Asymptotic expansion of the expected Minkowski functional for isotropic central limit random fields

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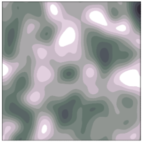
Excursion set for a smooth isotropic random field

- Isotropic random field $X(t)$, $t \in T \subset \mathbb{R}^n$:
  $\forall T'$(finite set) $\subset T$,

$$\{X(t)\}_{t\in T'} \overset{d}{=} \{X(Pt+b)\}_{t\in T'}, \ \forall (P,b) \in O(n) \times \mathbb{R}^n$$

- Excursion set is the sup-level set of a function $X(t)$:

$$T_v = \{t \in T \mid X(t) \geq v\} = X^{-1}([v,\infty))$$



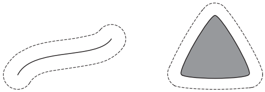

Left: Isotropic random field, Right: Its excursion set

- Filtration property: $T_{v_1} \supset T_{v_2}$ when $v_1 \leq v_2$

Minkowski functional (MF) and Lipschitz-Killing curvature

- Let $M \subset \mathbb{R}^n$ be a closed set. Tube about M with radius ρ:

$$\mathrm{Tube}(M,\rho) = \left\{x \in \mathbb{R}^n \mid \mathrm{dist}(x,M) \le \rho\right\}$$



- Steiner's formula: For small $\rho > 0$, and $\omega_d = \pi^{d/2}/\Gamma(d/2+1)$,

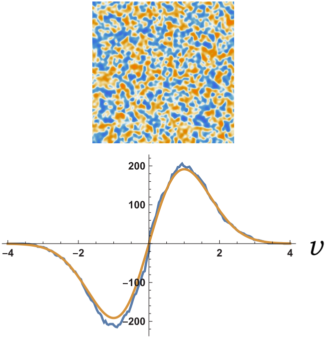
$$\mathrm{Vol}_n(\mathrm{Tube}(M,\rho)) = \sum_{j=0}^{n} \omega_{n-j}\rho^{n-j}\mathcal{L}_j(M) = \sum_{j=0}^{n} \rho^j \binom{n}{j} \mathcal{M}_j(M)$$

  $\mathcal{M}_j(M)$: Minkowski functional, $\mathcal{L}_j(M)$: Lipschitz-Killing curvature (defined independently of the ambient space)
- The Euler characteristic (EC) of M is

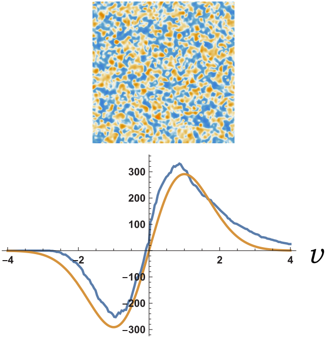
$$\chi(M) = \mathcal{L}_0(M) = \mathcal{M}_n(M)/\omega_n \quad \text{(Gauss-Bonnet theorem)}$$

MF of the excursion set T_v as a goodness-of-fit statistic

- The Minkowski functional $\mathcal{M}_j(T_v)$ of the excursion set T_v can be used as a statistic for testing goodness-of-fit.



Gaussian



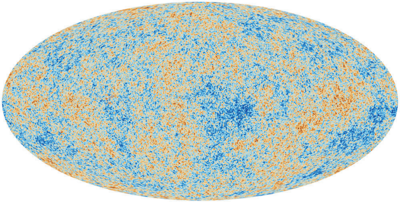
non-Gaussian

— $\chi(T_v)$

— $\mathbb{E}[\chi(T_v)]$ under the assumption of Gaussianity

Applications in cosmology: Cosmic fields

- Cosmic microwave background (CMB) (mode: 160.2GHz)



http://planck.cf.ac.uk/

The CMB has the information of the primitive universe.

- Cosmic inflation theory:

$$X(t) = \underbrace{\varphi(t)}_{O(1)} + \underbrace{\varphi^{(2)}(t)}_{O(\nu)} + \underbrace{\varphi^{(3)}(t)}_{O(\nu^2)} + \cdots, \quad t \in \mathbb{R}^2, \quad \nu \ll 1$$

φ: isotropic Gaussian field, $\varphi^{(2)}$: quadratic functional of φ, ...

- k-point correlation function:

$$\mathrm{cum}(X(t_1), \ldots, X(t_k)) = O(\nu^{k-2})$$

Simulator vs. Analytic approach

- Many versions of the inflation models exist.
- Theoretical MF (evaluated by cosmic simulator) and empirical MF are compared to check the assumed model.
- The computational cost of the cosmic simulator is very high.
- Our purpose is to provide an analytic approach to evaluate the MFs without using simulators.

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Kinematic Formula for isotropic random field

Proposition (Kinematic Formula)

When $X(t)$, $t \in T$, is a smooth isotropic random field,

$$\mathbb{E}[\chi(T_x)] = \mathbb{E}[\mathcal{L}_0(T_x)] = \sum_{d=0}^{n} \mathcal{L}_d(T)\, \Xi_d(x)$$

$$\mathbb{E}[\mathcal{L}_k(T_x)] = \sum_{d=0}^{n-k} \begin{bmatrix} k+d \\ k \end{bmatrix} \mathcal{L}_{k+d}(T)\, \Xi_d(x), \quad k = 0, \ldots, n$$

where $\Xi_d(x)$ is the Euler characteristic density.

Proposition (Tomita, 1986, *PTP*, and many)

Suppose that $\mathrm{Var}(\nabla X(t)) = \gamma I$. When $X(t)$ is Gaussian,

$$\Xi_d(x) = (\gamma/2\pi)^{d/2} \phi(x) H_{d-1}(x)$$

where $\phi(x)$: pdf of $\mathcal{N}(0,1)$, $H_j(x)$: Hermite polynomial

Isotropic central limit random fields

- Our purpose is to obtain the Euler characteristic density $\Xi_d(x)$ when $X(t)$ is non-Gaussian. We assume the central limit random fields model (Chamandy, et al., 2008):

$$X(t) = X_N(t) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} Z_{(i)}(t), \quad t \in T \subset \mathbb{R}^n$$

$Z_{(i)}$: zero mean i.i.d. isotropic non-Gaussian random field

- The isotropic k-point correlation function:

$$\begin{aligned} \mathrm{cum}(Z(t_1), \ldots, Z(t_k)) =& \kappa^{(k)}\Big((\tfrac{1}{2}\|t_a - t_b\|^2)_{1\le a<b\le k} \Big) \\ \mathrm{cum}(X(t_1), \ldots, X(t_k)) =& N^{-(k-2)/2} \kappa^{(k)}\Big((\tfrac{1}{2}\|t_a - t_b\|^2)_{1\le a<b\le k} \Big) \\ =& O(\nu^{k-2}), \quad \nu = 1/\sqrt{N} \end{aligned}$$

Arguments are pairwise distances of t_i's.

Asymptotic expansion of the Euler density

Assumption

(i) *$t \mapsto X_N(t)$ is of C^2 a.s.*

(ii) *Recall that $t = (t^j)_{1\le j\le n}$. There exists*

$$\frac{\partial^8 \mathbb{E}\big[X_N(t_1)X_N(t_2)X_N(t_3)X_N(t_4)\big]}{\partial t_1^{i_1}\partial t_1^{j_1}\cdots\partial t_4^{i_4}\partial t_4^{j_4}} \quad \text{around } t_1 = t_2 = t_3 = t_4$$

(iii) *For t fixed, $(X_N(t), \nabla X_N(t), \nabla^2 X_N(t))$ has a density p_N. p_N is bounded for some N. It has a moment of order $\binom{n+2}{2}+1$.*

Theorem

Under the assumptions above, as $N \to \infty$ uniformly in x,

$$\Xi_{d,N}(x) = \left(\frac{\gamma}{2\pi}\right)^{d/2}\phi(x)\Big(H_{d-1}(x)+\frac{1}{\sqrt{N}}\Delta_{1,d}(x)+\frac{1}{N}\Delta_{2,d}(x)\Big)+o(N^{-2})$$

$\Delta_{1,n}$ and $\Delta_{2,n}$

$$\Delta_{1,n}(x) = \tfrac{1}{2\gamma^2}\kappa_{11}(n)_2 H_{n-2}(x) - \tfrac{1}{2\gamma}\kappa_1 n H_n(x) + \tfrac{1}{6}\kappa_0 H_{n+2}(x)$$

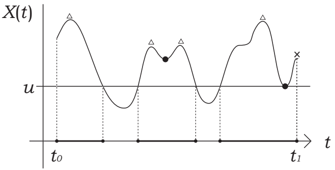
$$\begin{aligned}\Delta_{2,n}(x) = &\Big(-\tfrac{1}{6\gamma^3}(3\widetilde{\kappa}^a_{111} + \widetilde{\kappa}^d_{111}) + \tfrac{1}{8\gamma^4}(n-7)\kappa_{11}^2\Big)(n)_3 H_{n-3}(x)\\ &+ \Big(\tfrac{1}{8\gamma^2}(\widetilde{\kappa}^{aa}_{11}(n-2) + 4\widetilde{\kappa}^a_{11}(n-1)\\ &- \tfrac{1}{4\gamma^3}\kappa_1\kappa_{11}(n-1)(n-4)\Big) n H_{n-1}(x)\\ &+ \Big(-\tfrac{1}{4\gamma}\widetilde{\kappa}_1 + \tfrac{1}{24\gamma^2}(3\kappa_1^2(n-2) + 2\kappa_0\kappa_{11}(n-1))\Big) n H_{n+1}(x)\\ &+ \Big(\tfrac{1}{24}\widetilde{\kappa}_0 - \tfrac{1}{12\gamma}\kappa_0\kappa_1 n\Big) H_{n+3}(x) + \tfrac{1}{72}\kappa_0^2 H_{n+5}(x)\end{aligned}$$

where $\kappa_0 = \kappa^{(3)}(0,0,0)$, $\kappa_1 = \frac{\mathrm{d}\kappa^{(3)}(x,0,0)}{\mathrm{d}x}|_{x=0}$, $\kappa_{11} = \frac{\mathrm{d}^2\kappa^{(3)}(x,y,0)}{\mathrm{d}x\mathrm{d}y}|_{x=y=0}$, $\widetilde{\kappa}_0 = \kappa^{(4)}(0,0,0,0,0,0)$, $\widetilde{\kappa}_1 = \frac{\mathrm{d}\kappa^{(4)}(x_1,0,0,0,0,0)}{\mathrm{d}x_1}|_{x_1=0}$, etc.

Sketch of the proof

- Morse's theorem:

$$\chi(T_v) = \sum_{t:\text{critical}} \mathbb{1}(X(t) \geq v) \times \operatorname{sgn}\det(-\nabla^2 X(t))$$



- Kac-Rice formula for the EC density:

$$\Xi_n(v) = \mathbb{E}[\mathbb{1}(X(t) \geq v)\det(-\nabla^2 X(t))\delta(\nabla X(t))]$$

$\Xi_n(v)$ is independent of t (because X is isotropic).

- Obtain the Edgeworth expansion of the pdf (or mgf) of

$$(X(t), \nabla X(t), \nabla^2 X(t)) \in \mathbb{R}^{1+n+n(n+1)/2}$$

and evaluate $\Xi_n(v)$ formally.

- Validity is proved separately.

Key identities on the Hermite polynomial

- $A \sim \mathrm{GOE}(n)$, that is, $A = (a_{ij}) \in \mathrm{Sym}(n)$, $a_{ii} \sim \mathcal{N}(0,2)$, $a_{ij} \sim \mathcal{N}(0,1)$ $(i < j)$. Then, $\mathbb{E}[e^{\mathrm{tr}(\Theta A)}] = e^{\mathrm{tr}(\Theta^2)}$
- For $B = (b_{ij}) \in \mathrm{Sym}(n)$, define a matrix differential operator

$$(D_B)_{ij} = (1/2)(1 + \delta_{ij})(\partial/\partial b_{ij}) \quad (i \le j)$$

Lemma

Let $A \sim \mathrm{GOE}(n)$. *Let* $m = \sum_{i=1}^{\ell} c_i$. *Then,*

$$\begin{aligned}(-1/2)^{m-\ell}(n)_m H_{n-m}(x) &= \mathbb{E}\big[\mathrm{tr}(D_A^{c_1}) \cdots \mathrm{tr}(D_A^{c_\ell}) \det(xI_n + A)\big] \\ &= \det(xI + D_\Theta)\big(e^{\mathrm{tr}(\Theta^2)} \mathrm{tr}(\Theta^{c_1}) \cdots \mathrm{tr}(\Theta^{c_\ell})\big)\Big|_{\Theta=0}\end{aligned}$$

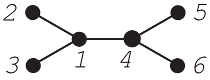
In particular, when $\ell = m = 0$,

$$H_n(x) = \mathbb{E}[\det(xI_n + A)] = \det(xI_n + D_\Theta) e^{\mathrm{tr}(\Theta^2)}\Big|_{\Theta=0}$$

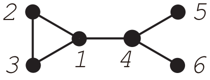
(Non)Detectable non-Gaussianity

- Diagram of the derivatives:

$$\frac{\partial}{\partial x_{12}}\frac{\partial}{\partial x_{13}}\frac{\partial}{\partial x_{14}}\frac{\partial}{\partial x_{45}}\frac{\partial}{\partial x_{46}}\kappa^{(6)}(x_{12},\dots,x_{56})\Big|_{x=0}$$



$$\frac{\partial}{\partial x_{12}}\frac{\partial}{\partial x_{13}}\frac{\partial}{\partial x_{14}}\frac{\partial}{\partial x_{23}}\frac{\partial}{\partial x_{45}}\frac{\partial}{\partial x_{46}}\kappa^{(6)}(x_{12},\dots,x_{56})\Big|_{x=0}$$



Theorem

The derivatives with loops do not appear in the asymptotic expansion formula.

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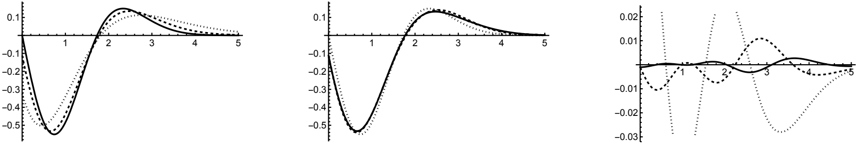
Chi-square random field

$$Y(t) = Y_N(t) = \frac{1}{\sqrt{2N}} \sum_{i=1}^{N} \big(Z_{(i)}(t)^2 - 1\big), \quad t \in T \subset \mathbb{R}^4,$$

$Z_{(i)}(t)$: zero mean Gaussian s.t. $\mathbb{E}[Z_{(i)}(s)Z_{(i)}(t)] = e^{-\frac{1}{4}\|s-t\|^2}$



Left: EC density ($\cdots$ $N = 10$, $--N = 100$, —$N = \infty$)

Middle: EC density, $N = 100$ (–·– true, $\cdots$ 0th approx, – –1st approx, —2nd approx)

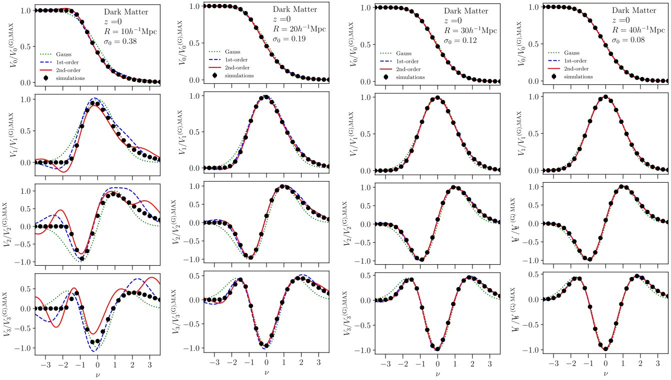
Right: difference from the true, $N = 100$ ($\cdots$0th approx, – –1st approx, —2nd approx)

Comparison with simulator (Matsubara, Hikage & K, 2022)

Cosmic model, parameters $\longrightarrow$ Simulation data

$\downarrow$ $\downarrow$

Skewness, Kurtosis $\longrightarrow$ Minkowski Functional (MF)



Simulator (dot) and expansion formulas (solid line) for $\mathcal{M}_j$, $j = 0, 1, 2, 3$

Radius of smoothing kernel $R = 10, 20, 30, 40h^{-1}$Mpc

Summary

- We introduced “isotropic random field”, its “excursion set”, and its “Minkowski functional (MF)” or “Lipschitz-Killing curvature” including “Euler characteristic (EC)”.
- We provided an asymptotic expansion formula of the EC density $\Xi_n(v)$ under the existence of skewness and kurtosis.
- The accuracy of the formula is confirmed by a chi-square field example.
- The proposed asymptotic expansion formula is useful in cosmic research.

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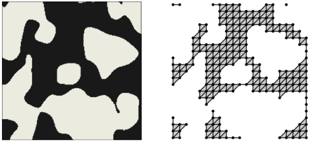
How to calculate the EC of 2D image

0. The excursion set image is represented as 0/1 at each pixel.



1. We convert the image into a triangle complex by connecting adjacent vertices and by filling triangles. Then,

$$\chi = \#\text{vertices} - \#\text{edges} + \#\text{triangles}$$

2. By increasing the threshold, one new vertex is generated. Incidentally, new edges and triangles are produced.

$$\Delta\chi = 1 - \#\text{new edges} + \#\text{new triangles}$$

Proof (1/5). Notations

- The covariance function and kth cumulant

$$\mathrm{Cov}(X(t_1), X(t_2)) = \rho(\tfrac{1}{2}\|t_1 - t_2\|^2)$$
$$\mathrm{cum}(X(t_1), \ldots, X(t_k)) = N^{-(k-2)/2}\kappa^{(k)}\Big((\tfrac{1}{2}\|t_a - t_b\|^2)_{1\le a<b\le k}\Big)$$

- Kac-Rice formula for the EC density:

$$\Xi_n(v) = \mathbb{E}[\mathbb{1}(X(t) \ge v)\det(-\nabla^2 X(t))\delta(\nabla X(t))]$$

- To obtain the Edgeworth-type expansion of

$$(X(t), \nabla X(t), \nabla^2 X(t)) \quad (t \text{ fixed})$$

we evaluate the cumulants of

$$X = X(t), \quad X_i = \partial X(t)/\partial t^i, \quad X_{ij} = \partial^2 X(t)/\partial t^i \partial t^j$$

Proof (2/5). Joint cumulants of X and its derivatives

- For example,

$$\mathbb{E}[X_i X_j] = \frac{\partial}{\partial s_i}\frac{\partial}{\partial t_j}\rho\big(\tfrac{1}{2}\|s-t\|^2\big)|_{s=t} = -\rho'(0)\delta_{ij}$$

- 2nd and 3rd cumulants:

$$\begin{aligned}
&\mathbb{E}[XX] = 1 \qquad \mathbb{E}[X_i X_j] = -\rho'(0)\delta_{ij} \qquad \mathbb{E}[X X_{ij}] = \rho'(0)\delta_{ij} \\
&\mathbb{E}[X_{ij}X_{kl}] = \rho''(0)(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
&\mathbb{E}[XXX] = \kappa_0 \qquad \mathbb{E}[X X_i X_j] = -\kappa_1\delta_{ij} \qquad \mathbb{E}[XXX_{ij}] = 2\kappa_1\delta_{ij} \\
&\mathbb{E}[X X_{ij} X_{kl}] = (3\kappa_{11} + \kappa_2)\delta_{ij}\delta_{kl} + \kappa_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
&\mathbb{E}[X_i X_j X_{kl}] = -2\kappa_{11}\delta_{ij}\delta_{kl} + \kappa_{11}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
&\mathbb{E}[X_{ij}X_{kl}X_{mn}] = (2\kappa_{111} + 6\kappa_{21})\delta_{ij}\delta_{kl}\delta_{mn} + 2\kappa_{21}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\delta_{mn}[3] \\
&\qquad\qquad + (-\kappa_{111})\delta_{il}\delta_{jn}\delta_{km}[8]
\end{aligned}$$

where $\kappa_{21} = \frac{\partial^3\kappa^{(3)}(x_{12},x_{13},x_{23})}{\partial x_{12}^2\partial x_{13}}|_{x_{ab}\equiv 0}$, etc.

Proof (3/5). Joint moment generating function (mgf)

- Define $R = \nabla^2 X - \rho'(0) X I_n$. Then $(X, \nabla X, R)$ are uncorrelated. The joint mgf is

$$\psi(s,T,\Theta) = \mathbb{E}\Big[e^{sX + \langle T, \nabla X\rangle + \mathrm{tr}(\Theta R)}\Big]$$

$$= \overbrace{e^{\frac{1}{2}s^2}}^{\psi_X^0(s)} \times \overbrace{e^{\frac{-\rho'(0)}{2}\|T\|^2}}^{\psi_{\nabla X}^0(T)} \times \overbrace{e^{\frac{2\rho''(0)}{2}\mathrm{tr}(\Theta^2) + \frac{\rho''(0)-\rho'(0)^2}{2}\mathrm{tr}(\Theta)^2}}^{\psi_R^0(\Theta)}$$

$$\times \Big\{1 + \underbrace{Q(t,T,\Theta)}_{\mathrm{non-Gaussianity}}\Big\} \qquad \Big(\rho''(0) > \tfrac{n}{n+2}\rho'(0)^2 > 0\Big)$$

where $Q(t,T,\Theta)$ is a polynomial in

$$s^k,\ \|T\|^{2k},\ \mathrm{tr}(\Theta^k),\ \ T^\top \Theta^k T$$

(because of the invariance under $(TT^\top, \Theta) \mapsto P^\top (TT^\top, \Theta) P$, $P \in O(n)$ and the "invariance polynomial" theory by Davis)

Proof (4/5). Derivative of mgf

- Define the mgf of R under $X = x$, $\nabla X = 0$:

$$\psi_{X=x,\nabla X=0}(\Theta) = \frac{1}{(2\pi)^{n+1}} \int_{\mathbb{R}^{n+1}} e^{-\sqrt{-1}sx} \psi(\sqrt{-1}s, \sqrt{-1}T, \Theta) \mathrm{d}T \mathrm{d}s$$

- The Kac-Rice formula is rewritten as

$$\begin{aligned}
\Xi_n(v) &= \mathbb{E}[\mathbb{1}(X(t) \geq v) \det(-\nabla^2 X(t)) \delta(\nabla X(t))] \\
&= \mathbb{E}[\mathbb{1}(X(t) \geq v) \det(-R - \rho'(0) X(t) I_n) \delta(\nabla X(t))] \\
&= \int_x^\infty \left[\det(-D_\Theta - \rho'(0) x I_n) \Big|_{\Theta=0} \psi_{X=x,\nabla X=0}(\Theta) \right] \mathrm{d}x
\end{aligned}$$

where D_Θ is an $n \times n$ symmetric matrix differential operator

$$(D_\Theta)_{ij} = \frac{1 + \delta_{ij}}{2} \frac{\partial}{\partial(\Theta)_{ij}} \quad (i \leq j)$$

Proof (5/5) Key identity

- Recall that

$$\psi_R^0(\Theta) = e^{\frac{2\rho''(0)}{2}\mathrm{tr}(\Theta^2) + \frac{\rho''(0)-\rho'(0)^2}{2}\mathrm{tr}(\Theta)^2}$$

Lemma

Let $\gamma = -\rho'(0)$.

$$\begin{aligned}\det(-D_\Theta + \gamma x I_n)\big(\psi_R^0(\Theta)\mathrm{tr}(\Theta^{c_1})\cdots\mathrm{tr}(\Theta^{c_k})\big)\Big|_{\Theta=0} \\ = (-1)^m\gamma^{n-m}(-1/2)^{m-k}(n)_m H_{n-m}(x),\end{aligned}$$

where $m = \sum_{i=1}^k c_i$.

- Note that $\rho''(0)$ disappears.
- The diagram of $\rho''(0) = -\frac{\partial}{\partial s_i}\frac{\partial}{\partial t_i}\rho\big(\frac{1}{2}\|s-t\|^2\big)|_{s=t}$ is