Peak Height Distributions of Gaussian Random Fields and Their Statistical Applications

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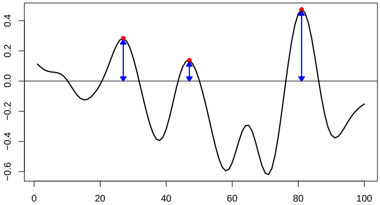
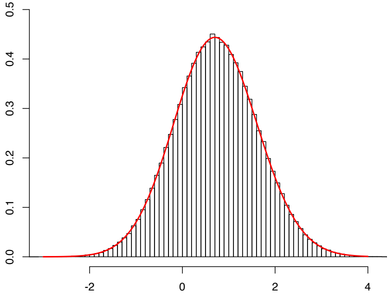
Smooth Gaussian Random Fields

- We call $\{X(t), t \in T\}$ a real-valued Gaussian random field (process), if any finite-dimensional collection $(X(t_1), \ldots, X(t_n))$ is a multivariate Gaussian random variable.
- Signal-plus-noise (spatiotemporal) model: $y(t) = \mu(t) + z(t)$.
- The noise $z(t)$ can be modeled by Gaussian random fields.

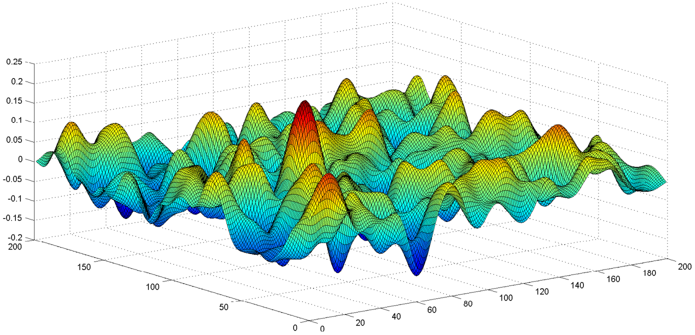
Peak Height Distribution of Smooth Gaussian Processes (1D)

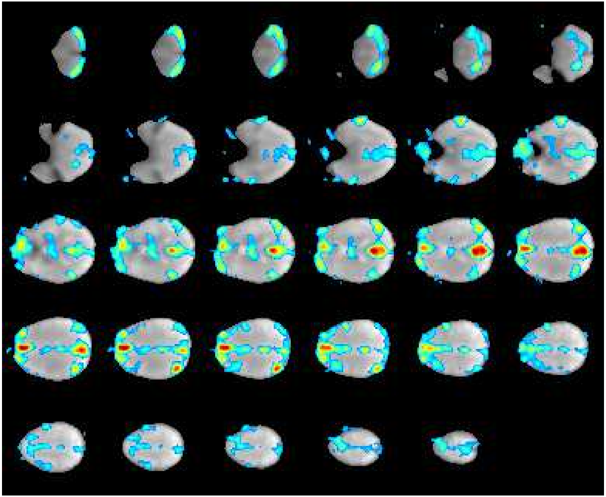




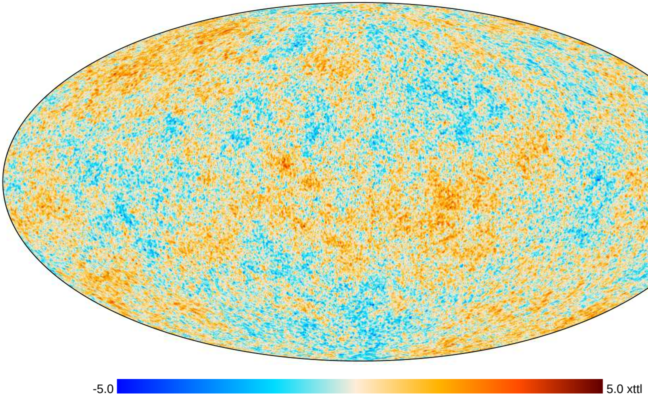
- A simulated smooth stationary Gaussian process (black curve)
- Peak height (blue lines)
- Simulated peak height density (relative frequency histogram)
- Theoretical peak height density (red curve)

Example of a smooth Gaussian random field on $\mathbb{R}^2$ (2D)





Brain Image



Cosmic Microwave Background (CMB) Data

Peak Height Distribution of Gaussian Fields

- Let $\{X(t), t \in T\}$ be a smooth Gaussian field.
- P-value computation in statistics: peak (signal) detection.
- The peak height distribution is defined as

$$\mathbb{P}\{X(t) > u \,|\, t \text{ is a local maximum of } X\},$$

  where $t \in T \subset \mathbb{R}^N$ is some fixed point.
- This is a conditional probability and the conditional event has zero probability.

Generally, for a smooth Gaussian random field $X(t)$, we have [C. and Schwartzman (2015)]

$$\begin{aligned}
F_t(u) &= \mathbb{P}(X(t) > u \mid t \text{ is a local maximum }) \\
&= \lim_{\varepsilon \to 0} \mathbb{P}(X(t) > u \mid \exists \text{ local maximum within } \varepsilon\text{-ball of } t) \\
&= \lim_{\varepsilon \to 0} \frac{\mathbb{P}\{X(t) > u, \exists \text{ local maximum within } \varepsilon\text{-ball of } t\}}{\mathbb{P}\{\exists \text{ local maximum within } \varepsilon\text{-ball of } t\}} \\
&= \lim_{\varepsilon \to 0} \frac{\mathbb{E}\{\# \text{ local maxima within } \varepsilon\text{-ball of } t \text{ s.t. } X(t) > u\}}{\mathbb{E}\{\# \text{ local maxima within } \varepsilon\text{-ball of } t\}} \\
&\overset{\text{Kac-Rice}}{=} \frac{\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{X(t) > u\}} \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}} | \nabla X(t) = 0\}}{\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}} | \nabla X(t) = 0\}},
\end{aligned}$$

where $\nabla X(t)$ and $\nabla^2 X(t)$ are respectively the gradient and Hessian, and $\nabla^2 X(t) \prec 0$ means that the Hessian is negative definite.

1D (nonstationary) Gaussian processes with unit variance

- In the 1D case, the peak height distribution becomes

$$F_t(u) = \frac{\mathbb{E}\left[X''(t)\mathbb{1}_{\{X(t)>u\}}\mathbb{1}_{\{X''(t)<0\}}|X'(t)=0\right]}{\mathbb{E}\left[X''(t)\mathbb{1}_{\{X''(t)<0\}}|X'(t)=0\right]}.$$

- We have that [C. (2023)]

$$F_t(u) = \Psi\left(\frac{u}{\sqrt{1-r^2(t)}}\right) - \sqrt{2\pi}r(t)\phi(u)\Phi\left(\frac{-r(t)u}{\sqrt{1-r^2(t)}}\right).$$

Here $\phi(\cdot)$, $\Phi(\cdot)$ and $\Psi(\cdot)$ are respectively pdf, cdf and tail prob. of $N(0,1)$, and

$$r(t) = \mathrm{Corr}[X(t), X''(t)|X'(t)=0] = \frac{-\lambda_1(t)}{\sqrt{\lambda_2(t) - \frac{\lambda_1'(t)^2}{4\lambda_1(t)}}},$$

where $\lambda_1(t) = \mathrm{Var}(X'(t))$ and $\lambda_2(t) = \mathrm{Var}(X''(t))$.

Isotropic Gaussian Random Fields on $\mathbb{R}^N$

- Assume additionally the field is isotropic (stationary), then $\nabla X(t)$ is independent of $X(t)$ and $\nabla^2 X(t)$ for each t, and hence

$$F(u) = \frac{\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{X(t)>u\}} \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\}}{\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\}}.$$

  Note that $F_t(u)$ does not depend on t under isotropy.
- Note that $|\det \nabla^2 X(t)| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}} = \prod_{j=1}^N |\lambda_j| \mathbb{1}_{\{\lambda_N < 0\}}$, the problem can now be transformed to the distributions of the ordered eigenvalues of Gaussian random matrices

$$\nabla^2 X(t) \quad \text{and} \quad (\nabla^2 X(t) | X(t) = x).$$

- We will study the properties of such Gaussian random matrices.

Isotropic Gaussian Random Fields on $\mathbb{R}^N$

Assuming the Gaussian field is isotropic with unit variance, we can write the covariance as $C(t,s) = \rho(\|t-s\|^2)$ for an appropriate function $\rho(\cdot) : [0,\infty) \to \mathbb{R}$. Denote

$$\rho' = \rho'(0), \quad \rho'' = \rho''(0), \quad \kappa = -\rho'/\sqrt{\rho''}.$$

Let $X_i(t) = \frac{\partial}{\partial t_i} X(t)$ and $X_{ij}(t) = \frac{\partial^2}{\partial t_i t_j} X(t)$. Then for each $t \in T \subset \mathbb{R}^N$ and $i, j, k, l \in \{1, \ldots, N\}$,

$$\begin{aligned}
\mathbb{E}\{X_i(t)X(t)\} &= \mathbb{E}\{X_i(t)X_{jk}(t)\} = 0, \\
\mathbb{E}\{X_i(t)X_j(t)\} &= -\mathbb{E}\{X_{ij}(t)X(t)\} = -2\rho'\delta_{ij}, \\
\mathbb{E}\{X_{ij}(t)X_{kl}(t)\} &= 4\rho''(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),
\end{aligned}$$

where δ_{ij} is the Kronecker delta.

Gaussian Orthogonally Invariance (GOI) Matrices

- We call an $N \times N$ random matrix $M = (M_{ij})_{1 \leq i,j \leq N}$ Gaussian Orthogonally Invariant (GOI) with *covariance parameter* c, denoted by $\mathrm{GOI}(c)$, if it is symmetric and all entries are centered Gaussian variables such that

$$\mathbb{E}[M_{ij}M_{kl}] = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + c\delta_{ij}\delta_{kl}.$$

- This is the class of matrices M whose distribution is invariant under all transformations of the form QMQ^T with orthogonal Q.
- An $N \times N$ Gaussian Orthogonal Ensemble (GOE) matrix $H = (H_{ij})_{1 \leq i,j \leq N}$ such that

$$\mathbb{E}[H_{ij}H_{kl}] = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),$$

is a special case of $\mathrm{GOI}(c)$ when $c = 0$.

Density of Eigenvalues of GOI Matrices (C. and Schwartzman (2020))

- The density of the ordered eigenvalues $\lambda_1 \leq \ldots \leq \lambda_N$ of $M \in \mathrm{GOI}(c)$ is given by

$$f_c(\lambda_1, \ldots, \lambda_N) = \frac{1}{K_N\sqrt{1+Nc}} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j| \mathbb{1}_{\{\lambda_1 \leq \ldots \leq \lambda_N\}} \times \exp\left\{ -\frac{1}{2}\sum_{i=1}^N \lambda_i^2 + \frac{c}{2(1+Nc)} \left(\sum_{i=1}^N \lambda_i\right)^2 \right\},$$

  where $K_N = 2^{N/2} \prod_{i=1}^N \Gamma\left(\frac{i}{2}\right)$.
- We denote by $\mathbb{E}^N_{\mathrm{GOI}(c)}$ the expectation taken under such density.

Connections between the Hessian and GOI Matrices

- Recall that a GOI(c) matrix M satisfies

$$\mathbb{E}[M_{ij}M_{kl}] = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + c\delta_{ij}\delta_{kl};$$

and for an isotropic Gaussian field X,

$$\begin{aligned}\mathbb{E}\{X_{ij}(t)X_{kl}(t)\} &= 4\rho''(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ &= 8\rho''\left[\frac{1}{2}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl}) + \frac{1}{2}\delta_{il}\delta_{jk}\right]\end{aligned}$$

- We have the following relations:

$$\nabla^2 X(t) \overset{d}{=} \sqrt{8\rho''}\mathrm{GOI}(1/2),$$

$$(\nabla^2 X(t)|X(t) = x) \overset{d}{=} \sqrt{8\rho''}\left[\mathrm{GOI}((1-\kappa^2)/2) - (\kappa x/\sqrt{2})I_N\right].$$

Since

$$\nabla^2 X(t) \overset{d}{=} \sqrt{8\rho''}\text{GOI}(1/2),$$
$$(\nabla^2 X(t)|X(t) = x) \overset{d}{=} \sqrt{8\rho''}\left[\text{GOI}((1-\kappa^2)/2) - \left(\kappa x/\sqrt{2}\right) I_N\right],$$

we obtain

$$\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\} = (8\rho'')^{N/2} \mathbb{E}^N_{\text{GOI}(1/2)} \left[\prod_{j=1}^N |\lambda_j| \mathbb{1}_{\{\lambda_N < 0\}} \right];$$

and

$$\begin{aligned} &\mathbb{E}\{|\det \nabla^2 X(t)| \mathbb{1}_{\{X(t)>u\}} \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\} \\ &= \int_u^\infty \phi(x) \mathbb{E}\left[|\det(\nabla^2 X(t))| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}} \middle| X(t) = x \right] dx \\ &= (8\rho'')^{N/2} \int_u^\infty \phi(x) \mathbb{E}^N_{\text{GOI}((1-\kappa^2)/2)} \left[\prod_{j=1}^N |\lambda_j - \kappa x/\sqrt{2}| \mathbb{1}_{\{\lambda_N < \kappa x/\sqrt{2}\}} \right] dx. \end{aligned}$$

Therefore [C. and Schwartzman (2020)],

$$F(u) = \frac{\mathbb{E}\{|\det\nabla^2 X(t)| \mathbb{1}_{\{X(t)>u\}} \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\}}{\mathbb{E}\{|\det\nabla^2 X(t)| \mathbb{1}_{\{\nabla^2 X(t) \prec 0\}}\}}$$

$$= \frac{\int_u^\infty \phi(x) \mathbb{E}^N_{\mathrm{GOI}((1-\kappa^2)/2)} \left[\prod_{j=1}^N |\lambda_j - \kappa x/\sqrt{2}| \mathbb{1}_{\{\lambda_N < \kappa x/\sqrt{2}\}}\right] dx}{\mathbb{E}^N_{\mathrm{GOI}(1/2)} \left[\prod_{j=1}^N |\lambda_j| \mathbb{1}_{\{\lambda_N < 0\}}\right]}.$$

- $F(u)$ only depends on κ.
- Denote by h the density of such distribution, i.e., $h(x) = -F'(x)$.
- Peak height densitie of isotropic Gaussian fields on $\mathbb{R}^2$:

$$h(x) = \sqrt{3}\kappa^2(x^2 - 1)\phi(x)\Phi\left(\frac{\kappa x}{\sqrt{2-\kappa^2}}\right) + \frac{\kappa x\sqrt{3(2-\kappa^2)}}{2\pi} e^{-\frac{x^2}{2-\kappa^2}}$$
$$+ \frac{\sqrt{6}}{\sqrt{\pi(3-\kappa^2)}} e^{-\frac{3x^2}{2(3-\kappa^2)}} \Phi\left(\frac{\kappa x}{\sqrt{(3-\kappa^2)(2-\kappa^2)}}\right).$$

Other Critical Points

- For $i = 0, \ldots, N$, the critical points of index i of X exceeding level u over a (unit-area) domain D is defined by

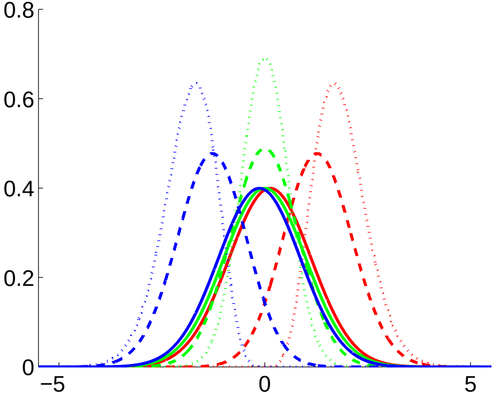
$$\left\{ t \in D : X(t) \geq u, \nabla X(t) = 0, \text{index}(\nabla^2 X(t)) = i \right\},$$

where the index of Hessian matrix is the number of negative eigenvalues.

- We can use similar techniques to obtain their height distributions:

$$F_i(u) = \frac{\mathbb{E}\left\{ |\det \nabla^2 X(t)| \mathbb{1}_{\{X(t)>u\}} \mathbb{1}_{\{\text{index}(\nabla^2 X(t))=i\}} \right\}}{\mathbb{E}\left\{ |\det \nabla^2 X(t)| \mathbb{1}_{\{\text{index}(\nabla^2 X(t))=i\}} \right\}}.$$

Densities of height distributions of critical points of isotropic Gaussian fields in $\mathbb{R}^2$



Red: height density of local maximum.

Green: height density of saddle point,

Blue: height density of local minimum,

The solid, dashed and dotted lines represent different values of κ.

Isotropic Gaussian Fields on Spheres

- Let $X = \{X(t) : t \in \mathbb{S}^N\}$ be a smooth isotropic Gaussian random field, where $\mathbb{S}^N$ is the N-dimensional unit sphere.
- Due to isotropy, we may write the covariance function of X as $C(\langle t, s\rangle)$, $t, s \in \mathbb{S}^N$, where $C(\cdot) : [-1, 1] \to \mathbb{R}$ and $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^{N+1}$.
- Define

$$C' = C'(1), \quad C'' = C''(1), \quad \kappa_1 = C'/C'', \quad \kappa_2 = C'^2/C''.$$

- Similarly to the Euclidean case, we have

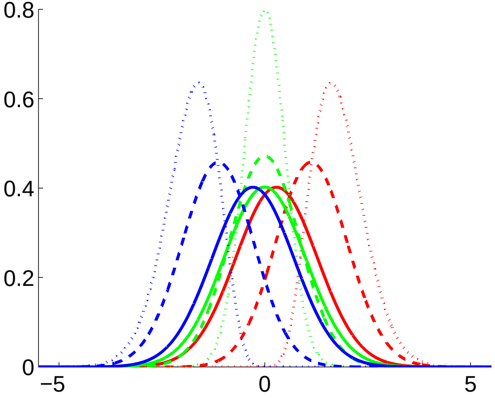
$$\begin{aligned} \mathbb{E}\{X_i(t)X(t)\} &= \mathbb{E}\{X_i(t)X_{jk}(t)\} = 0, \\ \mathbb{E}\{X_i(t)X_j(t)\} &= -\mathbb{E}\{X_{ij}(t)X(t)\} = C'\delta_{ij}, \\ \mathbb{E}\{X_{ij}(t)X_{kl}(t)\} &= C''(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + (C'' + C')\delta_{ij}\delta_{kl}. \end{aligned}$$

- We have the following relations:

$$\nabla^2 X(t) \overset{d}{=} \sqrt{2C''}\mathrm{GOI}((1+\kappa_1)/2),$$
$$(\nabla^2 X(t)|X(t)=x) \overset{d}{=} \sqrt{2C''}\left[\mathrm{GOI}((1+\kappa_1-\kappa_2)/2) - \left(\sqrt{\kappa_2/2}x\right)I_N\right].$$

- The height distribution of critical points can be solved similarly.

Densities of height distributions of critical points of isotropic Gaussian fields in $\mathbb{S}^2$



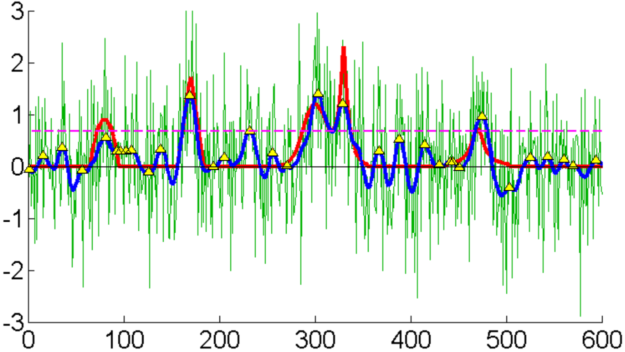
Red: height density of local maximum.

Green: height density of saddle point,

Blue: height density of local minimum,

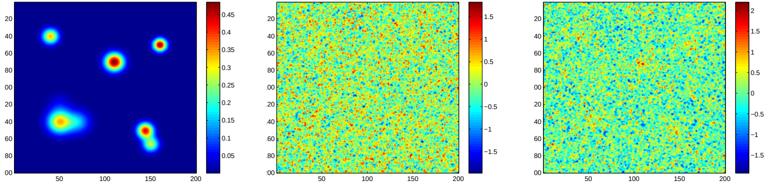
The solid, dashed and dotted lines represent different C' and C''.

Multiple Testing for Peak Detection in 1D [Schwartzman et al. (2011)]

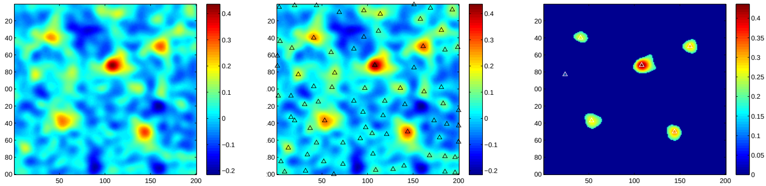


- Signal $\mu(t)$: red line
- Observed signal-plus-noise data $y(t) = \mu(t) + z(t)$: green line
- Smoothed signal-plus-noise model $y_\gamma(t) = \mu_\gamma(t) + z_\gamma(t)$: blue line
- Compute the p-value at each observed local maximum (yellow triangle) of $y_\gamma(t)$ to find significant peaks (above the peak line).

Multiple Testing for Peak Detection in Random Fields [C. and Schwartzman (2017)]



$\mu(t)$ (signal) $z(t)$ (noise) $y(t) = \mu(t) + z(t)$



$y_\gamma(t)$ candidate peaks significant peaks

BH procedure: level $\alpha = 0.2$, $\tilde{m} = 77$ tests.

The STEM Algorithm (Smooth and TEst Maxima)

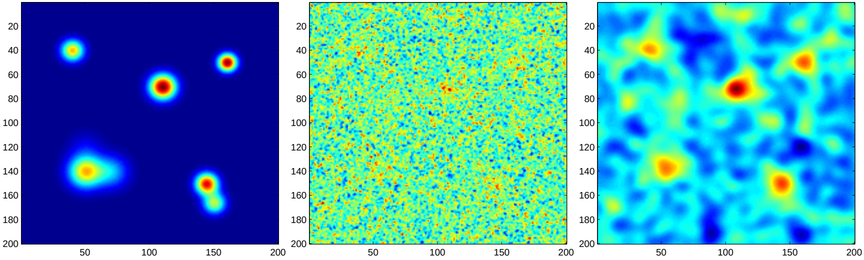
1. Smooth with a unimodal kernel: to increase the signal-to-noise ratio (SNR)
2. Find all the local maxima: candidate peaks
3. Compute the p-value of each local maximum
4. Apply a multiple testing procedure to detect those local maxima whose p-values are significant

1. Kernel Smoothing

- Unimodal kernel (best if same as signal)

$$y_\gamma(t) = w_\gamma(t) * y(t) = \int_{\mathbb{R}^N} w_\gamma(t-s)y(s)\,ds$$

$$w_\gamma(t) = w(t/\gamma)/\gamma$$

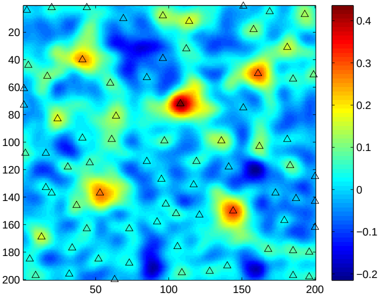


$\mu(t)$ (signal) $\quad y(t) = \mu(t) + z(t) \quad y_\gamma(t) == \mu_\gamma(t) + z_\gamma(t)$

2. Find Local Maxima

- Local maxima are candidate peaks

$$\tilde{T} = \left\{ t \in [0, L]^N : \nabla y_\gamma(t) = 0,\ \nabla^2 y_\gamma(t) \prec 0 \right\}.$$



Dimension reduction: $L^2 = 40000 \rightarrow \tilde{m} = 77$ (Random!)

3. Compute p-values

- Test at each local maximum $t \in \tilde{T}$ the hypotheses

$$H_0(t): \ \{\exists \delta_0 > 0 \text{ such that } \mu(s) = 0 \text{ for all } s \in B(t, \delta_0)\} \quad \text{vs.}$$
$$H_A(t): \ \{\forall \delta_0 > 0, \mu(s) > 0 \text{ for some } s \in B(t, \delta_0)\},$$

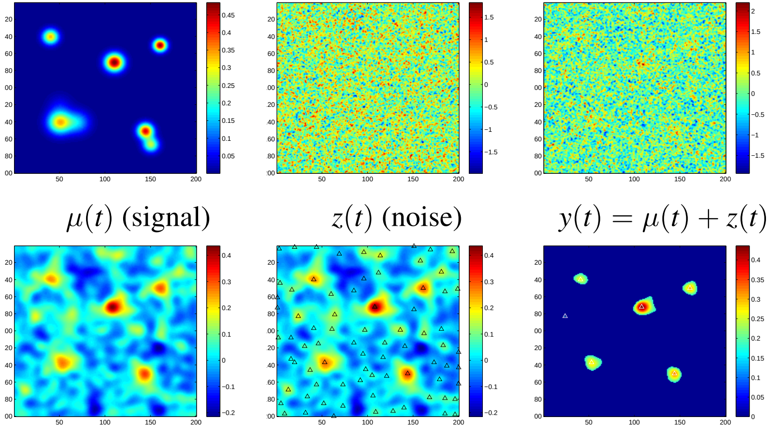
  where $B(t, \delta_0)$ is a ball of small radius δ_0 centered at t.
- Define the distribution of the height of a local maximum under the null hypothesis as

$$F_\gamma(u) = \mathbb{P}(z_\gamma(t) > u \mid t \text{ is a local maximum}).$$

- For each observed local maximum, its p-value is computed as

$$p_\gamma(t) = F_\gamma(y_\gamma(t)), \quad t \in \tilde{T}.$$

4. Multiple Testing



$\mu(t)$ (signal) $\quad$ $z(t)$ (noise) $\quad$ $y(t) = \mu(t) + z(t)$

$y_\gamma(t)$ $\quad$ candidate peaks $\quad$ significant peaks

BH procedure: level $\alpha = 0.2$, $\tilde{m} = 77$ tests.

Peak Detection for Gaussian Fields on the Sphere $\mathbb{S}^2$ [C. et al. (2020)]

- Signal-plus-noise model: $y_n(x) = \mu_n(x) + z(x), x \in \mathbb{S}^2$.
- The sigal $\mu_n(x)$ is a linear combination of "Gaussian shaped distributions" $h(x; \gamma_n, \xi_k)$ on $\mathbb{S}^2$ with center ξ_k and variance γ_n ($a_k > 0$ is signal strength)

$$\mu_n(x) = \sum_{k=1}^{n} a_k h(x; \gamma_n, \xi_k), \quad x \in \mathbb{S}^2.$$

- $z(x)$ is an isotropic Gaussian on $\mathbb{S}^2$ with a spectral representation:

$$z(x) = \sum_{\ell=0}^{\infty} z_\ell(x), \qquad z_\ell(x) = \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(x),$$

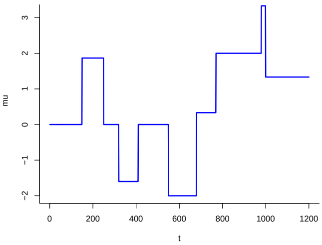
  where $\{Y_{\ell m}(\cdot)\}$ denotes the family of spherical harmonics and $\{a_{\ell m}\}$ denotes the random spherical harmonic coefficients.
- We apply filtering on $\mathbb{S}^2$ and the STEM algorithm to detect peaks.

Applications to Change Point Detection [Cheng et al. (2020, 2023)]

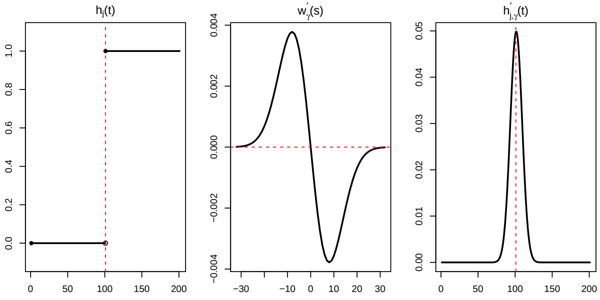
- Signal: piecewise constant of the form

$$\mu(t) = \sum_{j=0}^{\infty} a_j h_j(t), \qquad a_j \in \mathbb{R} \setminus \{0\},$$

  with $h_j(t) = \mathbb{1}(t \geq v_j)$ for $v_j \in \mathbb{R}$. Here, $a_j = c_j - c_{j-1}$ is the jump size or signal strength.
- v_j is called a change point.
- We want to detect the number and locations of v_j under noise background (observed signal-plus-noise data $y(t) = \mu(t) + z(t)$).
- Example:



- Key Observation: The derivatives of $\mu(t)$ are infinite at jumps v_j and 0 elsewhere. So, if we perform kernel smoothing for $\mu(t)$, the derivatives at jumps v_j would become local maxima or local minima.



- We also expect that such property can hold "asymptotically" even after adding the noise. This transforms the problem of detecting change points to detecting local extrema (maxima or minima).

Derivatives of Smoothed Signal

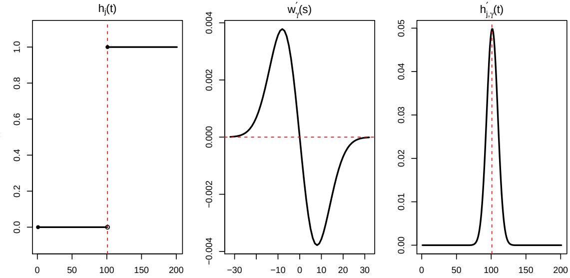
- Derivatives: $\mu'_\gamma(t) = w'_\gamma(t) * \mu(t) = \sum_{j=0}^{\infty} a_j h'_{j,\gamma}(t)$. A key observation is that

$$h'_{j,\gamma}(t) = \int_{\mathbb{R}} w'_\gamma(t-s) h_j(s)\, ds = \int_{\mathbb{R}} w'_\gamma(s) h_j(t-s)\, ds$$

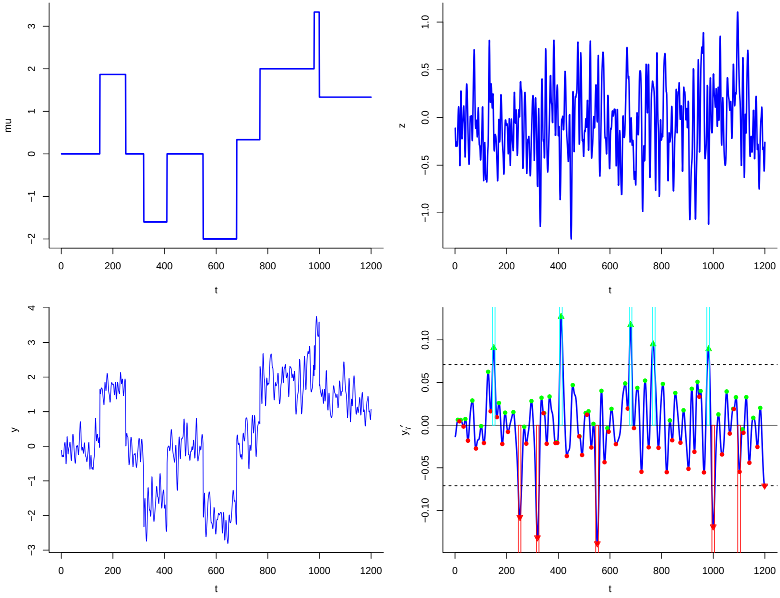
$$= \int_{\mathbb{R}} w'_\gamma(s) \mathbb{1}(t-s \geq v_j)\, ds = \int_{-\infty}^{t-v_j} w'_\gamma(s)\, ds = w_\gamma(t-v_j),$$

which is the original kernel $w_\gamma(t)$ shifted by v_j.

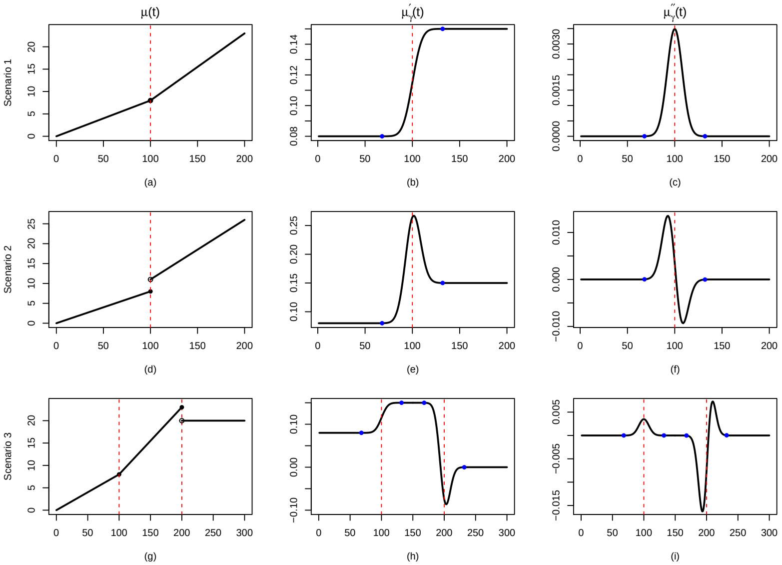
- The local maxima of $h'_{j,\gamma}(t)$ is at the jump (change point) v_j.



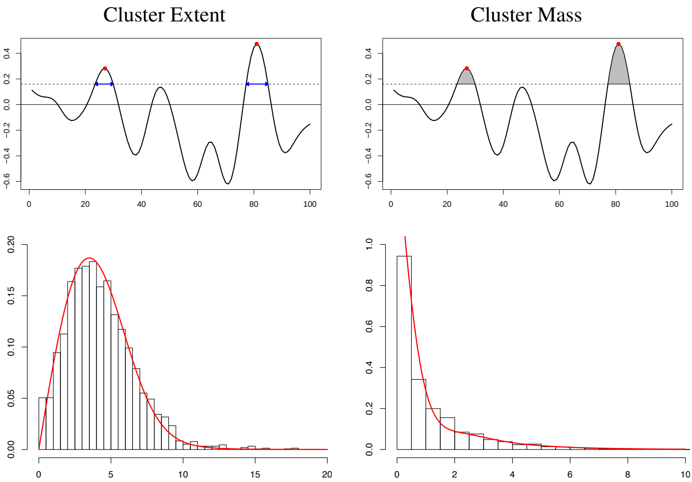
Toy Example



Extension to Detecting Structural Breaks (He et al. (2023))



Ongoing work: distribution of cluster extent and mass



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Thank you!