

Gaussian random fields

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Outline

- 1 Definition and main properties
 - reminder on the LLN and the CLT
 - Definition
 - Geometry of realizations
- 2 Unconditional simulation
 - The spectral method
 - The turning band method
- 3 Conditional simulation
- 4 Statistical fluctuations

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Results from probability

Let $(Y_n, n \in \mathbb{N})$ be a sequence of independent and identically distributed random variables

Theorem (Law of large numbers)

If their mean m is finite, then

$$\frac{Y_1 + \cdots + Y_n}{n} \xrightarrow[n \rightarrow \infty]{} m \quad a.s.$$

Theorem (Central limit theorem)

If their variance σ^2 is also finite, then

$$\mathcal{D} \left(\frac{\frac{Y_1 + \cdots + Y_n}{n} - m}{\frac{\sigma}{\sqrt{n}}} \right) = \mathcal{D} \left(\frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{Y_i - m}{\sigma} \right) \xrightarrow[n \rightarrow \infty]{} \mathcal{N}$$

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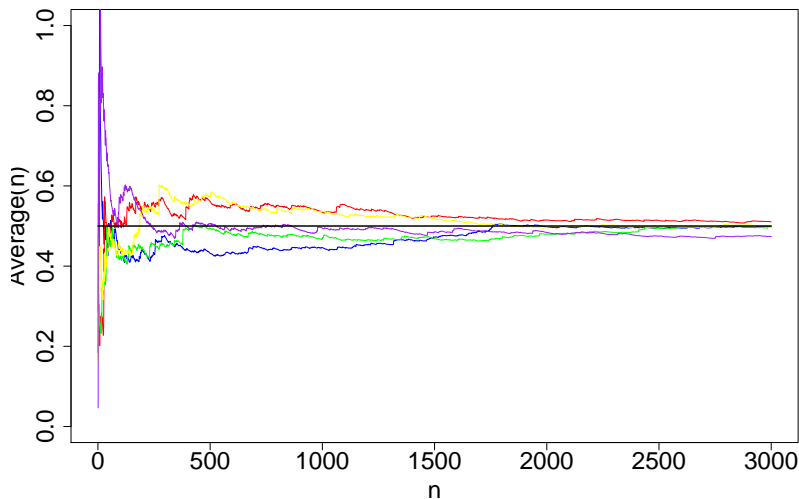
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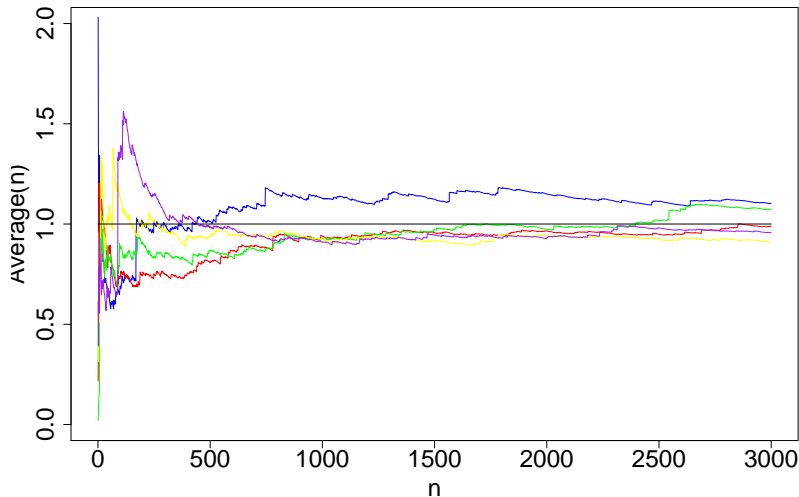
Example with finite mean and finite variance

$$f(y) = \frac{3}{(1+y)^4} \quad y \geq 0$$



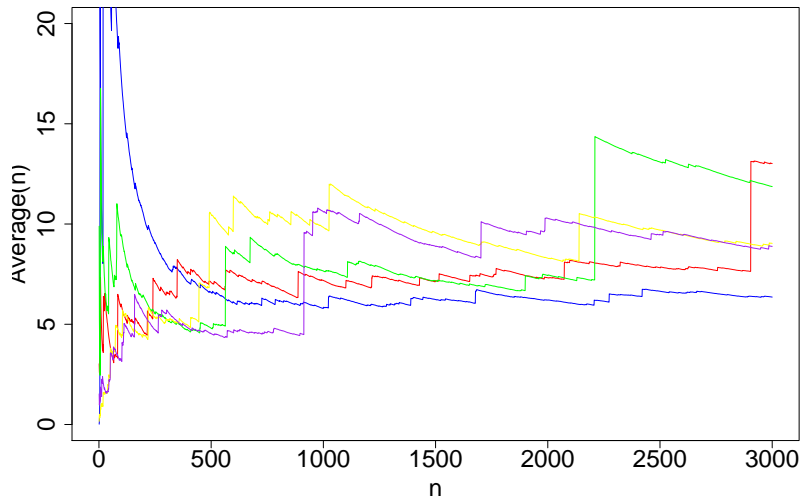
Example with finite mean and infinite variance

$$f(y) = \frac{2}{(1+y)^3} \quad y \geq 0$$



Example with infinite mean and infinite variance

$$f(y) = \frac{1}{(1+y)^2} \quad y \geq 0$$



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Second order stationary random field

Definition

A random field $Y = (Y(x), x \in \mathbb{R}^d)$ is said to be **second order stationary** if it satisfies the following 3 properties

- (i) $E\{Y(x)\} = m < \infty \quad \forall x \in \mathbb{R}^d$;
- (ii) $Var\{Y(x)\} = \sigma^2 < \infty \quad \forall x \in \mathbb{R}^d$;
- (iii) $Cov\{Y(x), Y(y)\} = C(x - y) \quad \forall x, y \in \mathbb{R}^d$.

A functional version of central limit theorem

Notation

Let $(Y_n, n \in \mathbb{N})$ be independent copies of a second order stationary random function with mean m , variance σ^2 and covariance C .

Definition

$$Y^{(n)} = \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{Y_i - m}{\sigma}$$

Property (central limit theorem)

The distribution of **any finite linear combination of variables** of $Y^{(n)}$ tend to be **Gaussian** as $n \rightarrow \infty$.

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Gaussian random field

Definition

A second order stationary random field $Y = (Y(x), x \in \mathbb{R}^d)$ is said to be **Gaussian** if any finite linear combination of its variables follows a **Gaussian** distribution:

$$\sum_{i=1}^n a_i Y(x_i) \sim \mathcal{N} \left(m \sum_{i=1}^n a_i, \sum_{i,j=1}^n a_i a_j C(x_i - x_j) \right)$$

Property

All statistical properties of Y are specified by its **mean** and its **covariance function**.

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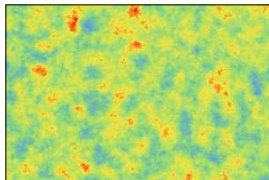
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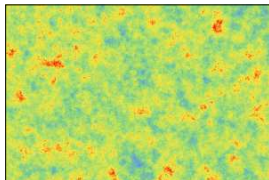
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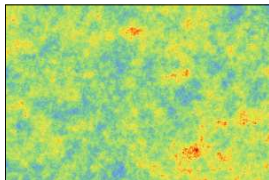
Examples (different covariance functions)



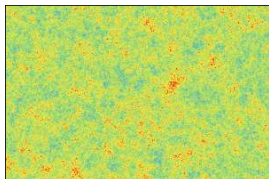
Spherical



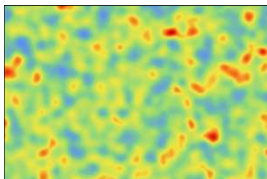
Exponential



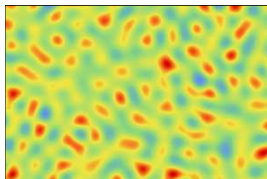
Hyperbolic



Stable



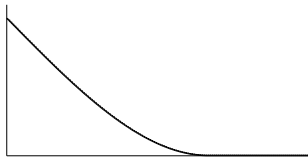
Gaussian



Cardinal sine

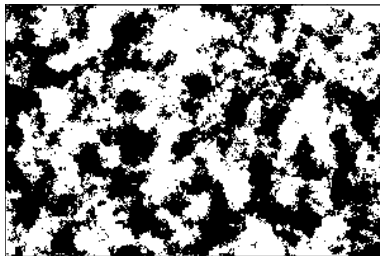
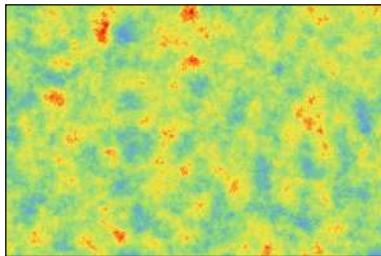
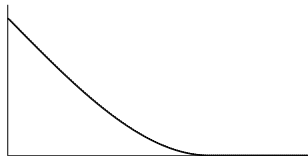
Spherical covariance

$$C(h) = \left(1 - \frac{3}{2} \frac{|h|}{a} + \frac{1}{2} \frac{|h|^3}{a^3}\right) 1_{|h| \leq a}$$



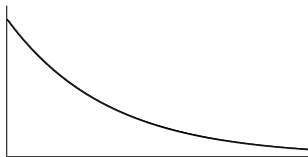
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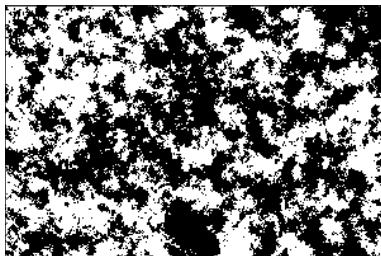
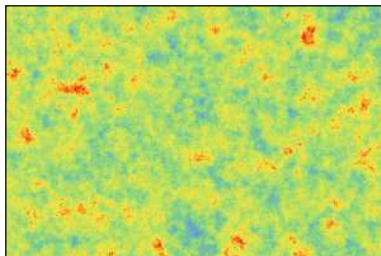
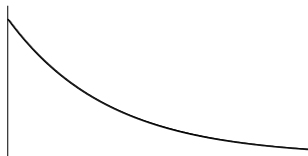
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$$C(h) = \exp \left\{ -\frac{|h|}{a} \right\}$$



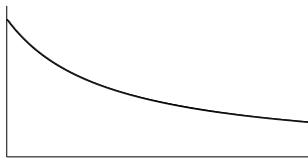
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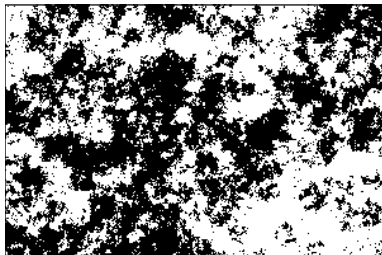
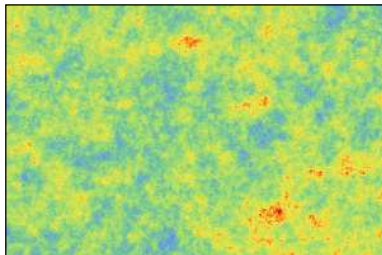
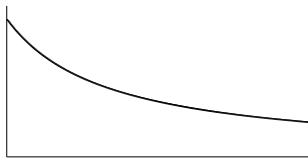
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$$C(h) = \frac{1}{1 + \frac{|h|}{a}}$$



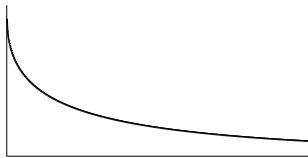
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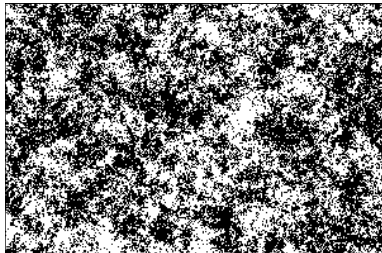
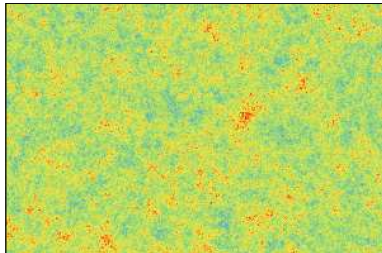
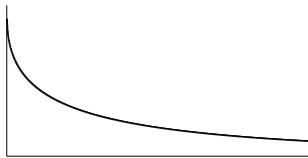
Stable covariance

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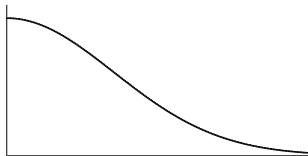
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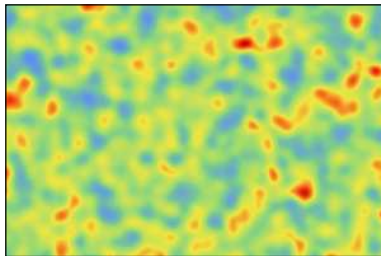
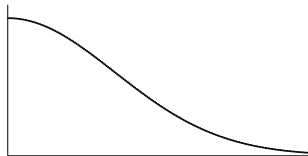
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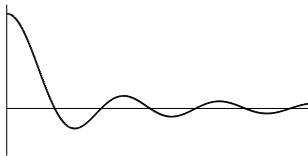
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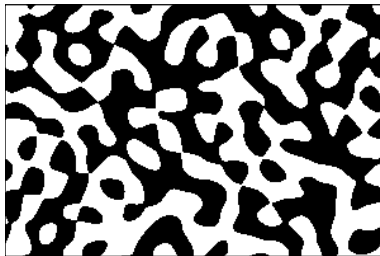
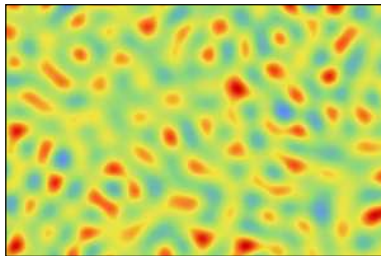
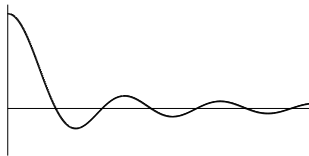
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$$C(h) = \frac{\sin \frac{|h|}{a}}{\frac{|h|}{a}}$$



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Simulation of a Gaussian random field

Problem

Produce realizations of a standardized (zero mean, unit variance) Gaussian random field with given covariance C in a **continuous** domain $D \subset \mathbb{R}^d$

Idea

Because of the **Central Limit Theorem**, it suffices to simulate a family of independent standardized random fields with covariance C .

$$Y^{(n)} = \frac{Y_1 + \cdots + Y_n}{\sqrt{n}}$$

Idea

Because \mathbb{R} is totally ordered, stochastic processes (defined on \mathbb{R}) are easier to simulate than random fields (defined on \mathbb{R}^d , $d > 1$).

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The spectral method

Theorem (Bochner)

If C is continuous at the origin, then there exists a probability measure F (spectral measure) such that

$$C(h) = \int_{\mathbb{R}^d} e^{i\langle \omega, h \rangle} dF(\omega)$$

Remark

Let $\Omega \sim F$ and $\Phi \sim \mathcal{U}([0, 2\pi])$ (independent). Then the random field defined by $Y(x) = \sqrt{2} \cos(\langle \Omega, x \rangle + \Phi)$ is standardized with covariance C .

P

Algorithm

- (i) generate $\omega_{1:n} \stackrel{iid}{\sim} F$ and $\phi_{1:n} \stackrel{iid}{\sim} \mathcal{U}([0, 2\pi])$;
- (ii) return $y(x) = \frac{\sqrt{2}}{\sqrt{n}} \sum_{i=1}^n \cos(\langle \omega_i, x \rangle + \phi_i)$ for each $x \in \mathbb{R}^d$.

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The spectral method: Example of the Gaussian covariance

$$C(h) = \exp \left\{ -\frac{|h|^2}{a^2} \right\}$$

Spectral measure

Because C is square integrable, the spectral measure F has a density f that is the inverse Fourier transform of C . Explicitly

$$f(\omega) = \left(\frac{a}{2\sqrt{\pi}} \right)^d \exp \left(-\frac{a^2|\omega|^2}{4} \right) \quad \omega \in \mathbb{R}^d$$

Algorithm (Generation of a spectral vector)

- (i) generate $u_{1:d} \stackrel{iid}{\sim} \mathcal{N}(0, \frac{2}{a^2})$;
- (ii) return $\omega = u_{1:d}$.

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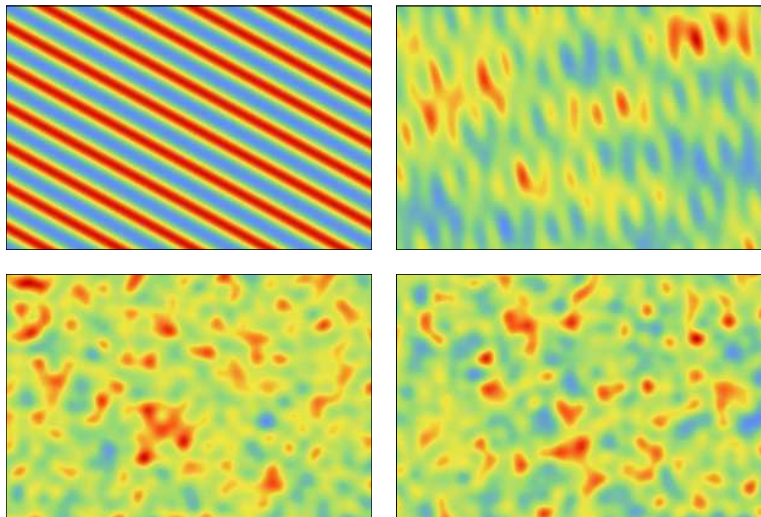
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Simulation of a GRF with Gaussian covariance



Simulations with 1, 10, 100 and 1000 basic fields.

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From the spectral method to the turning bands method

Remark

The spectral method rests on a proper sampling of the spectral measure. This is especially possible when this spectral measure has little dispersion, or equivalently when the covariance has a smooth behaviour around the origin.

Otherwise, the spectral method is not so efficient and its generalization, the turning bands methods, can be considered.

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Replace the **monochromatic** random fields of the spectral method by **polychromatic** random fields.

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The turning bands method

$$C(h) = \int_{\mathbb{R}^d} e^{i \langle \omega, h \rangle} dF(\omega)$$

Remark (Passing to polar coordinates)

Put $\omega = r\theta$ with $r \in \mathbb{R}$ and $\theta \in S_d$ (unit sphere). Then $dF(\omega) = dF_\theta(r) d\varpi(\theta)$, which gives

$$C(h) = \int_{S_d} \int_{\mathbb{R}} e^{ir \langle \theta, h \rangle} dF_\theta(r) d\varpi(\theta) = \int_{S_d} C_\theta(\langle \theta, h \rangle) d\varpi(\theta)$$

where the C_θ 's are **unidimensional covariances**.

Algorithm

- (i) generate directions $\theta_{1:n} \stackrel{iid}{\sim} \varpi$;
- (ii) for $i = 1, \dots, n$, generate a stochastic process y_i with mean 0 and covariances C_{θ_i} ;
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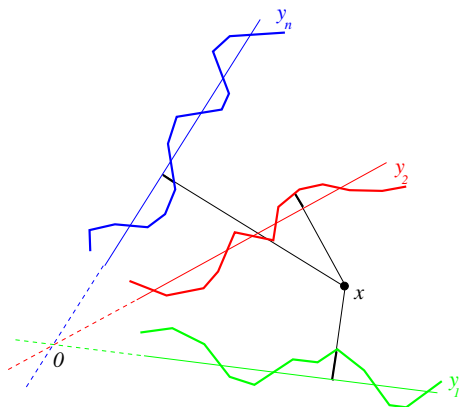
$$C(h) = \int_{S_d} \int_{\mathbb{R}} e^{ir \langle \theta, h \rangle} dF_\theta(r) d\varpi(\theta) = \int_{S_d} C_\theta(\langle \theta, h \rangle) d\varpi(\theta)$$

where the C_θ 's are **unidimensional covariances**.

Algorithm

- (i) generate directions $\theta_{1:n} \stackrel{iid}{\sim} \varpi$;
- (ii) for $i = 1, \dots, n$, generate a stochastic process y_i with mean 0 and covariances C_{θ_i} ;
- (iii) return $\frac{1}{\sqrt{n}} \sum_{i=1}^n y_i(\langle x, \theta_i \rangle)$ for each $x \in \mathbb{R}^d$.

The turning bands method: Geometric interpretation



$$y^{(n)}(x) = \frac{1}{\sqrt{n}} \sum_{i=1}^n y_i(< x, \theta_i >)$$

The turning bands method – Tridimensional isotropic case

Property

Put $C(h) = C_3(|h|)$. Then $C_\theta = C_1$ for each $\theta \in S_3$. Moreover, C_1 and C_3 are related by the formula

$$C_1(r) = \frac{d}{dr}(r C_3(r)) \quad r > 0$$

Algorithm

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The turning bands method – Tridimensional isotropic case

Spherical covariance

$$C_3(r) = \left(1 - \frac{3}{2} \frac{r}{a} + \frac{1}{2} \frac{r^3}{a^3}\right) 1_{r \leq a}$$

Property (Unidimensional covariance)

$$C_1(r) = \left(1 - 3 \frac{r}{a} + 2 \frac{r^3}{a^3}\right) 1_{r \leq a}$$

Remark (Comparison between C_3 and C_1)

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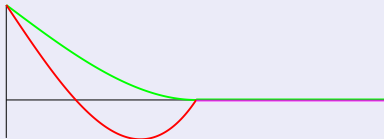
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Spherical covariance (2)

Algorithm (Generate a stochastic process with covariance C_1)

- (i) *put* $f(t) = 2\sqrt{3}t/a - \sqrt{3}$ *for each* $t \in]0, a[$;
- (ii) *generate* $x_0 \sim \mathcal{U}(]0, a[)$;
- (iii) *for each* $k \in \mathbb{Z}$, *generate* $\varepsilon_k \sim \mathcal{U}(\pm 1)$ *and put*
 $y(x) = \varepsilon_k f(x - x_0 - ka)$ *for each* $x \in]x_0 + ka, x_0 + (k+1)a[$.

Example

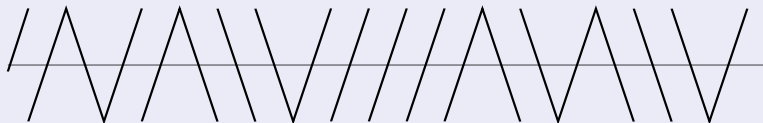
The turning bands method – Tridimensional isotropic case

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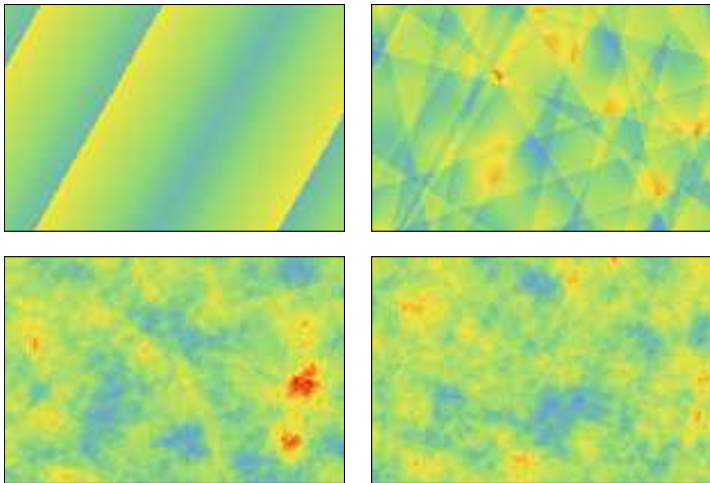
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Example



Simulation of a GRF with spherical covariance



Simulations using 1, 10, 100 and 1000 turning bands

The turning bands method – Tridimensional isotropic case

Exponential covariance

$$C_3(r) = \exp\left(-\frac{r}{a}\right)$$

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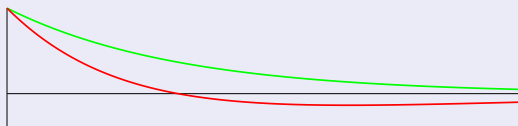
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The turning bands method – Tridimensional isotropic case

Exponential covariance (2)

Property

An exponential covariance can be seen as a spherical covariance with random range:

$$\exp\left(-\frac{|h|}{a}\right) = \int_0^\infty C_{sph}\left(\frac{|h|}{au}\right) w(u) du$$

where

- C_{sph} is the unit range **spherical covariance**;
- $w(u) = \frac{1}{3}e^{-u}u(1+u)$ is a **mixture of gamma distributions**.

Algorithm (Generate a stochastic process with covariance C_1)

- generate $u \sim w$;*
- generate a **spherical** stochastic process y with range au .*

The turning bands method – Tridimensional isotropic case

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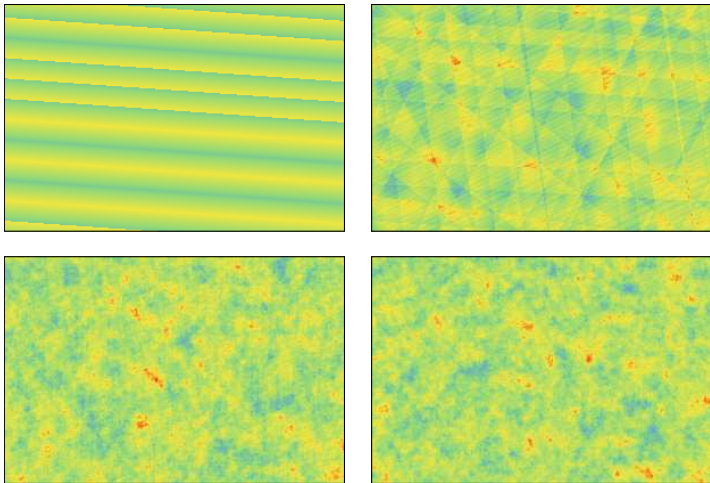
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Simulation of a GRF with exponential covariance



Simulations using 1, 10, 100 and 1000 turning bands

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Presentation of the problem

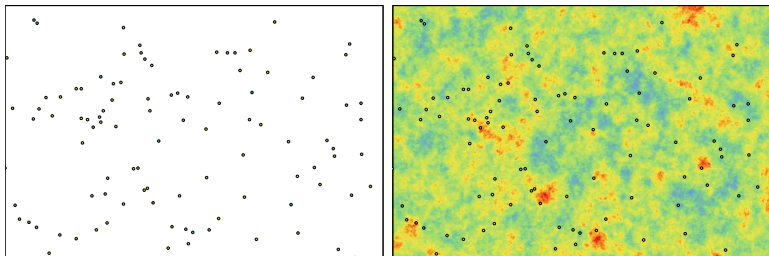
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Let $Y = (Y_x, x \in \mathbb{R}^d)$ be a Gaussian random field with mean m and covariance function C . These parameters are assumed to be known. How to produce a realization y of Y in a domain D , such that $Y_A = y_A$ (short notation for $Y_\alpha = y_\alpha$ for each $\alpha \in A$)?

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Example of conditional simulation. The realization (R) respects the values assigned to conditioning data point (L).

Principle

Definition

The **simple kriging** of Y_x on Y_A satisfies

$$Y_x^A - m = \sum_{\alpha \in A} \lambda_{\alpha} (Y_{\alpha} - m)$$

The kriging weights λ_{α} are chosen so as to minimize the estimation variance $Var\{Y_x - Y_x^A\}$. They are the solution of the system of linear equations

$$\sum_{\beta \in A} \lambda_{\beta} C_{\alpha, \beta} = C_{\alpha, s} \quad \alpha \in A$$

Property

Y^A and $Y - Y^A$ are **independent Gaussian random fields**.

Consequence

Y^A and $Y - Y^A$ can be generated independently.

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Conditional simulation algorithm

Idea

Starting from $Y = Y^A + Y - Y^A$, consider an independent copy S of Y and put $Y^{CS} = Y^A + S - S^A$.

Algorithm

- (i) generate an *unconditional* simulation s in D ;
- (ii) for each $x \in D$, return $y_x^{CS} = y_x^A + s_x - s_x^A$.

Remark (Verifications)

- if $x = \alpha$, then $y_\alpha^{SC} = y_\alpha + s_\alpha - s_\alpha = y_\alpha$;
- if $C_{x,\alpha} \approx 0$ for each $\alpha \in A$, then $y_x^{SC} \approx m + s_x - m = s_x$.

Remark (Simplification)

$$y_x^{CS} = s_x + \sum_{\alpha \in A} \lambda_\alpha (y_\alpha - s_\alpha)$$

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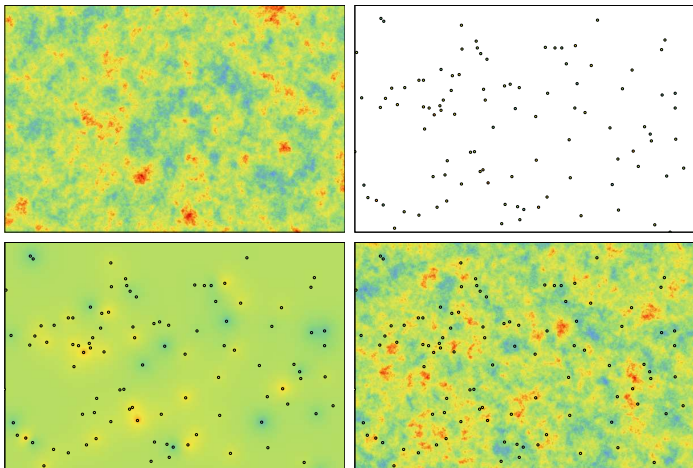
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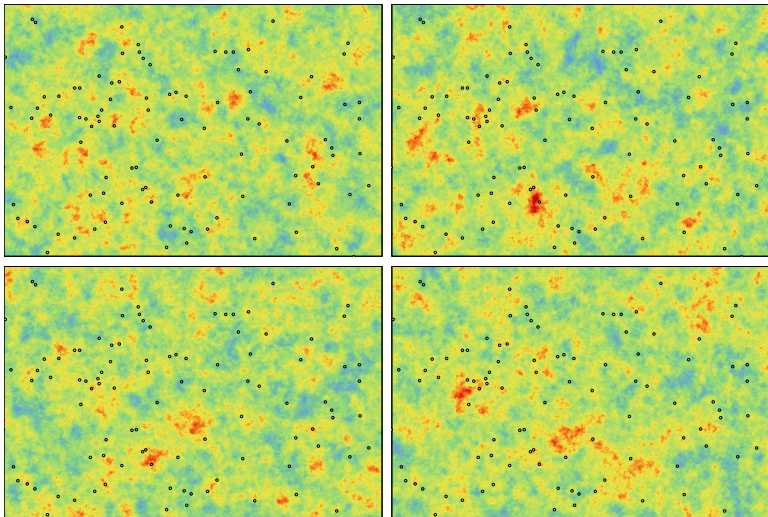
Illustration

Model $m = 0$, $C(h) = \exp(-|h|/15)$. Simulation field 600×400 .



Simulation (TL), conditioning data points (TR), simple kriging (BL) and conditional simulation (BR).

Four conditional simulations



Outline

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Presentation of the problem

Notation

Let $Y = (Y_x, x \in \mathbb{R}^d)$ be a **stationary Gaussian random function** with **mean** m and **covariance function** $C(h)$.

Notation

Let $(y_x, x \in D)$ be a **realization** of Y in domain D .

Problem

From this realization, a number of **empirical statistics** can be computed, such as its **average** over D or its **regional variogram**

$$y_D = \frac{1}{|D|} \int_D y_x dx \quad \gamma_D(h) = \frac{1}{2|D \cap \tau_h D|} \int_{D \cap \tau_h D} (y_x - y_{x+h})^2 dx$$

It appears that the retrieved statistics may be very different from those expected from the model. Why?

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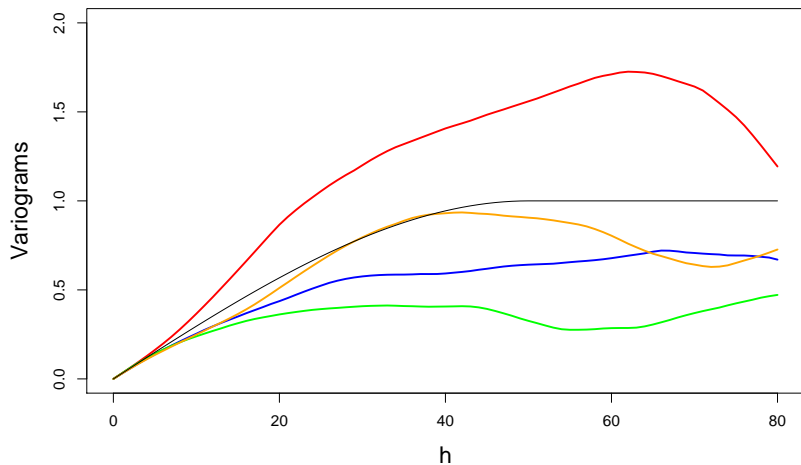
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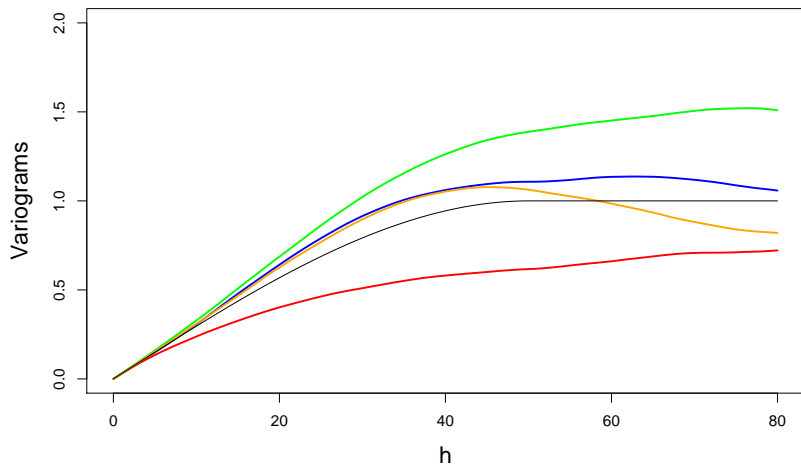
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Example



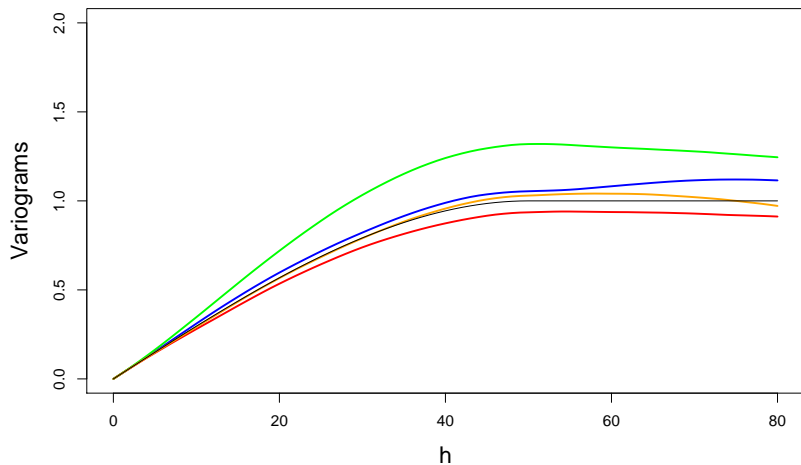
$$D = 100 \times 100 \quad \gamma = Sph(1, 50)$$

Example (2)



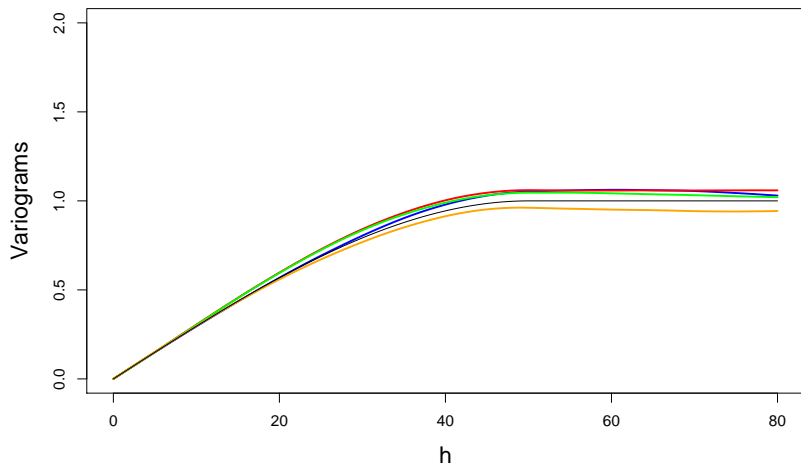
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Example (3)



$$D = 400 \times 400 \quad \gamma = Sph(1, 50)$$

Example (4)



$$D = 800 \times 800 \quad \gamma = Sph(1, 50)$$

Empirical observations and questions

Observation

- the experimental statistics of a simulation may **differ** from the model parameters;
- they depend on the simulation (**statistical fluctuations**);
- they tend to get closer to the model parameters as the simulation domain extends (**support effect**).

Question

- given a simulation domain, how large are the statistical fluctuations?
- how extended should the simulation domain be taken to get statistical fluctuations less than a prespecified level?

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Let y_D be the **average of the realization** over D :

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Let Y_D be its **probabilistic version**

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Property

Y_D is **normally distributed** with mean m and variance

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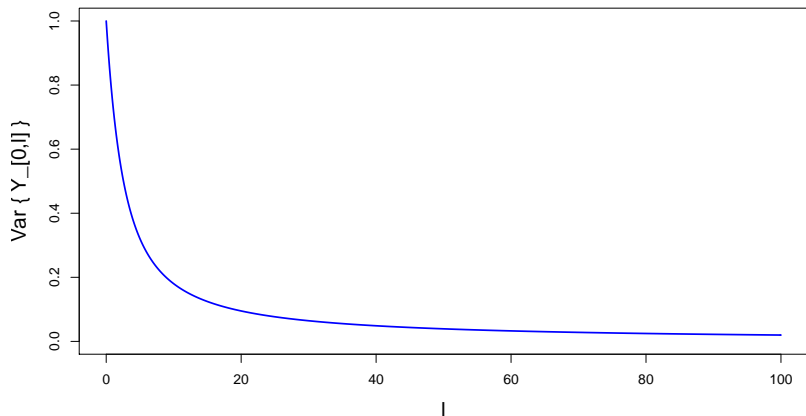
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Behaviour for large domains

Notation

Put $C(h) = \sigma^2 \rho(h)$, where σ^2 is the **point variance** and ρ the **correlation function**.

Definition

The **integral range** is the integral of the correlation function

$$A = \int_{\mathbb{R}^d} \rho(h) dh$$

Property

- A has the dimension of a d -volume;
- $0 \leq A \leq \infty$;
- if $0 < A < \infty$, and if D is large, then it can be shown that

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A sampling problem

Question

For which domain size do we have $P\{|Y_D - m| < 0.05\} > 0.9$?

Answer

$$|D| > 1076\sigma^2 A$$

P

Example (Standard spherical and exponential models)

<i>sph.</i>	1D	2D	3D
Integral range	3/4	$\pi/5$	$\pi/6$
d-volume	807	676	563

<i>exp.</i>	1D	2D	3D
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A functional version of central limit theorem

Notation

Let $(Y_n, n \in \mathbb{N})$ be independent copies of a second order stationary random function with mean m , variance σ^2 and covariance C . Put

$$Y^{(n)} = \frac{1}{\sqrt{n}} \sum_{i=1}^n \frac{Y_i - m}{\sigma}$$

Property (central limit theorem)

The distribution of **any finite linear combination of variables** of $Y^{(n)}$ tend to be **Gaussian** as $n \rightarrow \infty$.

Proof

Consider $a_1, \dots, a_k \in \mathbb{R}$ and $x_1, \dots, x_k \in \mathbb{R}^d$, and put $Y_{ij} = Y_i(x_j)$.

$$\sum_{j=1}^k a_j Y^{(n)}(x_j) = \frac{1}{\sqrt{n}} \sum_{j=1}^k a_j \sum_{i=1}^n \frac{Y_{ij} - m}{\sigma} = \frac{1}{\sqrt{n}} \sum_{i=1}^n \sum_{j=1}^k \frac{a_j (Y_{ij} - m)}{\sigma}$$

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On the geometry of Gaussian excursion sets

Definition (Excursion set at level λ)

$$X_\lambda = \{x \in \mathbb{R}^d : Y(x) \geq \lambda\}$$

Property (Covariance function of X_λ)

$$C_\lambda(h) = \frac{1}{2\pi} \int_0^{C(h)} \exp\left(\frac{-\lambda^2}{1+x}\right) \frac{dx}{\sqrt{1-x^2}} \quad h \in \mathbb{R}^d$$

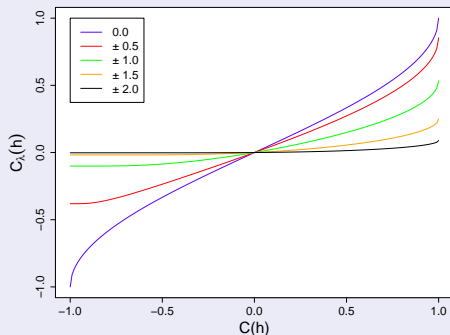
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Behaviour around the origin

Consequence

The variograms of Y and X_λ are related by the formula

$$\gamma_\lambda(h) \approx \kappa(\lambda) \sqrt{\gamma(h)} \quad |h| \approx 0$$

Property (Two-dimensional stationary isotropic random set)

The **specific perimeter** of X_λ , that is its mean boundary length per unit area is given by the formula $L_A = \pi \gamma'_\lambda(0)$.

Consequence

Suppose $\gamma(h) \approx |h|^\alpha$ when $|h| \approx 0$. Then $\gamma_\lambda(h) \approx |h|^{\alpha/2}$.
If $\alpha < 2$, then $L_A = \infty$. If $\alpha = 2$, then $L_A < \infty$.

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The spectral method

$$C(h) = \int_{\mathbb{R}^d} e^{i \langle \omega, h \rangle} dF(\omega)$$

Remark

$C(h) = C(-h)$ implies

$$C(h) = \int_{\mathbb{R}^d} \cos(\langle \omega, h \rangle) dF(\omega) = E\{\cos(\langle \Omega, h \rangle)\}$$

Proof

$$\begin{aligned} \text{Cov}\{Y(x), Y(y)\} &= 2E\{\cos(\langle \Omega, x \rangle + \Phi) \cos(\langle \Omega, y \rangle + \Phi)\} \\ &= E\{\cos(\langle \Omega, x + y \rangle + 2\Phi) + \cos(\langle \Omega, x - y \rangle)\} \\ &= E\{\cos(\langle \Omega, x - y \rangle)\} \\ &= C(x - y) \end{aligned}$$

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A sampling problem

Question

How large should the domain size be chosen so as to have

$$P\{|Y_D - m| < 0.05\} > 0.9?$$

Proof

If D is large, then $Y_D \approx m + \sigma\sqrt{A/|D|}U$ with $U \sim \mathcal{N}$. Accordingly, the question amounts to finding D such that

$$P\left\{|U| < \frac{0.05}{\sigma}\sqrt{\frac{|D|}{A}}\right\} > 0.9$$

But $P\{|U| < 1.64\} = 0.9$. Therefore the previous inequality will be satisfied as soon as

$$1.64 < \frac{0.05}{\sigma}\sqrt{\frac{|D|}{A}}$$

or equivalently $|D| > 1076\sigma^2 A$.

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