Spatio-temporal statistics (MATH4341) Michaelmas term, 2023

Handout 3: Point referenced data modeling / Geostatistics

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Aim. To introduce Point referenced data modeling / Geostatistics: regional variables, random field, variogram,

Reading list & references:

(1) Cressie, N. (2015; Part I). Statistics for spatial data. John Wiley & Sons.
(2) Gaetan, C., & Guyon, X. (2010; Ch 2 & 5.1). Spatial statistics and modeling (Vol. 90). New York: Springer.

Further reading.

(4) Wackernagel, H. (2003). Multivariate geostatistics: an introduction with applications. Springer Science & Business Media.
(5) Kent, J. T., & Mardia, K. V. (2022). Spatial analysis (Vol. 72). John Wiley & Sons.

Part 1. Building stochastic models & concepts

Note 1. We discuss basic stochastic models and concepts for modeling point references data int he Geostatistics framework.

1. Stochastic processes (or Random fields)

Definition 2. A stochastic process (or random field) $Z = (Z_s; s \in \mathcal{S})$ taking values in $\mathcal{Z} \subseteq \mathbb{R}^q$, $q \geq 1$ is a family of random variables $\{Z_s := Z_s(\omega); s \in \mathcal{S}, \omega \in \Omega\}$ defined on the same probability space $(\Omega, \mathfrak{F}, \Pr)$ and taking values in $\mathcal{Z}$. The label $s \in \mathcal{S}$ is called site, the set $\mathcal{S} \subseteq \mathbb{R}^d$ is called the (spatial) set of sites at which the process is defined, and $\mathcal{Z}$ is called the state space of the process.

Note 3. Given a set $\{s_1, ..., s_n\}$ of sites $s_i \in S$ the random vector $(Z(s_1), ..., Z(s_n))^\top$ has a well-defined probability distribution that is completely determined by its joint CDF

$$\mathrm{F}_{s_1,...,s_n}(z_1, ..., z_n) = \Pr(Z(s_1) \leq z_1, ..., Z(s_n) \leq z_n)$$

Finite dimensional distributions (or fidi's) of Z is called the ensemble of all such joint CDF's with $n \in \mathbb{N}$ and $\{s_i \in S\}$.

Note 4. To define a random field model, one must specify the joint distribution of $(Z(s_1), ..., Z(s_n))^\top$ for all choices of n and $\{s_i \in S\}_{i=1}^n$ in a consistent way, due to Kolmogorov thm.

Proposition 5. *(Kolmogorov consistency theorem) Let* $\Pr_{s_1,...,s_n}$ *be a probability on* $\mathbb{R}^n$ *with join CDF* $F_{s_1,...,s_n}$ *for every finite collection of points* $s_1, ..., s_n$*. If* $F_{s_1,...,s_n}$ *is symmetric w.r.t. any permutation* $\mathfrak{p}$

$$F_{\mathfrak{p}(s_1),...,\mathfrak{p}(s_n)}\left(z_{\mathfrak{p}(1)}, ..., z_{\mathfrak{p}(n)}\right) = F_{F_{s_1,...,s_n}}\left(z_1, ..., z_n\right)$$

for all $n \in \mathbb{N}$, $\{s_i \in S\}$, *and* $\{z \in \mathbb{R}\}$, *and all if all permulations* $\mathfrak{p}$ *are consistent in the sense*

$$\lim_{z_n \to \infty} F_{s_1,...,s_n}\left(z_1, ..., z_n\right) = F_{s_1,...,s_{n-1}}\left(z_1, ..., z_{n-1}\right)$$

or all $n \in \mathbb{N}$, $\{s_i \in S\}$, *and* $\{z \in \mathbb{R}\}$, *then there exists a random field* Z *whose fidi's coincide with those in* F*.*

Example 6. Let $n \in \mathbb{N}$, let $\{f_i : T \to \mathbb{R};\ i = 1, ..., n\}$ be a set of constant functions, and let $\{Z_i \sim \mathrm{N}(0,1)\}_{i=1}^n$ be a set of independent random variables. Then

$$\tilde{Z}_s = \sum_{i=1}^{n} Z_i f_i(s),\ s \in S$$

is a well defined stochastic process as it satisfies Thm 5.

1.1. **Mean and covariance functions.**

Definition 7. The mean function $\mu(\cdot)$ and covariance function $c(\cdot,\cdot)$ of a random field $Z = (Z_s)_{s \in S}$ are defined as

$$\mu(s) = \mathrm{E}(Z_s), \qquad \forall s \in S \tag{1.1}$$

$$c(s, s') = \mathrm{Cov}(Z_s, Z_{s'}) = \mathrm{E}\left(\left(Z_s - \mu(s)\right)\left(Z_{s'} - \mu(s')\right)^\top\right), \qquad \forall s, s' \in S \tag{1.2}$$

Example 8. Examples of covariace functions (c.f.)

(1) Exponential c.f. $c(s, s') = \frac{1}{2\beta} \exp\left(-\beta \left\|s - s'\right\|_1\right)$
(2) Gaussian c.f. $c(s, s') = \sigma^2 \exp\left(-\beta \left\|s - s'\right\|_2^2\right)$
(3) Nugget c.f. $c(s, s') = \sigma^2 1(s = s')$

1.1.1. *Construction of covariance functions.*

(The following provides the means for checking and constructing covariance functions.)

Proposition 9. *The function* $c : S \times S \to \mathbb{R}$, $S \subseteq \mathbb{R}^d$ is the covariance function iff $c(\cdot,\cdot)$ is semi-positive definite; i.e. the Gram matrix $(c(s_i, s_j))_{i,j=1}^n$ is non-negative definite for any $\{s_i\}_{i=1}^n$, $n \in \mathbb{N}$.

Example 10. $c(s, s') = 1(s = s')$ is a proper covariance function as

$$\sum_i \sum_j a_i a_j c(s_i, s_j) = \sum_i a_i^2 \geq 0, \quad \forall a$$

Note 11. Prop 12 uses the experience from basis functions, while Theorem 29 uses experience from characteristic functions to be incorporated int he process for modeling reasons.

Remark 12. One way to construct a c.f c is to set $c(s,s') = \psi(s)^\top \psi(s')$, for a given vector of basis functions $\psi(\cdot) = (\psi_1(\cdot), ..., \psi_n(\cdot))$.

Proof. From Prop 9, as

$$\sum_i \sum_j a_i a_j c(s_i, s_j) = (\psi a)^\top (\psi a) \geq 0, \ \ \forall a \in \mathbb{R}^n$$

□

2. Second order processes (or Random fields)

Definition 13. Second order process (or random field) $Z = (Z_s; s \in \mathcal{S})$ is called the stochastic process where $\mathrm{E}(Z_s^2) < \infty$ for all $s \in S$. Then the associated mean function $\mu(\cdot)$ and covariance function $c(\cdot,\cdot)$ exist.

3. Gaussian process

Definition 14. $Z = (Z_s; s \in S)$ indexed by $S \subseteq \mathbb{R}^d$ is a Gaussian process (GP) or random field (GRF) if for any finite set $\{s_1, ..., s_n\}$ of $n \in \mathbb{N}$ indices, the random vector $(Z_{s_1}, ..., Z_{s_n})^\top$ has a multivariate normal distribution.

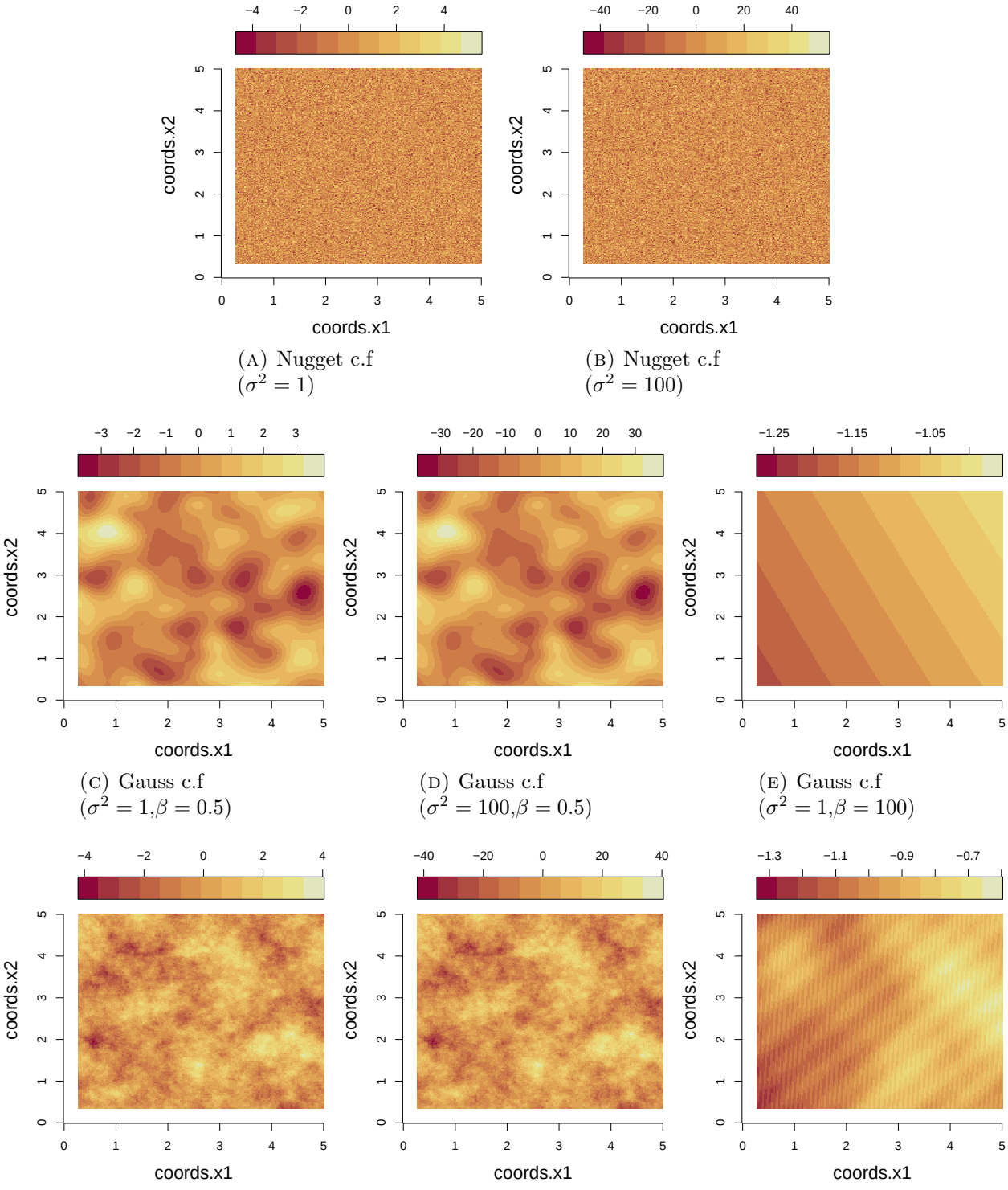
Also Example of Proposition

Proposition 15. *A GP $Z = (Z_s; s \in S)$ is fully characterized by its mean function $\mu : S \to \mathbb{R}$ with $\mu(s) = E(Z_s)$, and its covariance function with $c(s,s') = Cov(Z_s, Z_{s'})$.*

Notation 16. Hence, we denote the GP as $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$.

Example 17. Recall your linear regression lessons where you specified a sampling distribution $y_x|\beta,\sigma^2 \overset{\text{ind}}{\sim} \mathrm{N}\left(x^\top\beta, \sigma^2\right)$, $\forall x \in \mathbb{R}^d$; well that can be considered as a GP with $\mu_x = x^\top\beta$ and $c(x,x') = \sigma^2 1(x = x')$.

Example 18. Figure 3.1 presents realizations GRF $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$ with $\mu(s) = 0$ and differently parametrized covariance functions in 2D. Nugget c.f. is the usual noise where the ups and downs are random and controlled by σ^2 (Fig. 3.1a & 3.1b). In Gaussian c.f. the ups and downs are random and controlled by σ^2 (Fig. 3.1c & 3.1d), and the spatial dependence is controlled by β (Fig.3.1d & 3.1e). Realizations with different c.f. have behavior Fig. 3.1a, 3.1d & 3.1e)



(A) Nugget c.f ($\sigma^2 = 1$)

(B) Nugget c.f ($\sigma^2 = 100$)

(C) Gauss c.f ($\sigma^2 = 1, \beta = 0.5$)

(D) Gauss c.f ($\sigma^2 = 100, \beta = 0.5$)

(E) Gauss c.f ($\sigma^2 = 1, \beta = 100$)

(F) Exp c.f ($\sigma^2 = 1, \beta = 0.5$)

(G) Exp c.f ($\sigma^2 = 100, \beta = 0.5$)

(H) Exp c.f ($\sigma^2 = 1, \beta = 100$)

FIGURE 3.1. Realizations of GRF $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$ (using same seed)

4. Strong stationarity

Note 19. Assume $\mathcal{S} = \mathbb{R}^d$ for simplicity. [1]

Definition 20. A random field $Z = (Z_s)_{s\in\mathbb{R}^d}$ is strongly stationary if for all finite sets consisting of $s_1, ..., s_n \in \mathbb{R}^d$, $n \in \mathbb{N}$, for all $k_1, ..., k_n \in \mathbb{R}$, and for all $h \in \mathbb{R}^d$

$$\Pr\left(Z\left(s_1+h\right) \leq k_1, ..., Z\left(s_n+h\right) \leq k_n\right) = \Pr\left(Z\left(s_1\right) \leq k_1, ..., Z\left(s_n\right) \leq k_n\right)$$

5. Weak stationarity (or second order stationarity)

Note 21. Yuh... strong stationary may be a too "restricting" a characteristic for our modeling... Perhaps, we could only restrict the first two moments them properly; notice Def. 20 implies that, given $\mathrm{E}\left(Z_s^2\right) < \infty$, it is $\mathrm{E}\left(Z_s\right) = \mathrm{E}\left(Z_{s+h}\right) = \text{contst...}$ and $\mathrm{Cov}\left(Z_s, Z_{s'}\right) = \mathrm{Cov}\left(Z_{s+h}, Z_{s'+h}\right) \overset{h=-s'}{=} \mathrm{Cov}\left(Z_{s-s'}, Z_0\right) = \text{funct of lag...}$

Definition 22. A random field $Z = (Z_s)_{s\in\mathbb{R}^d}$ is weakly stationary (or second order stationary) if, for all $s, s' \in \mathbb{R}^d$,

(1) $\mathrm{E}\left(Z_s^2\right) < \infty$ (finite)
(2) $\mathrm{E}\left(Z_s\right) = m$ (constant)
(3) $\mathrm{Cov}\left(Z_s, Z_{s'}\right) = c\left(s'-s\right)$ for some even function $c : \mathbb{R}^d \to \mathbb{R}$ (lag dependency)

Definition 23. Weakly (or second order) stationary covariance function is called the c.f. of a weakly stationary stochastic process.

6. Covariogram

Note 24. The definition of the covariogram function requires the random field to be weakly stationary.

Definition 25. Let $Z = (Z_s)_{s\in\mathbb{R}^d}$ be a weakly stationary random field. The covariogram function of $Z = (Z_s)_{s\in\mathbb{R}^d}$ is defined by $c : \mathbb{R}^d \to \mathbb{R}$ with

$$c\left(h\right) = \mathrm{Cov}\left(Z_s, Z_{s+h}\right), \ \forall s \in \mathbb{R}^d.$$

Example 26. For the Gaussian c.f. $c\left(s,t\right) = \sigma^2 \exp\left(-\beta \left\|s-t\right\|_2^2\right)$ in (Ex. 8(2)), we may denote just

$$c\left(h\right) = c\left(s, s+h\right) = \sigma^2 \exp\left(-\beta \left\|h\right\|_2^2\right)$$

Note that, in Fig 3.1, the bigger the β, the smoother the realization (aka slower changes). This is

Proposition 27. *If $c : \mathbb{R}^d \to \mathbb{R}$ is the covariogram of a weakly stationary random field $Z = (Z_s)_{s\in\mathbb{R}^d}$ then:*

[1] Otherwise, we should set $s, s' \in \mathcal{S}$, $h \in \mathcal{H}$, such as $\mathcal{H} = \left\{h \in \mathbb{R}^d : s+h \in \mathcal{S}\right\}$.

(1) $c(0) \geq 0$
(2) $c(h) = c(-h)$ *for all* $h \in \mathbb{R}^d$
(3) $|c(h)| \leq c(0) = Var(Z_s)$ *for all* $h \in \mathbb{R}^d$
(4) $c(\cdot)$ *is semi-positive definite; i.e. for all* $n \in \mathbb{N}$, $a \in \mathbb{R}^n$, *and* $\{s_1, ..., s_n\} \subseteq S$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j c(s_i - s_j) \geq 0$$

Note 28. The following helps in the specification of cavariograms by considering properties of characteristic functions.

Theorem 29. *Let* $c : \mathbb{R}^d \to \mathbb{R}$ *be a continuous even real-valued function. Then* c *is positive semi-definite iff it is the Fourier transform of a symmetric positive finite measure on* $\mathbb{R}^d$*; i.e.*

$$c(h) = \int_{\mathbb{R}^d} \exp\left(i\omega^\top h\right) dF(\omega)$$

- *Here, we will focus on cases of the form* $dF(\omega) = f(\omega)\, d\omega$ *where* $f(\cdot)$ *is called spectral density of* $c(\cdot)$ *i.e.*

$$c(h) = \int_{\mathbb{R}^d} \exp\left(i\omega^\top h\right) f(\omega)\, d\omega$$

In this case, $\lim_{h\to\infty} c(h) = 0$

Theorem 30. *If* $c(\cdot)$ *is integrable,* $F(\cdot)$ *is absolutely continuous with spectral density* $f(\cdot)$ *of* $Z = (Z_s; s \in \mathcal{S})$ *then by Fast Fourier transformation*

$$f(\omega) = \left(\frac{1}{2\pi}\right)^d \int_{\mathbb{R}^d} \exp\left(-i\omega^\top h\right) c(h)\, dh$$

Example 31. Consider the Gaussian c.f. $c(h) = \sigma^2 \exp\left(-\beta \|h\|_2^2\right)$ for $\sigma^2, \beta > 0$ and $h \in \mathbb{R}^d$. Then the spectral density from Thm 29 is

$$\begin{aligned}
f(\omega) &= \left(\frac{1}{2\pi}\right)^d \int_{\mathbb{R}^d} \exp\left(-i\omega^\top h\right) \sigma^2 \exp\left(-\beta \|h\|_2^2\right) \mathrm{d}h \\
&= \sigma^2 \left(\frac{1}{2\pi}\right)^d \prod_{j=1}^{d} \int_{\mathbb{R}} \exp\left(-i\omega_j h_j - \beta h_j^2\right) \mathrm{d}h \\
&= \sigma^2 \left(\frac{1}{2\pi}\right)^d \prod_{j=1}^{d} \int_{\mathbb{R}} \exp\left(-\beta\left(h_j - \left(-i\omega/(2\beta)\right)\right)^2\right) \mathrm{d}h_j \\
&= \sigma^2 \left(\frac{1}{4\pi\beta}\right)^{d/2} \exp\left(-\|\omega\|_2^2/(4\beta)\right)
\end{aligned}$$

i.e. of a Gaussian form.

7. Intrinsic stationarity

Note 32. Getting greedier, we can further weaken the weak stationarity by considering lag dependent variance in the increments with purpose to be able to use more inclusive models; Def 22 implies that $\mathrm{Var}\left(Z_{s+h}-Z_s\right)=\mathrm{Var}\left(Z_{s+h}\right)+\mathrm{Var}\left(Z_s\right)-2\mathrm{Coc}\left(Z_{s+h},Z_s\right)=2c\left(0\right)-2c\left(h\right)$.

Definition 33. A random field $Z=\left(Z_s\right)_{s\in\mathbb{R}^d}$ is intrinsically stationary if, for all $h\in\mathbb{R}^d$, $\left(Z_{s+h}-Z_s\right)_{s\in\mathbb{R}^d}$ is weakly stationary; i.e.

(1) $\mathrm{E}\left(Z_{s+h}-Z_s\right)^2<\infty$
(2) $\mathrm{E}\left(Z_{s+h}-Z_s\right)=m$ (constant)
(3) $\mathrm{Var}\left(Z_{s+h}-Z_s\right)=2\gamma\left(h\right)$ for some function $\gamma:\mathbb{R}^d\to\mathbb{R}$ (lag dependent)

Definition 34. Intrinsically stationary covariance function is called the c.f. of an intrinsically stationary stochastic process.

Example 35. The following covariance function is not weakly but intrinsically stationary

$$c\left(s,t\right)=\frac{1}{2}\left(\left\|s\right\|^{2H}+\left\|t\right\|^{2H}-\left\|t-s\right\|^{2H}\right),\ H\in\left(0,1\right)$$

because for $h\in\mathbb{R}^d$

$$c\left(s,s+h\right)=\frac{1}{2}\left(\left\|s\right\|^{2H}+\left\|s+h\right\|^{2H}-\left\|h\right\|^{2H}\right)$$

and

$$\mathrm{Var}\left(Z_s-Z_{s+h}\right)=\mathrm{Var}\left(Z_s\right)+\mathrm{Var}\left(Z_{s+h}\right)-2\mathrm{Cov}\left(Z_s,Z_{s+h}\right)=\frac{1}{2}\left\|h\right\|^{2H}$$

8. (Semi) variogram

Note 36. The definition of the semi-variogram function requires the random field to be intrinsic stationarity; which is weaker assumption than weak stationary required by covariogram.

Definition 37. Let $Z=\left(Z_s\right)_{s\in\mathbb{R}^d}$ be intrinsically stationary. The semi-variogram of Z is defined by $\gamma:\mathbb{R}^d\to\mathbb{R}$ with

$$\gamma\left(h\right)=\frac{1}{2}\mathrm{Var}\left(Z_{s+h}-Z_s\right),\ \forall s\in\mathbb{R}^d$$

Definition 38. Variogram of an intrinsically stationary random field is called the quantity $2\gamma\left(h\right)$.

Note 39. Let $Z=\left(Z_s\right)_{s\in\mathbb{R}^d}$ be weakly stationary with covariogram $c\left(\cdot\right)$. Then Z is intrinsic stationary with semi-variogram

$$\gamma\left(h\right)=c\left(0\right)-c\left(h\right),\ \forall h\in\mathbb{R}^d$$

Example 40. For the Gaussian covariance function (Ex. 26) the semi-variogram is

$$\gamma(h) = c(0) - c(h) = \sigma^2 \left(1 - \exp\left(-\beta \|h\|_2^2\right)\right)$$