Geometric and topological functionals of smooth Gaussian fields

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Slides available at
`https://michael-mcauley.github.io`

Outline

1. Motivating example: the Euler characteristic
2. Geometric/local functionals
3. Topological/non-local functionals

Gaussian fields

Motivation: medical imaging

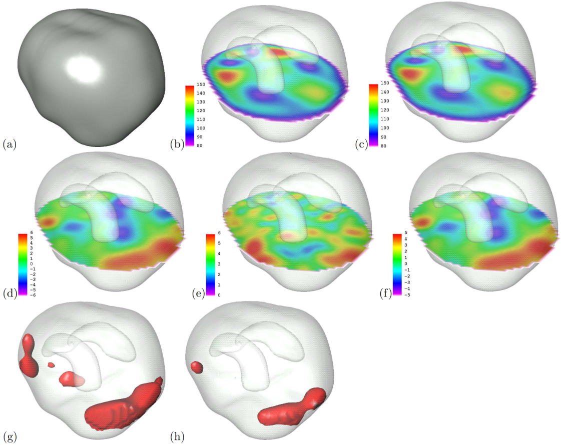

Figure: Measurements from a PET study of brain activity during a reading task. (Source: [14]). See [15] for a technical account.

- Let M be a smooth manifold and $f : M \to \mathbb{R}$ be a C^2 Gaussian field with mean zero and variance one (at each point).
- The distribution of the field is specified by its covariance function $K : M^2 \to [-1, 1]$ defined as

$$K(x, y) = \mathbb{E}[f(x)f(y)] \qquad \forall x, y \in M.$$

- We are interested in the geometry of the *excursion sets*

$$\{f \geq \ell\} := \{x \in M \mid f(x) \geq \ell\}$$

for $\ell \in \mathbb{R}$.

Euler characteristic

A rough definition

Figure: The Euler characteristics of a sliotar (solid ball), a tennis ball and a coffee cup are 1, 2 and 0 respectively.

1. The Euler characteristic is an integer valued topological invariant of ‘nice’ sets in Euclidean space.
2. The Euler characteristic of a set in $\mathbb{R}^3$ is the number of components minus the number of ‘handles’ plus the number of ‘holes’.
3. For large ℓ, if the excursion set $\{f \geq \ell\}$ is non-empty then it is most likely a single simply connected component, hence

$$\mathbb{E}[\mathrm{EC}[\{f \geq \ell\}]] \approx \mathbb{P}\left(\sup_M f \geq \ell\right).$$

Euler characteristic

Application to excursion sets

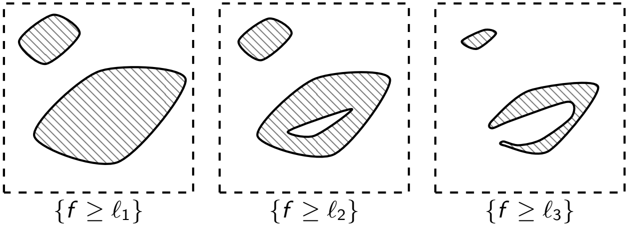

Figure: Excursion sets for a function f above levels $\ell_1 < \ell_2 < \ell_3$.

The Euler characteristic of an excursion set for a 'nice' function $f : M \to \mathbb{R}$ can be decomposed as

$$\mathrm{EC}[\{f \geq \ell\}] = \sum_{i=0}^{d} (-1)^i n_i + \text{Boundary terms}$$

where

$$n_i = \#\{x \in M \ : \ f(x) \geq \ell, \ \nabla f(x) = 0, \ \mathrm{index} \nabla^2 f(x) = d - i\}.$$

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Euler characteristic

Application to Gaussian fields

- The expected number of zeros of a one-dimensional random function $h : [0, T] \to \mathbb{R}$ can be computed by the Kac-Rice formula as:

$$\mathbb{E}\left[\int_0^T \delta_0(h(t))|h'(t)|\, dt\right] = \int_0^T \mathbb{E}\left[|h'(t)|\,\middle|\,h(t)=0\right] p_{h(t)}(0)\, dt.$$

- For $f : \mathbb{R}^d \to \mathbb{R}$ stationary, Gaussian

$$\mathbb{E}\left[\sum_i (-1)^i n_i\right] = (-1)^d \int_M \mathbb{E}\left[\det \nabla^2 f(x) \mathbb{1}_{f(x)\geq \ell}\,\middle|\,\nabla f(x) = 0\right] p_{\nabla f(x)}(0)\, dx$$

- In particular, when $M = [-R, R]^3$

$$\mathbb{E}[\mathrm{EC}[\{f \geq \ell\} \cap M]] = \frac{\sqrt{-\det \nabla^2 K(0)}}{(2\pi)^2}(2R)^3(\ell^2 - 1)e^{-\ell^2/2} + O(R^2)$$

Euler characteristic

Medical imaging

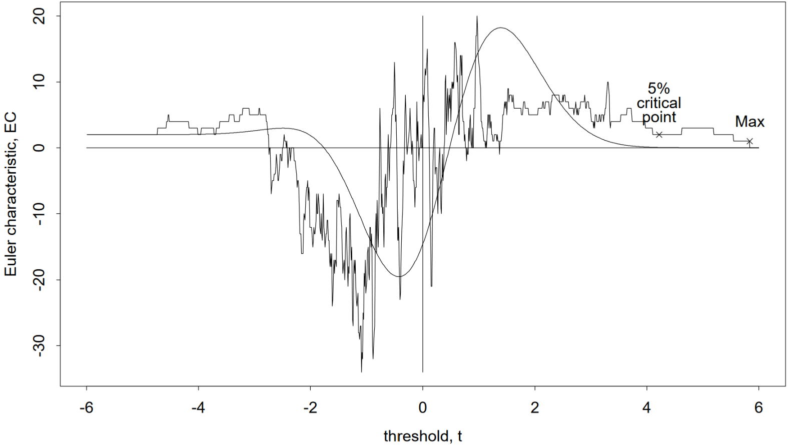

Figure: The observed Euler characteristic for PET data (jagged) and the expected value for a Gaussian field (smooth) at different thresholds. Source: [15].

For more details, see

- [14] for a non-technical overview of different applications;
- [1] for theoretical development of the Euler characteristic for Gaussian fields;
- [8] for a mathematical development of Gaussian fields with applications in cosmology.

Outline

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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.
- Examples:
  - Volume of the excursion set
  - Boundary length of the excursion set
  - Euler characteristic of the excursion set
- 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. $\varphi(y) = \mathbb{1}_{y \geq 0}$) and stationary $f : \mathbb{R}^d \to \mathbb{R}$.
- By Fubini's theorem,

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

  where $Z \sim \mathcal{N}(0, 1)$ for all $R > 0$.

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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

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

- If $X \sim \mathcal{N}(0,1)$ and $\mathbb{E}[\varphi^2(X)] < \infty$ 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 the Wiener chaos expansion

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

- The variance of $F_{R,\ell}$ can be computed by considering

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

- The overall variance therefore depends on the integrability/decay of K.

Second order properties

Covariance function examples

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

1. K is **integrable**
   - Example: the Bargmann-Fock field is the scaling limit of random homogeneous polynomials [2] and has covariance

$$K(x-y) = \exp\left(-\frac{\|x-y\|^2}{2}\right).$$

2. K is **regularly varying** at infinity with index $\alpha \in (0, d)$
   - Example: The Cauchy field has covariance

$$K(x-y) = (1+|x-y|^2)^{-\alpha/2}.$$

3. K is **oscillating and slowly decaying**
   - Example: The Random Plane Wave is the two-dimensional field with covariance

$$K(x) = J_0(|x|) \sim \sqrt{\frac{2}{\pi}}\cos(|x|-\pi/4)|x|^{-1/2} \quad \text{as } |x| \to \infty.$$

   It models high energy Laplace eigenfunctions in quantum chaos [4].

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Second order properties

Case 1: Integrable covariance

Recall:

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

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

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

  so each chaos has variance of order R^d.
- Moreover for each ℓ

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

- **(Breuer-Major theorem.)** If f is isotropic, then F_R satisfies a central limit theorem as $R \to \infty$.

- If K is regularly varying at infinity with index $\alpha \in (0, d)$ then for $n \neq 0$

$$\mathrm{Var}[Q_n] \sim c_{K,n} R^{\max\{2d-n\alpha, d\}}.$$

- At a 'generic' level ℓ, $a_1(\ell) \neq 0$ so the first chaos carries all variance asymptotically

$$F_R \sim a_1(\ell) \int_{[-R,R]^d} f(x)\, dx$$

  and so a central limit theorem holds with variance of order $R^{2d-\alpha}$.
- At some 'anomalous' levels, $a_1(\ell) = 0$ so F_R has lower order variance.
- The limiting distribution may be Gaussian or non-Gaussian depending on which chaos(es) dominate!

- Results in this setting mostly consider specific fields and functionals.
- Compared to the regularly varying case, the first chaos typically has lower order variance due to oscillations of K. Hence when $a_2(\ell) \neq 0$ the second chaos dominates

$$\mathrm{Var}[F_R] \sim a_2(\ell) \iint_{[-R,R]^{2d}} K^2(x-y)\, dxdy.$$

- At anomalous levels (i.e. $a_2(\ell) \neq 0$) the fourth chaos typically dominates, resulting in a lower order of variance.
- Central limit theorems are known in many cases, although degenerate behaviour is also possible [7].

Local functionals

Limit theorem references

- The classical Breuer-Major theorem established a CLT for local functionals of fields with fast correlation decay [5]. Modern proofs of this result typically use the Malliavin-Stein method [11].
- Non-CLTs were established for fields with slow (regularly varying) correlation decay [6] using multiple Wiener-Itô integrals.
- More recently, a general CLT has been proven for some fields with slowly decaying oscillating correlations [7].

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Non-local functionals

- Many natural topological functionals of a Gaussian field are non-local.
- Examples:
  - Number of connected components of the excursion set
  - Betti numbers of the excursion set
  - Volume of the unbounded component of the excursion set
- These functionals are of interest from both applied [13] and theoretical perspectives [2], but are much harder to study!

The component count

Law of large numbers

- Let $f : \mathbb{R}^d \to \mathbb{R}$ be a stationary, centred, smooth Gaussian field.
- Given $\ell \in \mathbb{R}$ and $R > 0$ we let $N(\ell, R)$ be the number of connected components of $\{f \geq \ell\} \cap [-R, R]^d$.

Theorem (Nazarov-Sodin[10])

If $K(x) \to 0$ as $|x| \to \infty$, then there exists $c(\ell) \geq 0$ such that

$$\lim_{R\to\infty} \frac{N(\ell, R)}{(2R)^d} = c(\ell)$$

almost surely and in L^1.

- The result is extremely general: in particular, there is no requirement of fast correlation decay.
- The proof shows that the component count is 'semi-local': its value on a macroscopic domain can be well approximated by summing its value on mesoscopic domains.

The component count

Law of large numbers: Proof

- Let $\Lambda_R = [-R, R]^d$. Let $N_x(R)$ and $\overline{N}_x(R)$ denote the number of components of $\{f \geq \ell\}$ which are inside or intersect $x + \Lambda_R$ respectively.
- **(Integral geometric sandwich)** For $0 < s < R$

$$\int_{\Lambda_{R-s}} \frac{N_x(s)}{(2s)^d}\, dx \leq N_0(R) \leq \int_{\Lambda_{R+s}} \frac{\overline{N}_x(s)}{(2s)^d}\, dx.$$

- Applying the ergodic theorem as $R \to \infty$

$$\limsup_{R\to\infty} \left| \frac{N_0(R)}{(2R)^d} - \frac{1}{(2R)^d} \int_{\Lambda_R} \frac{N_x(s)}{(2s)^d}\, dx \right| \leq \frac{\mathbb{E}[\overline{N}_0(s) - N_0(s)]}{(2s)^d}.$$

- $\overline{N}_0(s) - N_0(s)$ is the number of components intersecting $\partial\Lambda_s$ which has expectation $O(s^{d-1})$ as $s \to \infty$.
- These observations imply that $(2R)^{-d} N_0(R)$ is Cauchy almost surely and in L^1.

The component count

Central limit theorem

Assume that $f = q * W$ where W is a Gaussian white noise process on $\mathbb{R}^d$ and q satisfies some regularity conditions, including

$$\sup_{|\alpha|\leq 2} |\partial^\alpha q(x)| \leq c|x|^{-\beta}$$

for some $c > 0$ and $\beta > 9d$ and all $x \in \mathbb{R}^d$.

Theorem (Beliaev-M.-Muirhead[3])

Given $\ell \in \mathbb{R}$, there exists $\sigma^2(\ell) > 0$ such that as $R \to \infty$

$$\frac{\mathrm{Var}[N(\ell, R)]}{(2R)^d} \to \sigma^2(\ell)$$

and

$$\frac{N(\ell, R) - \mathbb{E}[N(\ell, R)]}{(2R)^{d/2}} \xrightarrow{d} \mathcal{N}(0, \sigma^2(\ell)).$$

- Matches results for local functionals when the covariance function is integrable.
- Method extends to other non-local functionals [9].

The component count

Proof of CLT

- The proof adapts a martingale CLT argument from discrete probability [12].
- Let $(\mathcal{F}_v)_{v\in\mathbb{Z}^d}$ be a 'lexicographic' filtration generated by the white noise W and
$$S_n := \frac{N(\ell,n)-\mathbb{E}[N(\ell,n)]}{(2n)^{d/2}}.$$
Then $S_{n,v} := \mathbb{E}[S_n|\mathcal{F}_v]$ defines a 'lexicographic martingale array'.
- A generalisation of the classical martingale CLT states that $S_n \to \mathcal{N}(0,\sigma^2)$ provided that the martingale differences $U_{n,v}$ satisfy certain moment bounds and $\sum_{v\in\mathbb{Z}^d} U_{n,v}^2 \to \sigma^2$ in L^1.
- The latter property follows from an elegant ergodic argument due to Penrose [12].
- The moments bounds follow from relating $U_{n,v}$ to the change in the component count when the white noise W is resampled on a cube of unit length centred at v.

Open questions:

- How is the component count affected by long-range dependence?
  - Do anomalous levels exist?
  - Do central/non-central limit theorems hold?
- What happens if we relax the assumptions of stationarity, Gaussianity or smoothness?

Thank you for listening!

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