is the 2×2 identity matrix.

Motivation: where P_n arises – II contd.

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

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- In the last example if V is non-quadratic, then P_n is the law of the spectrum of random normal matrices (Ameur, Y., Hedenmalm, H. and Makarov, N., 2011)

Law of the Empirical Measure

- “Mean-field” symmetries of the model suggest the study of Q_n , the empirical distribution of the particles

$$m_{\mathbf{x}^n}^n(\cdot) =: \frac{1}{n} \sum_{i=1}^n \delta_{\mathbf{x}_i}(\cdot),$$

under the distribution

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

Note that under P_n , $m_{\mathbf{x}^n}^n$ is a random element taking values in $\mathcal{P}(\mathbb{R}^d)$, the space of probability measures on \mathbb{R}^d

So Q_n is a probability measure on $\mathcal{P}(\mathbb{R}^d)$

Objective: Large Deviations

Goal:

Given a suitable sequence $\gamma_n \rightarrow \infty$, establish a **large deviation principle (LDP)** for $\{Q_n\}$: that is, identify a corresponding suitable sequence $\alpha_n \rightarrow \infty$ and function $I : \mathcal{P}(\mathbb{R}^d) \mapsto [0, \infty]$ such that

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$$Q_n(A) = P_n(m_{x^n}^n \in A) \approx e^{-\alpha_n I(A)}$$

for all nice subsets $A \subset \mathcal{P}(\mathbb{R}^d)$, where

$$I(A) = \inf_{x \in A} I(x)$$

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$\{\alpha_n\}$ is called the **speed** of the LDP and I is called the **rate function**

Large Deviations Principles

- Let (S, \mathcal{S}) be a topological space, and $\mathcal{P}(S)$ the space of Borel probability measures on that space.
- Given a sequence of measures $\{\theta_n\} \subset \mathcal{P}(S)$, let $\{\alpha_n\}$ be a sequence of positive real numbers such that $\lim_{n \rightarrow \infty} \alpha_n = \infty$, and let $\mathcal{H} : S \rightarrow [0, \infty]$ be a rate function (lowersemicontinuous with compact level sets). The sequence $\{\theta_n\}$ is said to satisfy a **large deviation principle (LDP)** with speed $\{\alpha_n\}$ and rate function \mathcal{H} if for each $E \in \mathcal{B}(S)$,

$$\begin{aligned} - \inf_{x \in E^o} \mathcal{H}(x) &\leq \liminf_{n \rightarrow \infty} \alpha_n^{-1} \log(R_n(E)) \leq \limsup_{n \rightarrow \infty} \alpha_n^{-1} \log(R_n(E)) \\ &\leq - \inf_{x \in \bar{E}} \mathcal{H}(x). \end{aligned}$$

Why Large Deviations Principles?

$$Q_n(A) = P_n(m_{x^n}^n \in A) \approx e^{-\alpha_n I(A)}$$

where

$$I(A) = \inf_{x \in A} I(x)$$

- Large deviations is an asymptotic theory that estimates probabilities of rare events (those with exponentially small probability) and represents them as the solution of a **variational problem**
- In many cases (when the rate function is strictly convex) the minimizer of the variational representation identifies the **limit of the empirical measures**
- Large deviations principles often provide information on the behavior of the distribution, conditioned on the rare event

Contraction Principle

“One gets LDPs for continuous functionals for free”

If $\{X_n\}$ satisfies an LDP at a speed $\{\alpha_n\}$ on a topological space (S, \mathcal{S}) with rate function I , and the map $F : (S, \mathcal{S}) \mapsto (S', \mathcal{S}')$ is continuous, then $\{F(X_n)\}$ also satisfies an LDP at a speed $\{\alpha_n\}$ with rate function

$J : T \mapsto [0, \infty]$ given by

$$J(y) = \inf\{I(x) : F(x) = y, x \in S\}, \quad y \in T$$

Recall our Goal

To establish LDPs for the sequence $\{Q_n\}$ of the law of the (random) empirical measures

$$m_{\mathbf{x}^n}^n(\cdot) =: \frac{1}{n} \sum_{i=1}^n \delta_{\mathbf{x}_i}(\cdot),$$

under

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

where

$$H_n(\mathbf{x}^n) \equiv H_n(\mathbf{x}_1, \dots, \mathbf{x}_n) =: \frac{1}{n} \sum_{i=1}^n V(\mathbf{x}_i) + \frac{1}{2n^2} \sum_{i,j=1, i \neq j}^n W(\mathbf{x}_i, \mathbf{x}_j)$$

Topologies on the Space $\mathcal{P}(\mathbb{R}^d)$

Recall we are interested in LDPs for the sequence of probability measures Q_n on $\mathcal{P}(\mathbb{R}^d)$

- Let $\mathcal{P}(\mathbb{R}^d)$ be the space of probability measures on \mathbb{R}^d , equipped with the weak topology; recall μ_n converges to μ in the weak topology if and only if

$$\forall f \in C_b(\mathbb{R}^d), \int_{\mathbb{R}^d} f(\mathbf{x}) \mu_n(d\mathbf{x}) \rightarrow \int_{\mathbb{R}^d} f(\mathbf{x}) \mu(d\mathbf{x}),$$

Let d_W denote the so-called Lévy-Prohorov metric on $\mathcal{P}(\mathbb{R}^d)$ that induces this topology.

Stronger Topologies on the Space $\mathcal{P}(\mathbb{R}^d)$

Fix a positive, continuous function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^+$ that satisfies the growth condition

$$\lim_{c \rightarrow \infty} \inf_{\mathbf{x}: \|\mathbf{x}\|=c} \psi(\mathbf{x}) = \infty.$$

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Define

$$\mathcal{P}_\psi(\mathbb{R}^d) \doteq \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \psi(\mathbf{x}) \mu(d\mathbf{x}) < +\infty \right\}.$$

and endow it with the metric

$$d_\psi(\mu, \nu) \doteq d_w(\mu, \nu) + \left| \int_{\mathbb{R}^d} \psi(\mathbf{x}) \mu(d\mathbf{x}) - \int_{\mathbb{R}^d} \psi(\mathbf{x}) \nu(d\mathbf{x}) \right|,$$

where d_w is the Lévy-Prohorov metric that topologizes weak convergence.

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Note: The choice of $\psi(\mathbf{x}) = \|\mathbf{x}\|^p$ for some $p \in [1, \infty)$ coincides with the p -Wasserstein topology

Results for Case 1: $\gamma_n/n \rightarrow \infty$

Dupuis, Laschos and R '15

Under suitable boundedness and growth conditions on V and W , and an additional approximability assumption, the sequence $\{Q_n\}$ satisfies an LDP on $\mathcal{P}(\mathbb{R}^d)$ (respectively $\mathcal{P}^\psi(\mathbb{R}^d)$) with rate function \mathcal{J}_* (respectively, \mathcal{J}_*^ψ), where

$$\mathcal{J}_* := \mathcal{J}(\mu) - \inf_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathcal{J}(\mu),$$

and

$$\mathcal{J}_*^\psi := \mathcal{J}(\mu) - \inf_{\mu \in \mathcal{P}^\psi(\mathbb{R}^d)} \mathcal{J}(\mu),$$

with $\mathcal{J} : \mathcal{P}(\mathbb{R}^d) \rightarrow (-\infty, \infty]$, given by

$$\mathcal{J}(\mu) \doteq \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{S}\mathbb{R}^d} (V(\mathbf{x}) + V(\mathbf{y}) + W(\mathbf{x}, \mathbf{y})) \mu(d\mathbf{x}) \mu(d\mathbf{y})$$

Results for Case 2: $\gamma_n = n$

Classical Special Case: $W = 0$

$$P_n(d\mathbf{x}_1, \dots, d\mathbf{x}_n) =: \frac{\exp(-\gamma_n H_n(\mathbf{x}_1, \dots, \mathbf{x}_n))}{Z_n} \ell(d\mathbf{x}_1) \cdots \ell(d\mathbf{x}_n),$$

Particles are iid with marginal distribution

$$\theta(d\mathbf{x}) \propto \exp(-\gamma_n V(\mathbf{x}))$$

Sanov's Theorem

Then $\{Q_n\}$ satisfies an LDP with rate function \mathcal{R} , where $\mathcal{R}(\cdot|\theta)$ is the relative entropy functional: for $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$,

$$\mathcal{R}(\mu|\nu) \doteq \begin{cases} \int_{\mathbb{R}^d} \frac{d\mu}{d\nu}(\mathbf{x}) \log \left(\frac{d\mu}{d\nu}(\mathbf{x}) \right) \nu(d\mathbf{x}), & \text{if } \mu \ll \nu, \\ \infty, & \text{otherwise,} \end{cases}$$

where $\mu \ll \nu$ denotes that μ is absolutely continuous with respect to ν .

Results II: $\gamma_n = n$

Theorem (Dupuis, Laschos and R '15)

Under suitable boundedness and growth conditions on V and W , and an additional approximability assumption, the sequence $\{Q_n\}$ satisfies an LDP with rate function \mathcal{I}_* (respy, \mathcal{I}_*^ψ on $\mathcal{P}(\mathbb{R}^d)$ (respy, $\mathcal{P}^\psi(\mathbb{R}^d)$), where

$$\mathcal{I}_*(\mu) = \mathcal{I}(\mu) - \inf_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathcal{I}(\mu),$$

and

$$\mathcal{I}_*^\psi(\mu) = \mathcal{I}(\mu) - \inf_{\mu \in \mathcal{P}^\psi(\mathbb{R}^d)} \mathcal{I}(\mu),$$

with

$$\mathcal{I}(\mu) \doteq \mathcal{R}(\mu | e^{-V} \ell) + \mathcal{W}(\mu),$$

where $\mathcal{R}(\cdot | \cdot)$ is the relative entropy functional and

$$\mathcal{W}(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(\mathbf{x}, \mathbf{y}) \mu(d\mathbf{x}) \mu(d\mathbf{y}).$$

- Specific results for random matrices were obtained by Ben-Arous-Guionnet (1997), Ben-Arous-Zeitouni (1998), Petz and Hievi (2998) and A. Hardy (2012)
- In this generality, LDPs with respect to the weak topology were obtained when ℓ is Lebesgue measure and $\gamma_n/n \log n \rightarrow \infty$ in work by Chafaï, Gozlan and Zitt (2014).
- Our work significantly extends this work by allowing for
 - (i) more general measures ℓ
 - (ii) arbitrary $\gamma_n/n \rightarrow \infty$
 - (iii) considering stronger topologies
- Our methodology is also different (based on weak convergence methods for large deviations) and based on a common framework

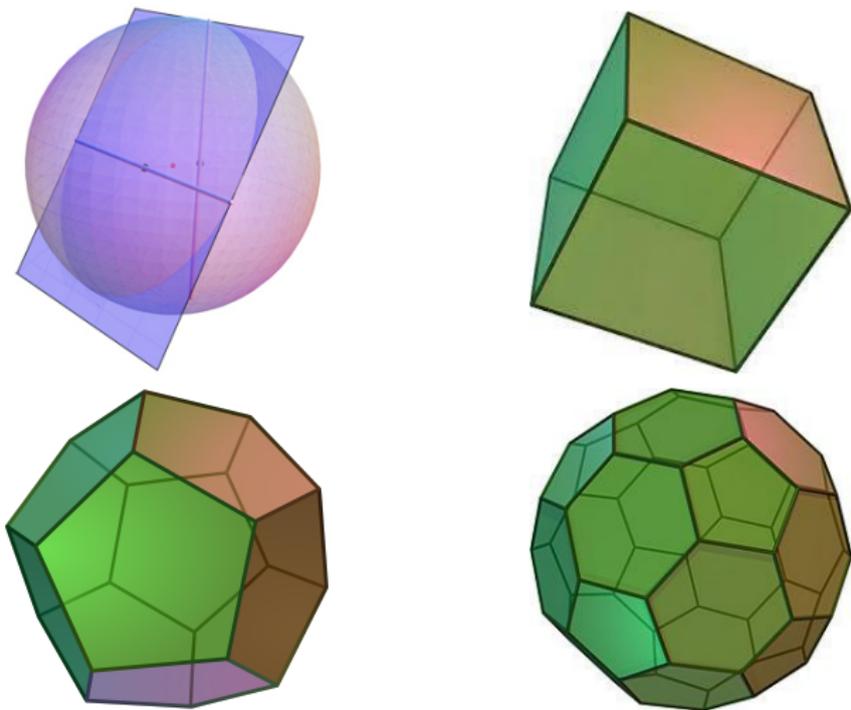
Random Projections of High-Dimensional Measures

Theme:

Study high-dimensional objects
by looking at their
(random) lower-dimensional projections

- Asymptotic (Convex) Geometry : study of the geometry of convex bodies in high dimensions
- The presence of high dimensions forces certain regularity on the geometry of convex bodies that has a probabilistic flavor

Asymptotic Convex Geometry



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Second Motivation

High-dimensional Probability and Statistics
low-dimensional projections are of relevance in
e.g., sparse recovery, information retrieval, statistics
(although will not discuss these applications)

A Striking Result

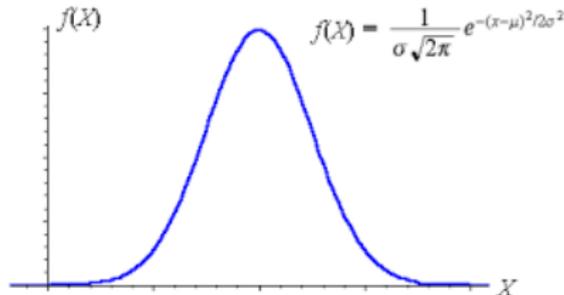
Conjectured by

Anttila, Ball and Perissanski (2003); Brehm and Voigt (2000);
(Diaconis & Freedman, Klartag, Meckes-Meckes, Bobkov, ...)

The CLT for Convex Sets

Let $X^{(n)}$ be uniformly distributed on a convex body in \mathbb{R}^n

Then $\langle X^{(n)}, \theta^{(n)} \rangle_n$ is approximately Gaussian for almost all $\theta^{(n)}$ on S^{n-1}



A Precise Statement of one such result

- A probability measure μ^n (or its density) on \mathbb{R}^n is said to be **isotropic** if it satisfies

$$\int_{\mathbb{R}^n} x \mu(dx) = 0 \text{ and } \int_{\mathbb{R}^n} x_i x_j \mu(dx) = \delta_{ij}.$$

- A convex body K is said to be isotropic if the normalized uniform measure on the body is isotropic

Theorem (CLT for Convex Sets; Klartag '07)

There exist sequences $\varepsilon_n \downarrow 0$, $\delta_n \downarrow 0$ for which the following holds: if $K \subset \mathbb{R}^n$ is an isotropic convex body and $X^{(n)}$ is the random vector that is distributed uniformly in K , then there exists a subset $\mathbb{S} \subset \mathcal{S}^{n-1}$ with $\sigma_{n-1}(\mathbb{S}) \geq 1 - \delta_n$ such that

$$d_{TV} \left(\langle X^{(n)}, \theta^{(n)} \rangle_n, Z \right) \leq \varepsilon_n$$

for all $\theta^{(n)} \in \mathbb{S}$, where $Z \sim \mathcal{N}(0, 1)$ and σ_{n-1} is the inv. measure on \mathcal{S}^{n-1}

Several Extensions of the CLT

- CLT can be extended to high-dimensional measures that satisfy a certain concentration condition (Meckes-Meckes)
- And it can also be extended to multidimensional projections (Klartag, Meckes, etc.)

Projection-Pursuit Algorithm

Kruskal (1969)

Friedman and Tukey (1974)

Diaconis and Friedman (1987)

- 1 Finding the “most interesting” possible projections in high-dimensional data
- 2 “Most interesting” are those that deviate more from a normal distribution

A Natural Question

- Fluctuation analysis suggests that
“Typical projections of certain high-dimensional measures that satisfy a geometric condition behave like sums of i.i.d. random variables”
- We know from a classical result called **Cramér's theorem** that sums of i.i.d. random variables satisfy large deviations principles (LDP).

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Question

Can we establish LDPs for random projections of high-dimensional measures?

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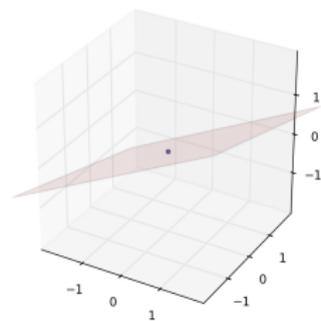
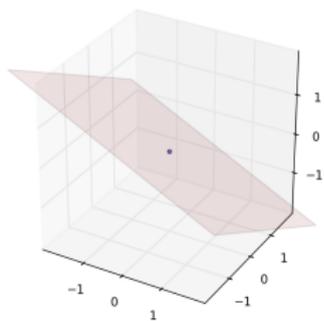
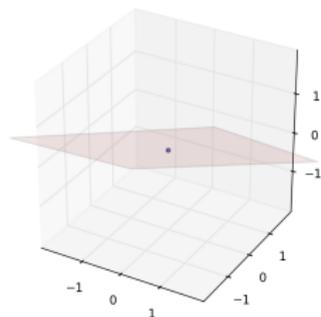
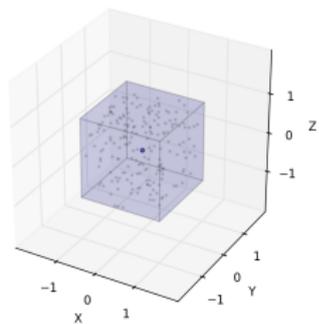
Question

Can we establish LDPs for random projections of high-dimensional measures?

May more easily distinguish the high-dimensional objects

Would lead to an LDP of a geometric flavour

Random Orthonormal Bases



The Stiefel Manifold

The **Stiefel manifold** of orthonormal k -frames in \mathbb{R}^n , $k < n$,

$$\mathbb{V}_{n,k} \doteq \{\mathbf{A} \in \mathbb{R}^{n \times k} : \mathbf{A}^T \mathbf{A} = \mathbf{I}_k\},$$

where \mathbf{I}_k is the $k \times k$ identity matrix.

Random orthonormal frames/bases are chosen with respect to the invariant measure on the (compact) Stiefel manifold.

Random Projections onto Random subspaces

- Suppose $X^{(n)}$ is a random vector in \mathbb{R}^n and

$$\mathbf{A}_{n,k} = [\mathbf{A}_{n,k}(i,j)]_{i=1,\dots,n;j=1,\dots,k}$$

is an $n \times k$ matrix drawn from the Haar measure on the Stiefel manifold $\mathbb{V}_{n,k}$, independent of $X^{(n)}$.

- Then the coordinates of the projection of $X^{(n)}$ onto the k -dimensional subspace with basis determined by $\mathbf{A}_{n,k}$ is given by

$$W_A^{(n)} \doteq \mathbf{A}_{n,k}^T X^{(n)}.$$

Results on Multidimensional Projections

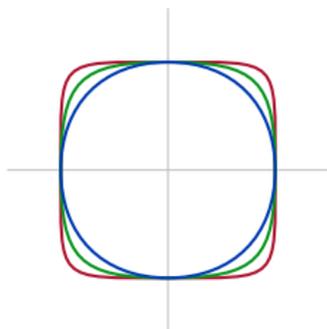
Assumption: The ATS (Asymptotic Thin-Shell) Condition

Suppose $\|X^{(n)}\|_2/\sqrt{n}$ satisfies an LDP in \mathbb{R} with speed n and rate function $J_X : \mathbb{R} \mapsto [0, \infty)$.

Theorem (Kim and R '17)

Suppose the sequence $\{X^{(n)}\}$ satisfies the ATS condition. Then $W_A^{(n)}, n \in \mathbb{N}$, where recall $W_A^{(n)} \doteq A_{n,k}^T X^{(n)}$, satisfies an LDP at speed n with a rate function that can be written explicitly in terms of J_X .

A natural sequence – ℓ^p Balls in \mathbb{R}^n



$$\begin{aligned}\|x\|_{n,p} &\doteq (x_1^p + \dots + x_n^p)^{1/p} \\ \mathbb{B}_{n,p} &\doteq \{x \in \mathbb{R}^n : \|x\|_{n,p} \leq 1\}.\end{aligned}$$

Let $\mathbf{X}^{(n,p)}$ be uniformly distributed on the ℓ^p ball $\mathbb{B}_{n,p}$.
Then the renormalized scalar projection is given by

$$\mathfrak{W}_{\Theta}^{(n,p)} \doteq \frac{n^{1/p}}{n^{1/2}} \langle \mathbf{X}^{(n,p)}, \Theta^{(n)} \rangle_n.$$

Scaling rationale: “typical” coordinate of $\mathbf{X}^{(n,p)}$ is $\sim n^{-1/p}$ and “typical” coordinate of $\Theta^{(n)}$ is $\sim n^{-1/2}$.

ℓ_p -balls (Kim and R '17)

- I. $X^{(n)}$ uniformly distributed on a suitably normalized ℓ_p ball in \mathbb{R}^n for $p \geq 2$

The Gibbs Case (Kim and R '17)

II. $X^{(n)} \sim P_n$ (with $d = 1$, $\gamma_n = n$)

Results: Examples that verify Assumption ATS

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This justifies the need for establishing the LDP in stronger topologies !!

- Laws of interacting particles (equivalently, non-product measures in high-dimensions) arise in many applications, ranging from statistics to statistical mechanics
- The study of their large deviations behavior is of general interest and leads to the study of certain associated variational problems
- The rate function in large deviations provides interesting qualitative information about the system