Geometry and topology of smooth Gaussian fields

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Slides available at
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Outline

Smooth Gaussian fields

Basic setting

- Let $f : \mathbb{R}^d \to \mathbb{R}$ be a stationary C^2 Gaussian field with mean zero.
- The distribution of f is specified by its covariance function $K : \mathbb{R}^d \to \mathbb{R}$ defined as

$$K(x-y) = \mathrm{Cov}[f(x), f(y)] \qquad \forall x, y \in \mathbb{R}^d.$$

- We will consider the geometry/topology of the **excursion sets**

$$\{f \geq \ell\} := \left\{ x \in \mathbb{R}^d \;\middle|\; f(x) \geq \ell \right\} \qquad \text{for } \ell \in \mathbb{R}.$$

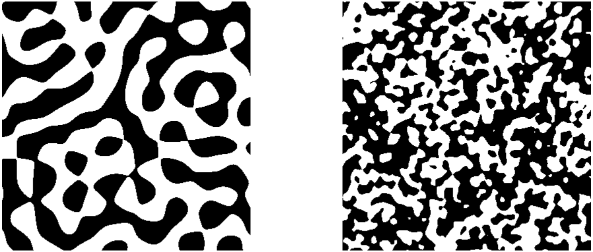

Figure: Excursion sets $\{f \geq 0\}$ in white for the fields on $\mathbb{R}^2$ with $K(x) = J_0(|x|)$, the 0-th Bessel function, (left) and $K(x) = \exp(-|x|^2/2)$ (right).

A Gaussian field can be viewed as a measure on a particular class of functions. Statements about the field can be interpreted as statements about 'typical' functions in the class.

1. **Berry's conjecture:** on generic 2-dimensional manifolds, high-frequency eigenfunctions of the Laplacian can be approximated by the Gaussian field with $K(x) = J_0(|x|)$ [6].
2. **Hilbert's 16th problem** concerns the zero set of homogeneous polynomials. There is a canonical Gaussian measure on such polynomials which behaves locally like the stationary field with $K(x) = \exp(-|x|^2/2)$ [11].

- **Percolation theory** studies the large scale topological properties of spatial random models.
- **Phase transition**: for a given field, there is a critical level ℓ_c such that, with probability one
  - for $\ell > \ell_c$, $\{f \geq \ell\}$ contains only bounded components,
  - for $\ell < \ell_c$, $\{f \geq \ell\}$ contains a unique unbounded component.

  See [2] for a survey.

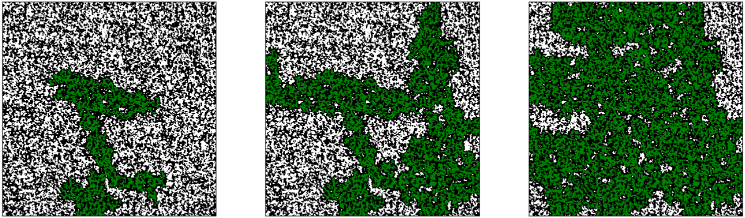

Figure: The excursion sets $\{f \geq \ell\}$ for $\ell = 0.05$ (left), $\ell = 0$ (middle) and $\ell = -0.05$ (right). Largest component highlighted in green.

Motivation

3) Statistical applications

- Gaussian fields arise in many areas of science:
  - Medical imaging [20],
  - Cosmology [18],
  - Topological data analysis [1].
- Geometric/topological properties of excursion sets can be used as test statistics. (See [19] for an overview.)

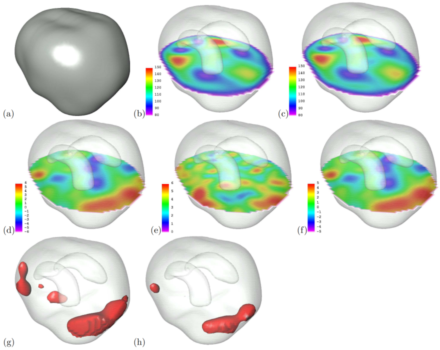

Figure: Measurements from a PET study of brain activity during a reading task. (Source: [19]).

Smooth Gaussian fields

Questions of interest

- What are the geometric and topological properties of smooth Gaussian excursion sets?
- We would like to analyse:

  Geometric functionals
  - volume
  - boundary volume
  - Euler characteristic

  Topological functionals
  - number of connected components
  - Betti numbers
- What is the expectation, variance and distribution of such functionals on a bounded domain?
- How does this depend on the size of the domain? the level of the excursion set? the covariance of the field?

Outline

Geometric/local functionals

A rough definition

- A functional of a random field is described as **local** (or geometric) if it is an integral of a pointwise function of the field and its derivatives:

$$\int_D \varphi(f(x), \nabla f(x), \nabla^2 f(x))\, \mu(dx)$$

- We will consider functionals of the form

$$F_R = \int_{[-R,R]^d} \varphi(f(x) - \ell)\, dx$$

  for some $\varphi : \mathbb{R} \to \mathbb{R}$ (e.g. $\varphi(y) = \mathbb{1}_{y \geq 0}$).
- How does this behave as $R \to \infty$?
- First order behaviour is trivial: by Fubini's theorem,

$$\mathbb{E}[F_R] = (2R)^d \mu(\ell)$$

  where $\mu(\ell) := \mathbb{E}[\varphi(f(0) - \ell)]$.

The variance and limiting distribution of local functionals can be studied using Hermite polynomials.

- The Hermite polynomials $(H_n)_{n\geq 0}$ can be defined inductively by setting

$$H_0(x) = 1 \quad \text{and} \quad H_{n+1}(x) = xH_n(x) - H_n'(x)$$

which yields

$$H_1(x) = x, \quad H_2(x) = x^2 - 1, \quad H_3(x) = x^3 - 3x.$$

- Hermite polynomials are orthogonal with respect to the Gaussian measure: if X, Y are jointly normal with mean zero and variance one then

$$\mathbb{E}[H_n(X)H_m(Y)] = \begin{cases} n!\mathrm{Cov}[X,Y]^n & \text{if } n = m \\ 0 & \text{if } n \neq m. \end{cases}$$

- If $\mathbb{E}[\varphi^2(Z)] < \infty$ for $Z \sim \mathcal{N}(0,1)$ then

$$\varphi = \sum_{n=0}^{\infty} a_n H_n$$

where $\sum_n a_n^2 n! < \infty$.

- Considering the expansion $\varphi(\cdot - \ell) = \sum_n a_n(\ell) H_n$ yields

$$F_R = \sum_{n=0}^{\infty} a_n(\ell) \int_{[-R,R]^d} H_n(f(x))\, dx =: \sum_{n=0}^{\infty} Q_n.$$

- The variance of F_R can be computed by considering

$$\begin{aligned}\mathrm{Cov}\,[Q_n, Q_m] &= a_n(\ell) a_m(\ell) \iint_{[-R,R]^{2d}} \mathrm{Cov}[H_n(f(x)), H_m(f(y))]\, dxdy \\ &= \begin{cases} a_n(\ell)^2 n! \iint_{[-R,R]^{2d}} K(x-y)^n\, dxdy & \text{if } n = m \neq 0, \\ 0 & \text{otherwise.} \end{cases}\end{aligned}$$

- Hence $\mathrm{Var}[F_R] = \sum_n \mathrm{Var}[Q_n]$ which depends on the integrability of K.

Three general classes of covariance function are considered in the literature:

1. K is **integrable**
   - Example: the Bargmann-Fock field has covariance
   $$K(x) = \exp\left(-\frac{|x|^2}{2}\right).$$
2. K is **regularly varying** at infinity with index $\alpha \in (0, d)$
   - Example: The Cauchy field has covariance
   $$K(x) = (1 + |x|^2)^{-\alpha/2}.$$
3. K is **oscillating and slowly decaying**
   - Example: The Random Plane Wave is the two-dimensional field with covariance
   $$K(x) = J_0(|x|) \sim \sqrt{\frac{2}{\pi}} \cos(|x| - \pi/4)|x|^{-1/2} \quad \text{as } |x| \to \infty.$$

Second order properties

Case 1: Integrable covariance

Recall:

$$F_R = \sum_{n=0}^{\infty} Q_n, \qquad \mathrm{Var}[Q_n] = a_n(\ell)^2 n! \int_{[-R,R]^{2d}} K(x-y)^n \, dxdy$$

- If K is integrable then for $n \neq 0$

$$\mathrm{Var}[Q_n] \sim \left(a_n(\ell)^2 n! \int_{\mathbb{R}^d} K(x)^n \, dx \right) (2R)^d$$

  so each chaos has variance of order R^d (or 0).
- Since $\sum_n a_n(\ell)^2 n! < \infty$, for each ℓ

$$\mathrm{Var}[F_R] \sim c_\ell R^d \text{ as } R \to \infty$$

  where $c_\ell > 0$ assuming φ is not too degenerate.

Using similar, but more involved, computations one can compute the higher order moments of F_R to prove:

Theorem (Breuer-Major theorem)

If f has rotation invariant distribution, then as $R \to \infty$

$$\frac{F_R - \mu(\ell)}{\mathrm{Var}[F_R]} \xrightarrow{d} \mathcal{N}(0,1)$$

Remark

More modern proofs of this result use the Malliavin-Stein method (in particular the fourth-moment theorem) which also yields a rate of convergence.

- If $K(x) \sim c|x|^{-\alpha}$ then for $n \neq 0$

$$\mathrm{Var}[Q_n] = a_n(\ell)^2 n! \int_{[-R,R]^d} K(x-y)^n \, dxdy$$

$$\sim a_n(\ell)^2 c_{K,n} \times \begin{cases} R^{2d-n\alpha} & \text{if } n\alpha < d, \\ R^d \log R & \text{if } n\alpha = d, \\ R^d & \text{if } n\alpha > d. \end{cases}$$

- Hence a finite number of the Q_n terms have higher orders of variance.
- Since $\sum_n a_n(\ell)^2 n! < \infty$

$$\sum_{n>d/\alpha} \mathrm{Var}[Q_n] \sim c_\ell R^d$$

and so $F_R = \sum_n Q_n$ will be asymptotically dominated by a single term if $a_n(\ell) \neq 0$ for some $n \leq d/\alpha$.

Theorem (Dobrushin-Major theorem)

Let $n^*(\ell) = \inf\{n : a_n(\ell) \neq 0\}$. If f satisfies some technical conditions, then

$$\mathrm{Var}[F_R] \sim c_{K,\varphi,\ell} \times \begin{cases} R^{2d-n^*\alpha} & \text{if } n^*\alpha < d, \\ R^d \log R & \text{if } n^*\alpha = d, \\ R^d & \text{if } n^*\alpha > d, \end{cases} \qquad \text{as } R \to \infty.$$

Moreover if $n^* = 1$ or $n^*\alpha > d$ then

$$\frac{F_R - \mu(\ell)}{\mathrm{Var}[F_R]} \xrightarrow{d} \mathcal{N}(0,1).$$

For other values of n^*, the limiting distribution is a Hermite distribution.

Remark

- *Typically $n^*(\ell) = 1$ for all but finitely many values of ℓ, which are described as anomalous levels.*
- *If φ is regular then $a_n(\ell) = (-1)^n \mu^{(n)}(\ell)/n!$ so that anomalous levels correspond to critical points of μ.*

- The classical Breuer-Major theorem [7]. A modern proof using the Malliavin-Stein method [17].
- The Dobrushin-Major theorem [8] was proven using multiple Wiener-Itô integrals.
- More recently, a general CLT has been proven for some fields with slowly decaying oscillating correlations [12].

Outline

1. Introduction

2. Geometric functionals

3. Topological functionals

Topological functionals
What is known?

- Much less is known about non-local/topological functionals of Gaussian fields.
- The previous approach fails due to the lack of an integral representation.
- There is no unifying theory, but many partial results using a variety of methods:

Type of result	Methods
Law of large numbers [15]	Ergodic argument
Variance bounds[16, 5, 4]	Coupling, interpolation formulae
Central limit theorem [3, 13, 10]	Martingale techniques

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- In joint work with Stephen Muirhead [14], we adapt the Hermite expansion approach to non-local functionals.
- Let $f : \mathbb{Z}^d \to \mathbb{R}$ be the Gaussian free field (in $d \geq 3$), so that

$$K(x-y) \sim c_d |x-y|^{-(d-2)}.$$

- The *cluster count* $N_R(f)$ is the number of clusters (i.e. connected components) of the graph $\{f \geq \ell\} \cap [-R, R]^d$.

Wiener chaos expansion

Let H be a set of centred jointly Gaussian variables. Let $\mathcal{P}_n$ be the space of all polynomials of degree n in H.
The n-th *Wiener chaos* of H is $H^{:n:} := \overline{\mathcal{P}_n} \cap \overline{\mathcal{P}_{n-1}}^{\perp}$.

Theorem

Let the random variable X be square integrable and $\sigma(H)$-measurable, then

$$X \stackrel{L^2}{=} \sum_{n=0}^{\infty} Q_n[X]$$

where Q_n denotes projection onto $H^{:n:}$.

Remark

- *While the result is very general, in practice the chaos projections can be difficult to characterise (especially if H is large).*
- *When H has a single element, this is just the Hermite expansion.*

Proposition

Let $D \subset \mathbb{Z}^d$ be finite and $\Phi : \mathbb{R}^D \to \mathbb{R}$ be smooth and bounded. Then

$$Q_n[\Phi(f)] = \frac{1}{n!} \sum_{x_1,\dots,x_n \in D} \mathbb{E}[\partial_{x_1} \dots \partial_{x_n} \Phi(f)] \, {:}f(x_1) \dots f(x_n){:}$$

where $:f(x_1) \dots f(x_n): \; = Q_n[f(x_1) \dots f(x_n)]$.

- The proof uses Gaussian integration by parts and is quite elementary.
- The term $:f(x_1) \dots f(x_n):$ is called a *Wick polynomial* and can be evaluated using a diagram formula.

The discrete derivative d_x is defined as

$$d_x N_R(f) = N_R(\{f \geq \ell\} \cup \{x\}) - N_R(\{f \geq \ell\} \setminus \{x\})$$

Proposition

For $R \geq 1$

$$Q_n[N_R(f)] = \frac{1}{n!} \sum_{x_1,\ldots,x_n \in [-R,R]^d \cap \mathbb{Z}^d} P_R(x_1, \ldots, x_n) :f(x_1) \ldots f(x_n):$$

where the pivotal intensity P_R is defined for distinct points $\underline{x} = (x_1, \ldots, x_n)$ as

$$P_R(\underline{x}) = \mathbb{E}[d_{x_1} \ldots d_{x_n} N_R(f) | f(\underline{x}) = \ell] \varphi_{f(\underline{x})}(\ell),$$

and $\varphi_{f(\underline{x})}$ is the density of $f(\underline{x})$.

Wiener chaos expansion

'Semi-locality' via percolation results

- For a local functional, $\partial_{x_1} \dots \partial_{x_n} \Phi(f) = 0$ unless $x_1 = \dots = x_n$ so the chaos is supported on diagonal terms.
- If P_R decays rapidly away from the diagonal, then we can analyse the variance and limiting distribution on each chaos as in the local case. We can view this as *'semi-locality'* of the cluster count.

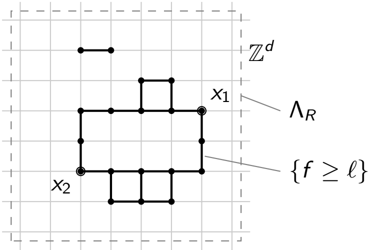

Figure: For this configuration $d_{x_1} d_{x_2} N_R(f) = 1$.

- In general, if $d_{x_1} \dots d_{x_n} N_R(f) \neq 0$ then $x_1, \dots, x_n$ must be joined by bounded clusters of $\{f \geq \ell\}$.

Theorem (Truncated arm decay [9])

Let $f : \mathbb{Z}^d \to \mathbb{R}$ be the Gaussian free field for $d \geq 3$. There exists $\ell_c \in \mathbb{R}$ such that for every $\ell \neq \ell_c$, the probability that 0 is contained in a bounded cluster of $\{f \geq \ell\}$ of diameter at least n is at most e^{-cn^ρ} for some $c, \rho > 0$.

Corollary

For $\ell \neq \ell_c$ there exists $c, C, \rho > 0$ such that

$$P_R(\underline{x}) \leq Ce^{-c\mathrm{diam}(\underline{x})^\rho}$$

where $\mathrm{diam}(\underline{x})$ denotes the diameter of $\underline{x}$.

Let $\mu(\ell) = \lim_{R\to\infty} \mathbb{E}[N_R(f)]/(2R)^d$ be the *mean clusters-per-vertex*.

Theorem

Let $f : \mathbb{Z}^3 \to \mathbb{R}$ be the Gaussian free field and $\ell \neq \ell_c$.

$$\mathrm{Var}[N_R(f)] \sim c_\ell \times \begin{cases} R^5 & \text{if } \mu'(\ell) \neq 0 \\ R^4 & \text{if } \mu'(\ell) = 0, \mu''(\ell) \neq 0 \\ R^3 \log R & \text{if } \mu'(\ell) = \mu''(\ell) = 0, \mu'''(\ell) \neq 0 \\ R^3 & \text{otherwise.} \end{cases}$$

In case 2, the (normalised) limiting distribution is a Hermite distribution, in all other cases it is Gaussian.

- Analogous results hold for $d \geq 4$ and other fields but are omitted here for brevity.
- Similar to results in local case, but the requirement that $\ell \neq \ell_c$ is new.

Summary

Open questions:

- Can this approach be extended to smooth fields?
- Does this approach enable the Malliavin-Stein method for non-local functionals?
- What happens at the critical level?

Thank you for listening!

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