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.

Specialized reading.

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

Part 1. Intro to building stochastic models & concepts

Note 1. We discuss basic stochastic models and concepts for modeling point referenced data in the 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, with $s_i \in S$, 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. According to Kolmogorov Thm 5, to define a random field model, one must specify the joint distribution of $(Z(s_1), ..., Z(s_n))^\top$ for all of n and all $\{s_i \in S\}_{i=1}^n$ in a consistent way.

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* $\mathfrak{p}$

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

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

$$\tilde{Z}_s = \sum_{i=1}^{n} Z_i f_i(s), \quad s \in S \tag{1.1}$$

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

$$\mu(s) = \mathrm{E}(Z_s), \qquad \forall s \in S \tag{1.2}$$

$$c(s,s') = \mathrm{Cov}(Z_s, Z_{s'}) = \mathrm{E}\left((Z_s - \mu(s))(Z_{s'} - \mu(s'))^{\top}\right), \qquad \forall s, s' \in S \tag{1.3}$$

Example 8. For (1.1), the mean function is $\mu(s) = \mathrm{E}\left(\tilde{Z}_s\right) = 0$ and covariance function is

$$c(s,s') = \mathrm{Cov}(Z_s, Z_{s'}) = \mathrm{Cov}\left(\sum_{i=1}^{n} Z_i f_i(s), \sum_{j=1}^{n} Z_j f_j(s')\right)$$
$$= \sum_{i=1}^{n} f_i(s) \sum_{j=1}^{n} f_j(s')\, \mathrm{Cov}(Z_i, Z_j) \overset{1(i=j)}{=} \sum_{i=1}^{n} f_i(s) f_i(s')$$

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

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

Note 11. Prop 12 uses the experience from basis functions, while Theorem 30 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 $n \in \mathbb{N}$ and for any finite set $\{s_1, ..., s_n; s_i \in \mathcal{S}\}$, 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. When using the GP as a model we may need to parameterize its parameters. An example of mean functions are polynomial expansions, such as $\mu(s) = \sum_{j=0}^{p-1} \beta_j s^j$ for some tunable unknown parameter β. Some examples of covariance functions (c.f.), for some tunable unknown parameter β,σ^2 are

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

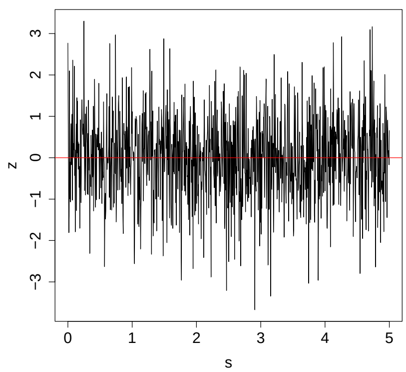
Example 18. Recall your linear regression lessons where you specified a sampling distribution $y_x|\beta, \sigma^2 \overset{\text{ind}}{\sim} \mathrm{N}\left(x^\top \beta, \sigma^2\right)$, $\forall x \in \mathbb{R}^d$; well that can be considered as a GP with $\mu_x = x^\top \beta$ and $c(x, x') = \sigma^2 1(x = x')$ in (3).

Example 19. Figs. 3.1 & 3.2 presents realizations of GRF $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$ with $\mu(s) = 0$ and differently parameterized covariance functions in 1D and 2D. In 1D the code to simulate the GP is given in Algorithm 1. Note that we actually discretize it and simulate it from the fidi.

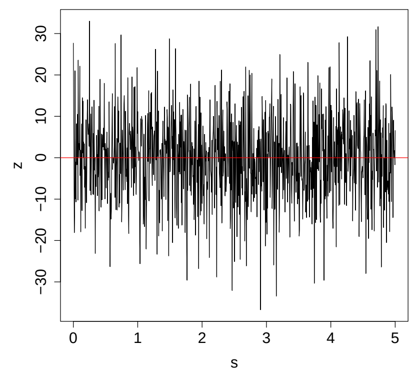
Algorithm 1 R script for simulating from a GP $(Z_s; s \in \mathbb{R}^1)$ with $\mu(s) = 0$ and $c(s,t) = \sigma^2 \exp\left(-\beta \|s-t\|_2^2\right)$

```
# set the GP parameterized mean and covariance function
mu_fun <- function(s) { return (0) }
cov_fun_gauss <- function(s,t,sig2,beta) { return (
sig2*exp(-beta*norm(c(s-t),type="2")**2) ) }
# discretize the problem in n = 100 spatial points
n <- 100
s_vec <- seq(from = 0, to = 5, length = n)
mu_vec <- matrix(nrow = n, ncol = 1)
Cov_mat <- matrix(nrow = n, ncol = n)
# compute the associated mean vector and covariance matrix of the n=100 dimensional
Normal r.v.
sig2_val <- 1.0 ;
beta_val <- 5
for (i in 1:n) {
    mu_vec[i] <- mu_fun(s_vec[i])
    for (j in 1:n) {
        Cov_mat[i,j] <- cov_fun_gauss(s_vec[i],s_vec[j],sig2_val,beta_val)
    }
}
# simulate from the associated distribution
z_vec <- mu_vec + t(chol(Cov_mat))%*%rnorm(n, mean=0, sd=1)
# plot the path (R produces a line plot)
plot(s_vec, z_vec, type="l")
abline(h=0,col="red")
```

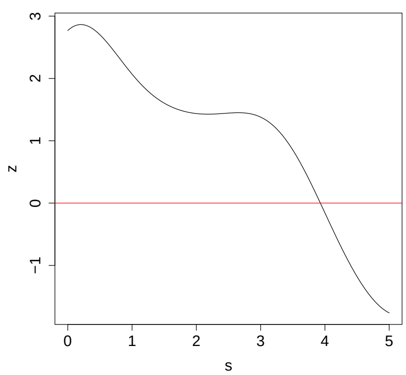
Nugget c.f. is the usual noise where the height of ups and downs are random and controlled by σ^2 (Fig. 3.1a & 3.1b ; Fig. 3.2a & 3.2b). In Gaussian c.f. the height of ups and downs are random and controlled by σ^2 (Fig.3.1c & 3.1d ; Fig. 3.2c & 3.2d), and the spatial dependence / frequency of the ups and downs is controlled by β (Fig. 3.1d & 3.1e ; Fig. 3.2d & 3.2e). Realizations with different c.f. have different behavior (Fig. 3.1a, 3.1d & 3.1e ; Fig. 3.2a, 3.2d & 3.2e)



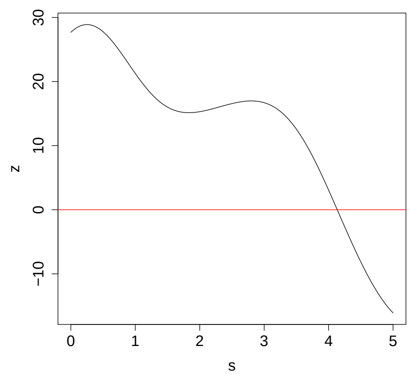
(A) Nugget c.f
($\sigma^2 = 1$)



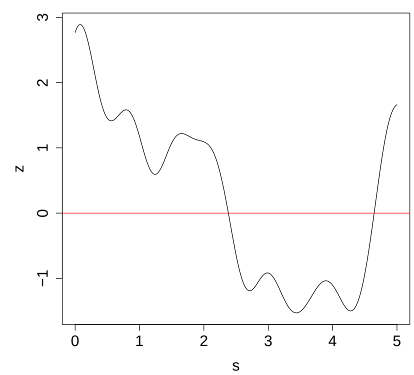
(B) Nugget c.f
($\sigma^2 = 100$)



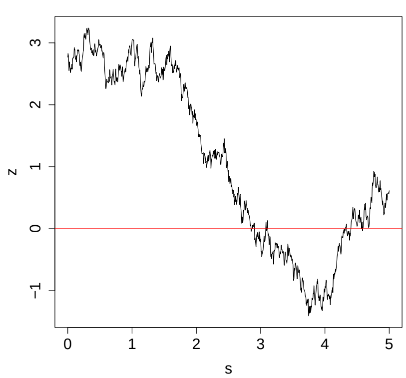
(C) Gauss c.f
($\sigma^2 = 1$,$\beta = 0.5$)



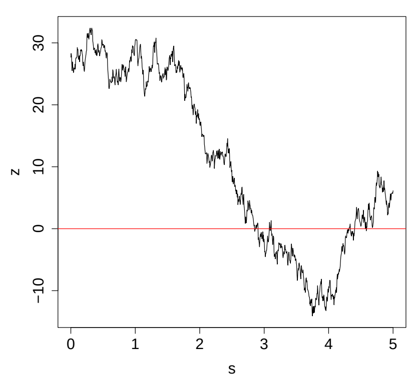
(D) Gauss c.f
($\sigma^2 = 100$,$\beta = 0.5$)



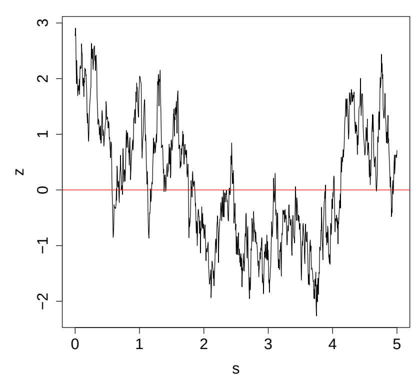
(E) Gauss c.f
($\sigma^2 = 1$,$\beta = 5$)



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

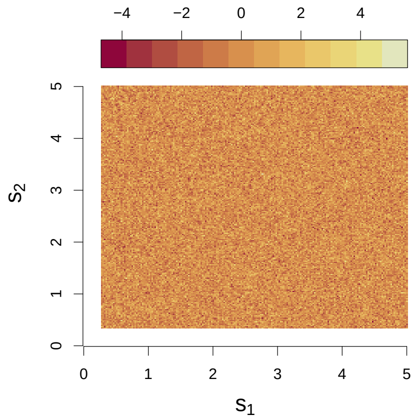


(G) Exp c.f
($\sigma^2 = 100$,$\beta = 0.5$)

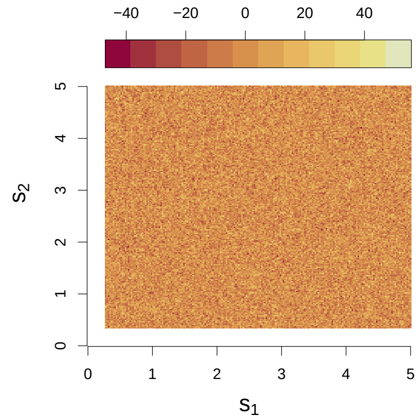


(H) Exp c.f
($\sigma^2 = 1$,$\beta = 5$)

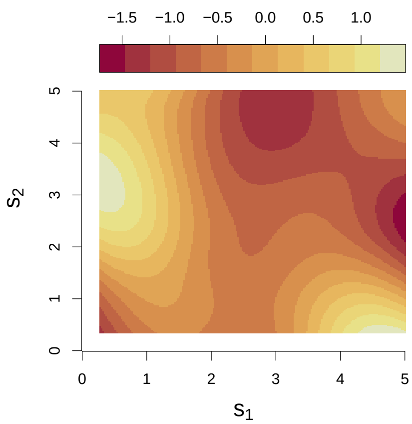
FIGURE 3.1. Realizations of GRF $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$ when $s \in [0,5]$ (using same seed)



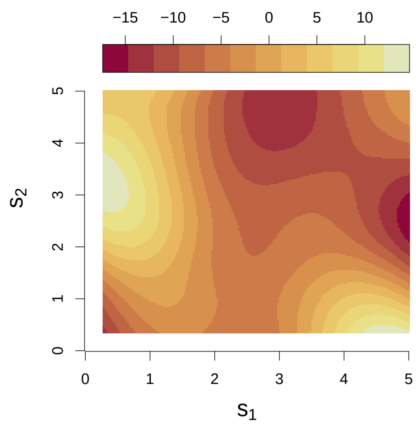
(A) Nugget c.f
($\sigma^2 = 1$)



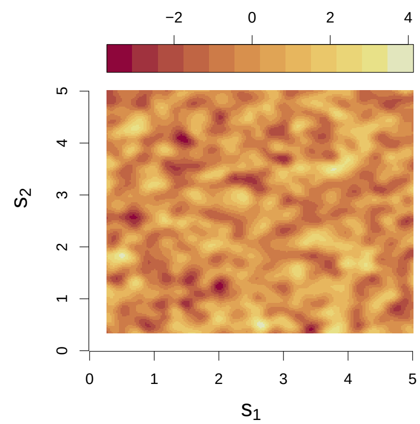
(B) Nugget c.f
($\sigma^2 = 100$)



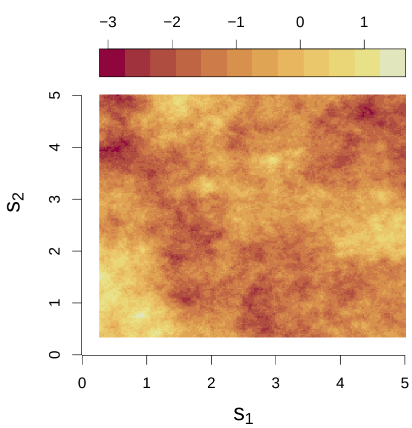
(C) Gauss c.f
($\sigma^2 = 1, \beta = 0.5$)



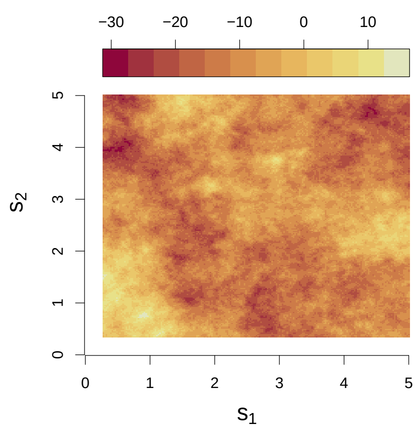
(D) Gauss c.f
($\sigma^2 = 100, \beta = 0.5$)



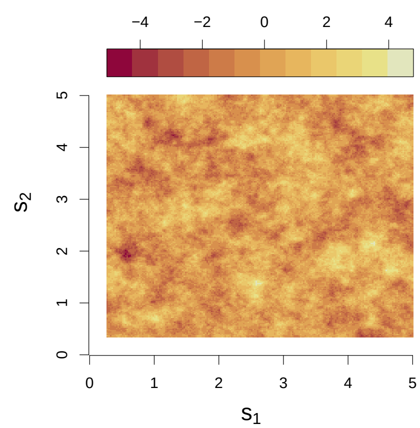
(E) Gauss c.f
($\sigma^2 = 1, \beta = 5$)



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



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



(H) Exp c.f
($\sigma^2 = 1, \beta = 5$)

FIGURE 3.2. Realizations of GRF $Z(\cdot) \sim \mathcal{GP}(\mu(\cdot), c(\cdot,\cdot))$ when $s \in [0,5]^2$ (using same seed)

4. Strong stationarity

Note 20. Assume $\mathcal{S} = \mathbb{R}^d$ for simplicity. [1]

Definition 21. 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 22. 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. 21 implies that, given $\mathrm{E}\left(Z_s^2\right) < \infty$, it is $\mathrm{E}\left(Z_s\right) = \mathrm{E}\left(Z_{s+h}\right) =$ contst... and $\mathrm{Cov}\left(Z_s, Z_{s'}\right) = \mathrm{Cov}\left(Z_{s+h}, Z_{s'+h}\right) \overset{h=-s'}{=} \mathrm{Cov}\left(Z_{s-s'}, Z_0\right) =$ funct of lag...

Definition 23. 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 24. Weakly (or second order) stationary covariance function is called the c.f. of a weakly stationary stochastic process.

6. Covariogram

Note 25. The definition of the covariogram function requires the random field to be weakly stationary.

Definition 26. 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 27. For the Gaussian c.f. $c\left(s, t\right) = \sigma^2 \exp\left(-\beta \left\|s - t\right\|_2^2\right)$ in (Ex. 17(2)), we may denote just

$$c\left(h\right) = c\left(s, s + h\right) = \sigma^2 \exp\left(-\beta \left\|h\right\|_2^2\right) \tag{6.1}$$

Observe that, in Figs 3.1 &3.2, the smaller the β, the smoother the realization (aka slower changes). One way to justify this observation is to think that smaller values of β essentially bring the points closer by re-scaling spatial lags $h$in the c.f.

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

Proposition 28. *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) $c(0) \geq 0$

(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 29. The following helps in the specification of cavariograms by considering properties of characteristic functions.

Theorem 30. *(Bochner's theorem) A continuous even real-valued function $c : \mathbb{R}^d \to \mathbb{R}$ is a covariance function of a weakly stationary random process if and only if it can be represented as*

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

where $\mathrm{d}F(\omega)$ is a *symmetric positive finite measure on* $\mathbb{R}^d$.

- *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 31. *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 32. Consider the Gaussian c.f. $c\left(h\right)=\sigma^{2}\exp\left(-\beta\left\Vert h\right\Vert _{2}^{2}\right)$ for $\sigma^{2},\beta>0$ and $h\in\mathbb{R}^{d}$. Then the spectral density from Thm 30 is

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

i.e. of a Gaussian form.

7. Intrinsic stationarity

Note 33. 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 23 implies that $\mathrm{Var}\left(Z_{s+h}-Z_{s}\right)=\mathrm{Var}\left(Z_{s+h}\right)+\mathrm{Var}\left(Z_{s}\right)-2\mathrm{Cov}\left(Z_{s+h},Z_{s}\right)=2c\left(0\right)-2c\left(h\right)$.

Definition 34. 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 $\gamma:\mathbb{R}^{d}\rightarrow\mathbb{R}$ (lag dependent)

Definition 35. Intrinsically stationary covariance function is called the c.f. of an intrinsically stationary stochastic process.

Example 36. The following covariance function is not weakly but intrinsically stationary

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

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

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

and

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

Note 37. 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 38. Let $Z = (Z_s)_{s\in\mathbb{R}^d}$ be intrinsically stationary. The semi-variogram of Z is defined by $\gamma : \mathbb{R}^d \to \mathbb{R}$ with

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

Definition 39. Variogram of an intrinsically stationary random field is called the quantity $2\gamma(h)$.

Note 40. Let $Z = (Z_s)_{s\in\mathbb{R}^d}$ be weakly stationary with covariogram $c(\cdot)$. Then Z is intrinsic stationary with semi-variogram

$$\gamma(h) = c(0) - c(h), \ \ \forall h \in \mathbb{R}^d \tag{8.1}$$

Example 41. For the Gaussian covariance function (Ex. 27) the semi-variogram is

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

Proposition 42. *Properties of semi-variogrames. Let $Z = (Z_s)_{s\in\mathbb{R}^d}$ be an intrinsically stationary process.*

1. *It is $\gamma(h) = \gamma(-h)$, $\gamma(h) \geq 0$, and $\gamma(0) = 0$*
2. *Semi-variogram is conditionally negative definite (c.n.d.): for all $a \in \mathbb{R}^n$ s.t. $\sum_{i=1}^n a_i = 0$, and for all $\forall\{s_1, ..., s_n\} \subseteq S$*
$$\sum_{i=1}^n\sum_{j=1}^n a_i a_j \gamma(s_i - s_j) \leq 0$$
3. *If $\gamma(h)$ is a semi-variogram, and A is a linear transformation in $\mathbb{R}^d$ then $\tilde{\gamma}(h) = \gamma(Ah)$ is a semi-variogram too.*
4. *The following functions are semi-variograms*
   (a) *$\gamma(\cdot) = \sum_{i=1}^n a_i\gamma_i(\cdot)$, if $a_i \geq 0$, and $\{\gamma_i(\cdot)\}$ are semi-variograms*
   (b) *$\gamma(\cdot) = \int \gamma_u(\cdot)\,dF(u)$, if $\gamma_u(\cdot)$ is a semi-variogram parametrized by $u \sim F$*
   (c) *$\gamma(\cdot) = \lim_{n\to\infty}\gamma_n(\cdot)$ if $\gamma_n(\cdot)$ is semi-variogram and the limit exists*
5. *Consider intrinsically stationary stochastic processes $Y = (Y_s)_{s\in\mathbb{R}^d}$ and $E = (E_s)_{s\in\mathbb{R}^d}$ where Y and E are independent each other. Let $Z_s = Y_s + E_s$. Then*
$$\gamma_Z(h) = \gamma_Y(h) + \gamma_E(h)$$

8.1. **Behavior of variogram (Nugget effect, Sill, Range).** The variogram $\gamma(h)$ is very informative when plotted against the lag h, below we discuss some of the characteristics of it, using Fig. 8.1

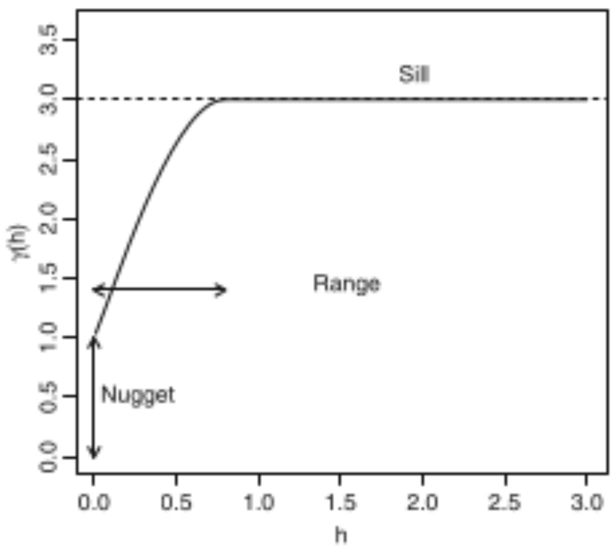


FIGURE 8.1. Variogram's characteristics

Note 43. A semivariogram tends to be an increasing function of the lag $\|h\|$. Recall in weakly stationary processes, $\gamma(h) = c(0) - c(h)$ where common logic suggests that $c(h)$ is decreases with $\|h\|$.

Note 44. If $\gamma(h)$ is a positive constant for all lags $h \neq 0$, then $Z(s_1)$ and $Z(s_2)$ are uncorrelated regardless of how close $s_1$and s_2 are; and $Z = (Z_s)_{s\in\mathbb{R}^d}$ is often called white noise.

Note 45. Conversely, a non zero slope of the variogram indicates structure.

Nugget Effect.

Note 46. Nugget effect is the semivariagram's limiting value

$$\sigma_\varepsilon^2 = \lim_{\|h\|\to 0} \gamma(h)$$

In particular when $\sigma_\varepsilon^2 \neq 0$.

Note 47. Nugget effect $\sigma_\varepsilon^2 \neq 0$ may expected or assumed to appear due to (1) measurement errors (e.g., if we collect repeated measurements at the same location s) or (2) due to some microscale variation causing discontinuity in the origin that cannot be detected from the data i.e. the spatial gaps because we collect a finite set of measurements at spatial locations. Hence theoretically, we could consider a more detailed decomposition $\sigma_\varepsilon^2 = \sigma_{\text{MS}}^2 + \sigma_{\text{MS}}^2$ where σ_{MS}^2 refers to the microscale and σ_{MS}^2 refers to the measurement error; however (my experience) this is non-identifiable.

Note 48. For a continuous processes $Z = (Z_s)_{s\in\mathbb{R}^d}$, it is expected

$$\lim_{\|h\|\to 0} \mathrm{E}\left(Z_{s+h} - Z_s\right)^2 = 0$$

which is equivalent to a continuous semivariagram $\gamma(h)$ for all h, and in particular, $\lim_{\|h\|\to 0}\gamma(h) = \gamma(0) = 0$, because $\gamma(0) = 0$. However, when modeling a real problem we may need to consider (or it may appear from the data) that $\gamma(h)$ should have a discontinuity $\lim_{\|h\|\to 0}\gamma(h) = \sigma_\varepsilon^2 \neq 0$.

Note 49. Nugget effect is often mathematically described by considering a decomposition ;

$$Z(s) = Y(s) + \varepsilon(s) \tag{8.2}$$

where Y can be a continuous stationary process with $\gamma_Y(\cdot)$, and ε can be a process (called errors-in-variables model) with (nugget) semivariogram $\gamma_\varepsilon(h) = \sigma_\varepsilon^2 1(h \neq 0)$. In this case,

$$\gamma_Z(h) = \gamma_Y(h) + \gamma_\varepsilon(h) \overset{\|h\|\to 0}{\to} \sigma_\varepsilon^2$$

Sill.

Definition 50. Sill is the variogram's limiting value $\lim_{\|h\|\to\infty}\gamma(h)$.

Note 51. For weakly stationary processes the sill is always finite. However, for intrinsic processes, the sill may be infinite.

Partial sill.

Definition 52. Partial sill is $\lim_{\|h\|\to\infty}\gamma(h) - \lim_{\|h\|\to 0}\gamma(h)$ which takes into account the nugget.

Range. Range is the distance at which the semivariogram reaches the Sill; it can be infinite.
Other.

Note 53. An abrupt change in slope indicates the passage to a different structuration of the values in space. This is often modeled via decompoditions of processes with different semivariograms as in (8.2).

9. Isotropy

Note 54. Isotropy as a notion imposes the assumption of "rotation invariance" in the stochastic process.

Definition 55. An intrinsic stochastic process $(Z_s)_{s\in\mathbb{R}^d}$ is isotropic iff

$$\forall s,t \in \mathcal{S},\ \frac{1}{2}\mathrm{Var}(Z_s - Z_t) = \gamma(\|t-s\|),\ \text{for some function } \gamma:\mathbb{R}^+ \to\mathbb{R}. \tag{9.1}$$

Definition 56. Isotropic semi-variogram $\gamma:\mathbb{R}^d \to \mathbb{R}$ is the semi-variogram of the isotropic stochastic process. (sometimes for simplicity of notation we use $\gamma:\mathbb{R}^+ \to \mathbb{R}$ with $\gamma(\|h\|) = \frac{1}{2}\mathrm{Var}(Z_s - Z_{s-h})$.

Definition 57. Isotropic covariance function $C : \mathcal{S}\times\mathcal{S} \to \mathbb{R}$ is called the covariance function satisfying (9.1).

Definition 58. Isotropic covariogram $c : \mathbb{R}^d \to \mathbb{R}$ of a weakly stationary process is the covariogram associated to an isotropic semi-variogram (sometimes for simplicity of notation we use $c : \mathbb{R}^+ \to \mathbb{R}$ with $c(\|h\|)$ from (9.1)).

9.1. Parametric forms of frequently used isotropic covariance functions.

Note 59. Given the covariogram $c(\cdot)$, and the semi-variogram can be computed from $\gamma(h) = c(0) - c(h)$ for any h.

9.1.1. *Nugget-effect.* For $\sigma^2 > 0$,

$$c(h) = \sigma^2 1_{\{0\}}(\|h\|).$$

It is associate to white noise. It is used to model a discontinuity in the origin of the covariogram / sem-variogram.

9.1.2. *Matern c.f.* For $\sigma^2 > 0$, $\phi > 0$, and $\nu \geq 0$

$$c(h) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\|h\|}{\phi}\right)^{\nu} K_{\nu}\left(\frac{\|h\|}{\phi}\right)$$

Parameter ν controls the variogram's regularity at 0 which in turn controls the quadratic mean (q.m.) regularity of the associated process. For $\nu = 1/2$, we get the exponential c.f.,

$$c(h) = \sigma^2 \exp\left(-\frac{1}{\phi}\|h\|_1\right)$$

which is not differentiable at $h = 0$, while for $\nu \to \infty$, we get the Gaussian c.f.

$$c(h) = \sigma^2 \exp\left(-\frac{1}{\phi}\|h\|_2^2\right)$$

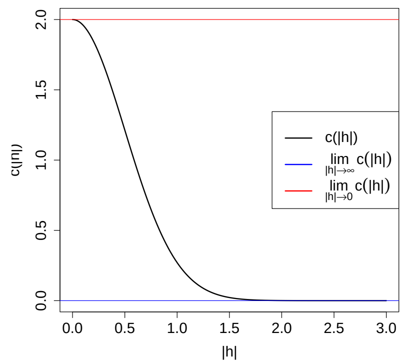
which is infinite differentiable. ϕ is a range parameter, and σ^2 is the (partial) sill parameter.

9.1.3. *Spherical c.f.* [2]For $\sigma^2 > 0$ and $\phi > 0$

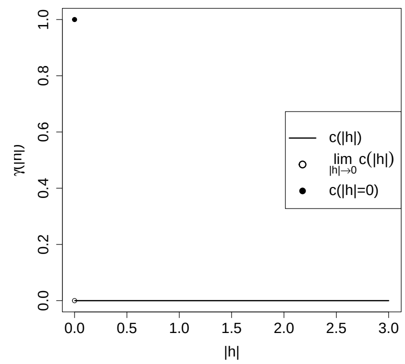
$$c(h) = \begin{cases} \sigma^2\left(1 - \frac{3}{2}\frac{\|h\|_1}{\phi} + \frac{1}{2}\left(\frac{\|h\|_1}{\phi}\right)^3\right) & \|h\|_1 \leq \phi \\ 0 & \|h\|_1 > \phi \end{cases}, \quad h \in \mathbb{R}^3. \tag{9.2}$$

The c.f. starts from its maximum value σ^2 at the origin, then steadily decreases, and finally vanishes when its range ϕ is reached. ϕ is a range parameter, and σ^2 is the (partial) sill parameter.

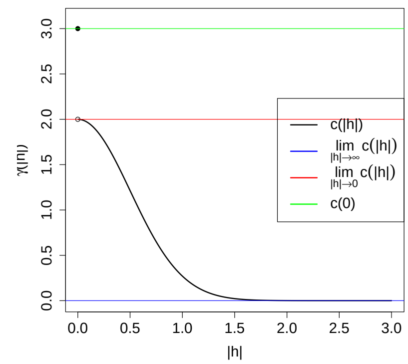
[2]For it's derivation see Ch 8 in [3]



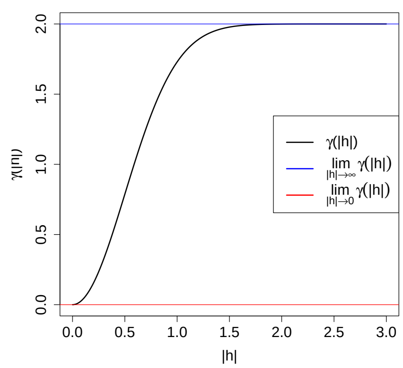
(A) $c_{\text{Gauss}}\left(\cdot\right)$



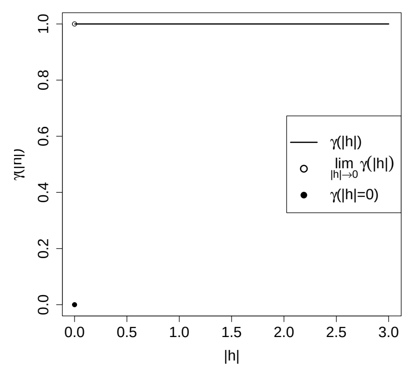
(B) $c_{\text{Nugget}}\left(\cdot\right)$



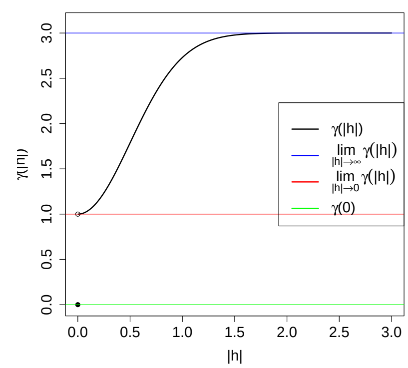
(C) $c_{\text{Gauss}}\left(\cdot\right) + c_{\text{Nugget}}\left(\cdot\right)$



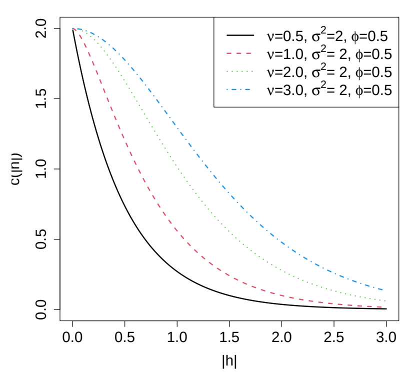
(D) $\gamma_{\text{Gauss}}\left(\cdot\right)$



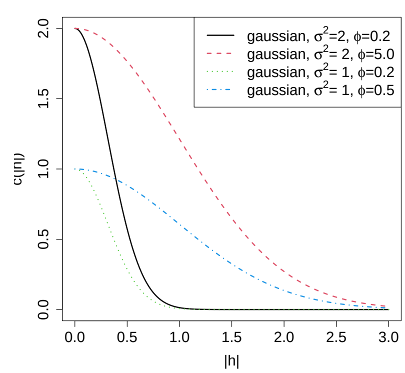
(E) $\gamma_{\text{Nugget}}\left(\cdot\right)$



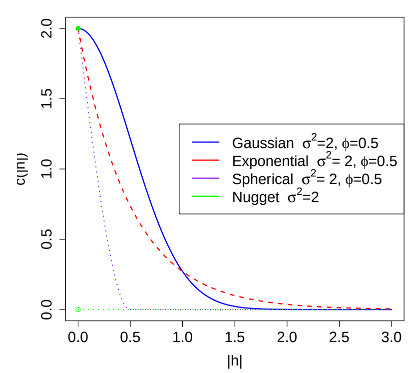
(F) $\gamma_{\text{Gauss}}\left(\cdot\right) + \gamma_{\text{Nugget}}\left(\cdot\right)$



(G) c_{Matern}

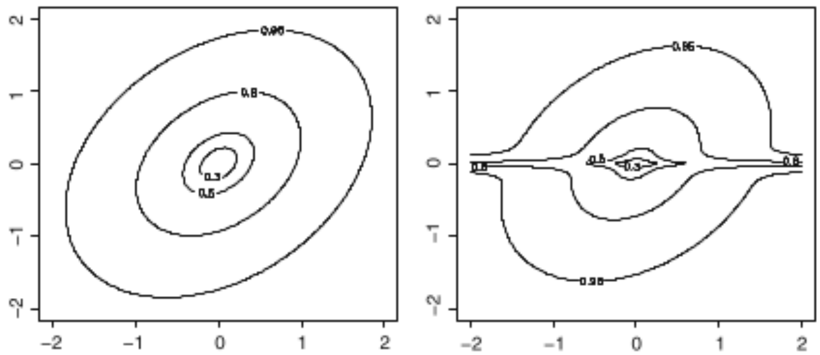


(H) $c_{\text{Gauss}}\left(\cdot;\sigma^2,\phi\right)$



(I) $c_{\cdot}\left(\cdot\right)$

FIGURE 9.1. Covariogrames $c\left(\cdot\right)$ and semivariogrames $\gamma\left(\cdot\right)$



(A) Geometric anisotropy

(B) Zonal anisotropy

FIGURE 10.1. Isotropy vs Anisotropy

10. ANISOTROPY

Note 60. Dependence between $Z(s)$ and $Z(s+h)$ is a function of both the magnitude and the direction of separation h. This can be caused by the underlying physical process evolving differently in space (e.g., vertical and horizontal axes).

Definition 61. The variogram $\gamma : \mathbb{R}^d \to \mathbb{R}$ is anisotropic if there are h_1 and h_2 with same length $\|h_1\| = \|h_2\|$ but different direction $h_1/\|h_1\| \neq h_2/\|h_2\|$ that produce different variograms $\gamma(h_1) \neq \gamma(h_2)$.

Definition 62. The intrinsically stationary process $(Z_s)_{s\in\mathbb{R}^d}$ is anisotropic if its variogram is anisotropic.

Definition 63. The covariogram $c : \mathbb{R}^d \to \mathbb{R}$ is anisotropic if there are h_1 and h_2 with same length $\|h_1\| = \|h_2\|$ but different direction $h_1/\|h_1\| \neq h_2/\|h_2\|$ that produce different covariogram $c(h_1) \neq c(h_2)$.

Definition 64. The weakly stationary process $(Z_s)_{s\in\mathbb{R}^d}$ is anisotropic if its covariogram is anisotropic.

Note 65. For brevity, below we discuss about intrinsically stationary process and variograms, however the concepts/definitions apply to weakly stationary process and covariograms when defined, as in Defs 61 & 63.

10.1. **Geometric anisotropy.**

Definition 66. The semi-variogram $\gamma_{\text{g.a.}} : \mathbb{R}^d \to \mathbb{R}$ exhibits geometric anisotropy if it results from an A-linear deformation of an isotropic semi-variogram with function $\gamma_{\text{iso}}(\cdot)$; i.e.

$$\gamma_{\text{g.a.}}(h) = \gamma_{\text{iso}}(\|Ah\|_2)$$

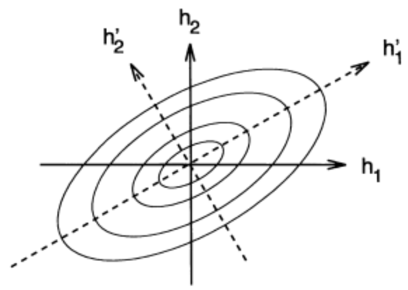


FIGURE 10.2. Rotation of the 2D coordinate system

Note 67. Such variograms have the same sill in all directions but with ranges that vary depending on the direction. See Fig 10.1a.

Example 68. For instance, if $\gamma_{\text{g.a.}}(h) = \gamma_{\text{iso}}\left(\sqrt{h^\top Q h}\right)$, where $Q = A^\top A$.

Example 69. [Rotating and dilating an ellipsoid in 2D] Consider a coordinate system for $h = (h_1, ..., h_n)^\top$. We wish to find a new coordinate system for h in which the iso-variogram lines are spherical.

(1) [Rotate] Apply rotation matrix R to h such as $h' = Qh$. In 2D, it is

$$R = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}, \quad \text{for } \theta \in (0, 2\pi), \text{ is the rotation angle.}$$

(2) [Dilate] Apply a dilation of the principal axes of the ellipsoid using a diagonal matrix $\sqrt{\Lambda} = \text{diag}\left(\sqrt{\lambda_1}, ..., \sqrt{\lambda_n}\right)$, as $\tilde{h} = \sqrt{\Lambda} h'$.

Now the ellipsoids become spheres with radius $r = \left\|\tilde{h}\right\|_2 = \sqrt{\tilde{h}^\top \tilde{h}}$. This yields the equation of an ellipsoid in the h coordinate system

$$h^\top \left(R^\top \Lambda R\right) h = r^2$$

where the diameters d_j (principal axes) of the ellipsoid along the principal directions are

$$d_j = 2r/\sqrt{\lambda_j}$$

and the principal direction is the j-th column of the rotation matrix $R_{:,j}$.

Hence the anisotropic semivariogram is $\gamma_{\text{g.a.}}(h) = \gamma_{\text{iso}}\left(\sqrt{h^\top Q h}\right)$ with $Q = R^\top \Lambda R$. This derivation extends to d dimensions.

10.2. **Zonal (or stratified) anisotropy.**

Definition 70. Support anisotropy is called the type of anysotropy when the semi-variogram $\gamma(h)$ of the process depends only on certain coordinates of h.

Example 71. If it is $\gamma(h = (h_1, h_2)) = \gamma(h_1)$, then I ve support anisotropy

Definition 72. Zonal anisotropy occurs when the semi-variogram $\gamma(h)$ is the sum of several components each with a support anisotropy.

Example 73. Let γ' and γ'' be semi-variograms. If it is $\gamma(h = (h_1, h_2)) = \gamma'(\|h_1\|) + \gamma''\left(\sqrt{\|h_1\| + \|h_2\|}\right)$, then I 've Zonal anisotrotropy.

Note 74. We have Zonal anisotropy then the variograms calculated in different directions suggest a different value for the sill (and possibly the range).

Note 75. If in 2D case, the sill in h_1 is larger than that in h_2, we can model zonal anysotropy of stochastic process (Z_s) by assuming $Z(s) = I(s) + A(s)$, where $I(s)$ is an isotropic process with isotropic semi-variogram γ_I along dimension of h_1 and $A(s)$ is an process with anisotropic semi-variogram γ_I without effect on dimension h_1; i.e. $\gamma_Z(h) = \gamma_I(h) + \gamma_A(h)$.

10.3. **Non-linear deformations.**

Note 76. A (rather too general) non-stationary model can be specified by considering semi-variogram $2\text{Var}(Z(s) - Z(t)) = 2\gamma_o(\|G(s) - G(t)\|)$ where we have performed a bijective non-linear (function) deformation $G(\cdot)$ of space $\mathcal{S}$ and applied on the isotropic semi-variogram γ_o. For instance, $\gamma_o(h) = \sigma^2 \exp(-\|h\|/\phi)$ and $G(s) = s^2$ as a deterministic function. Now, if function $G(\cdot)$ is considered as unknown, one can model it as a stochastic process $(G_s)_{s\in\mathcal{S}}$, and then we will be talking about deep learning modeling stuff.

11. Geometrical properties

(!): We discuss basic geometric properties of the basic models we will use for modeling, as it can give us a deeper intuition on how to design appropriate spatial statistical models.

Definition 77. (Continuity in quadratic mean (q.m.)) Second-order process $Z = (Z_s)_{s\in S}$ is q.m. continuous at $s \in \mathcal{S}$ if

$$\lim_{h\to 0} \mathrm{E}(Z(s+h) - Z(s))^2 = 0.$$

Proposition 78. *For $Z = (Z_s)_{s\in S}$ it is*

$$E(Z(s+h) - Z(s))^2 = (E(Z(s+h)) - E(Z(s)))^2 + Var(Z(s+h) - Z(s))$$

- *If Z is intrinsically stationary, then*

$$E(Z(s+h) - Z(s))^2 = \frac{1}{2}\gamma(h)$$

  and hence q.m. continuous iff $\lim_{h\to 0}\gamma(h) = \gamma(0)$.
- *If Z is weakly stationary, then*

$$E(Z(s+h) - Z(s))^2 = \frac{1}{2}(c(0) - c(h))$$

and hence q.m. continuous iff $\lim_{h\to 0} c(h) = c(0)$ *(i.e. ,c is continuous).*

Note 79. It has been shown that if a random field $Z = (Z_s)_{s\in S}$ has a variogram which is everywhere continuous apart from the origin i.e. $\lim_{s\to 0} \gamma(s) \neq \gamma(0)$ then Z it can be represented as $Z_s = Y_s + \varepsilon_s$ where (Y_s) has everywhere a continuous variogram and (ε_s) has a nugget effect, and Y_s, ε_s are independent. [2; Ch 1.4.1]

Definition 80. Differentiable in quadratic mean (q.m.)) Second-order process $Z = (Z_s)_{s\in\mathbb{R}}$ is q.m. differentiable at $s \in \mathbb{R}$ there exist

$$\dot{Z}(s) = \lim_{h\to 0} \frac{Z(s+h) - Z(s)}{h}. \text{ in } q.m. \tag{11.1}$$

Proposition 81. *Let* $c(s,t)$ *be the covariance function of* $Z = (Z_s)_{s\in S}$ *. Then* Z *is everywhere differentiable if* $\frac{\partial^2}{\partial s \partial t} c(s,t)$ *exists and it is finite. Also,* $\frac{\partial^2}{\partial s \partial t} c(s,t)$ *is the covariance function of (11.1).*

Example 82. The process with Gaussian c.f. $c(h) = \sigma^2 \exp(-|h|/\phi)$ is continuous because $\lim_{h\to 0} c(h) = \sigma^2 = c(0)$ but not differentiable because $\frac{\partial^2}{\partial h^2} c(h)$ does not exist at $h = 0$.

12. The Geostatistical model

12.1. **Linear Model of Regionalization.** A spatial phenomenon can be thought as being the sum of several independent subphenomena acting at different characteristic scales. A linear model can be set up to splits the stochastic process representing the phenomenon into several uncorrelated stochastic processes, each with a different variogram or covariance function and characterizing different aspect of the overall phenomenon under investigation. Decomposition of the stochastic process.

Note 83. The linear model of regionalization consider the decomposition of the stochastic process of interest $Z(s)$ as a summation of m independent zero-mean stochastic processes $\{Z_j(s)\}_{j=0}^m$ each of them characterizing different spatial scales, as

$$Z(s) = \mu(s) + Z_1(s) + ... + Z_m(s) \tag{12.1}$$

with $\mu(s) = \mathrm{E}(Z(s))$ be a deterministic function.

Note 84. In (12.1), let $Z_j(\cdot)$ be intrinsically stationary with semi-variogram $\gamma_j(\cdot)$, then the semi-variogram of $Z(\cdot)$ is $\gamma(\cdot) = \sum_{j=1}^m \gamma_j(\cdot)$.

Example 85. For instance consider (12.1) with $\mu(s) = 0$, $m = 3$, $Z_1(s)$ with a spherical semi-variogram (9.2) with range $\phi_1 = 3.5$, $Z_2(s)$ with a spherical semi-variogram (9.2) with range $\phi_2 = 6.5$, and $Z_3(s)$ with a nugget semi-variogram. See the "sudden" changes of the line in Fig. 12.1 representing change of spatial behavior.

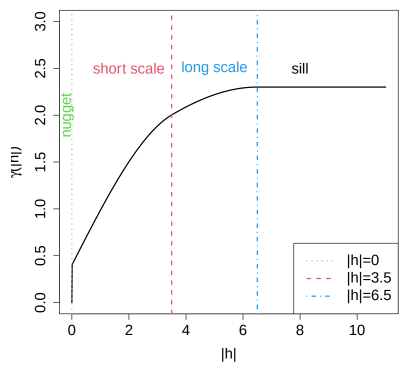


FIGURE 12.1. Variogram $\gamma(\cdot)$ of $Z(s) = Z_1(s) + Z_2(s) + Z_3(s)$ with spherical s.v. $\gamma_1\left(|h|;\sigma^2 = 0.8, \phi = 3.5\right)$, spherical s.v. $\gamma_1\left(|h|;\sigma^2 = 1.1, \phi = 6.5\right)$, and nugget $\gamma_3\left(|h|;\sigma^2 = 0.4\right)$.

12.2. Scale of variation.

Note 86. Cressi [1] Consider the following intuitive decomposition

$$Z(s) = \mu(s) + W(s) + \eta(s) + \varepsilon(s), \; s \in S \tag{12.2}$$

where

$\mu(s) = \mathbf{E}(Z(s))$: is the deterministic mean structure. It aims to represent the "large scale variation".

$W(s)$: is a zero mean second order continuous intrinsically stationary process whose range is larger than gaps between the sites (sampling grid). It aims to represent "smooth small scale variation".

$\eta(s)$: is a zero mean intrinsically stationary process whose variogram range exists and is smaller than the gaps between the sites. It aims to represent "microscale variation"

$\varepsilon(s)$: is a zero-mean white-noise process (modeled as nugget effect). It aims to represent "measurement error or noise"

$W(s)$, $\eta(s)$, $\varepsilon(s)$ are mutually independent.

Note 87. Reasonably, larger scale components, such as $\mu(s)$, $W(s)$ can represented in the variogram if the diameter of the sampling domain is large $\mathcal{S}$ is large enough.

Note 88. Clearly, smaller scale components, such as $\eta(s)$, $\varepsilon(s)$ could be identified if the sampling grid is sufficiently fine.

Note 89. Decomposition 86 is not unique and the components are not clearly identifiable from the data when modeled; e.g. one may find two pairs of $\mu(s), W(s)$ doign the same thing; yet, separating $\eta(s)$ and $\varepsilon(s)$ is difficult as they often describe changes with range smaller than that of the sites (!)

Note 90. The geostatistical model (decomposition) is often presented (with reference to (12.2)) as

$$Z(s) = \mu(s) + w(s) + \varepsilon(s), \ s \in S$$

where $w(s) = W(s) + \eta(s)$ contains all the spatial variation.

Note 91. Alternatively, the hierarchical statistical model (Handout 1, 3.5) is used

$$Z(s) = Y(s) + \varepsilon(s), \ s \in S$$

where $Y(s) = \mu(s) + W(s) + \eta(s)$ is the spatial process model, or latent process or signal process or noiseless process.

Note 92. A simpler decomposition is

$$Z(s) = \mu(s) + \delta(s), \ s \in S$$

where $\delta(s) = W(s) + \eta(s) + \varepsilon(s)$ is the called the correlated process.

13. Training & inference

Note 93. Suppose that the intrinsic stationary random field $(Z_s)_{s\in\mathcal{S}}$, $\mathcal{S} \in \mathbb{R}^d$ is observed at n sites $S = \{s_1, ..., s_n\}$, and we get n observed dataset $\{(s_i, Z(s_i))\}_{i=1}^{n}$.

Example 94. (Meuse river data set) The Meuse river dataset set, used as a running example gives locations and topsoil heavy metal concentrations, along with a number of soil and landscape variables at the observation locations, collected in a flood plain of the river Meuse, near the village of Stein (NL). Here, we use the topsoil zinc concentration, mg kg-1 soil ("ppm") as quantity of interest (Z). Heavy metal concentrations are from composite samples of an area of approximately 15m × 15m. See Fig. 13.1a. This is the R dataset `meuse{sp}`.

Example 95. (Wolfcamp-aquifer dataset) We also consider the Wolfcamp-aquifer dataset in Ex 5 in the Exercise sheet. See Fig. 13.2a

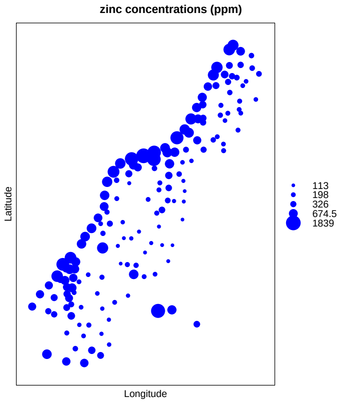
13.1. **The variogram cloud.**

Definition 96. Dissimilarity between pairs of data values $Z(s_a)$ and $Z(s_b)$ is called the measure

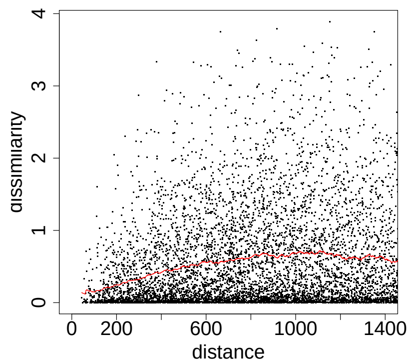
$$\gamma^\star(s_a, s_b) = \frac{1}{2}(Z(s_b) - Z(s_a))^2 \tag{13.1}$$

Definition 97. If we let dissimilarity between pairs of data values $Z(s)$ and $Z(s_b)$ depend on the separation $h = s_b - s$ (distance and orientation) then we get

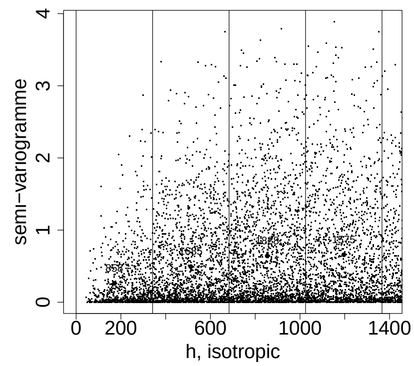
$$\gamma^\star(h) = \frac{1}{2}(Z(s+h) - Z(s))^2 .$$



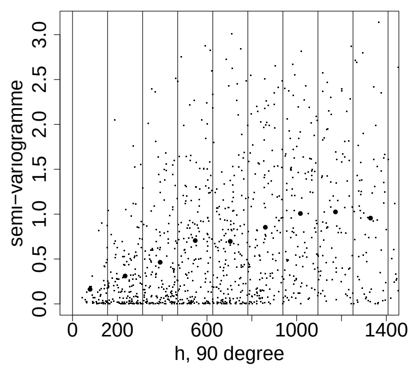
(A) Bubble plot of zinc (origial scale) vs location



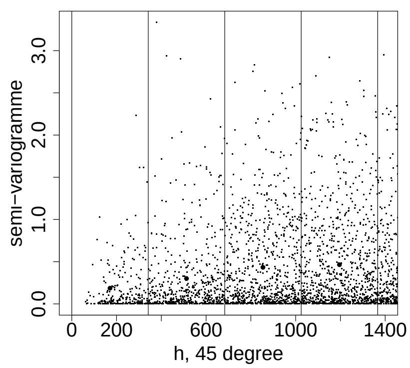
(B) Variogram cloud



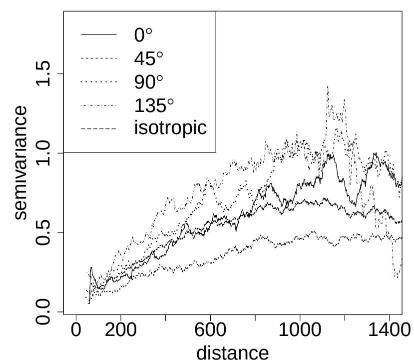
(C) Empirical estimate (isotropic)



(D) Empirical estimate (90°)



(E) Empirical estimate (45°)



(F) Empirical estimate (different directions)

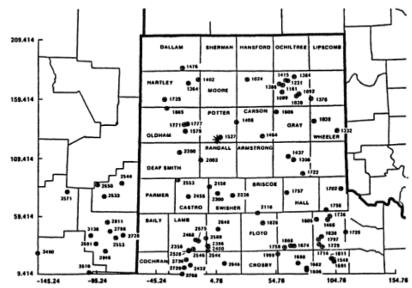
FIGURE 13.1. Meuse dataset variogram estimations (Zinc in log scale)

Definition 98. The variogram cloud is the set of $n(n-1)/2$ points

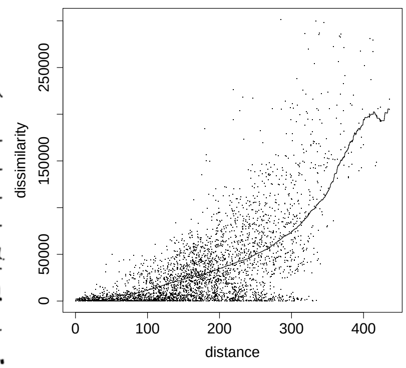
$$\mathfrak{C}_S = \{(\|s_i - s_j\|, \gamma^\star(s_j, s_i)),\ i, j = 1, ..., n, \text{ and } s_i \neq s_j\}$$

Note 99. Note that (13.1) is an unbiased estimator of the variogram and hence the variogram cloud is too.

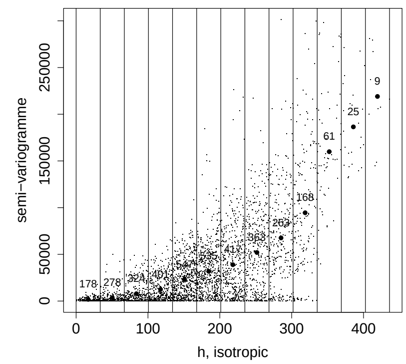
Note 100. Often there is a smoothing of the cloud is superimposed onto the cloud itself to help us see variogram's characteristics (e.g., sill, nugget, range) which may be "hidden" due to potential outliers in the plot.



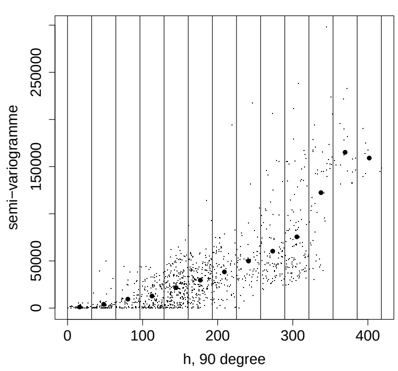
(A) Data



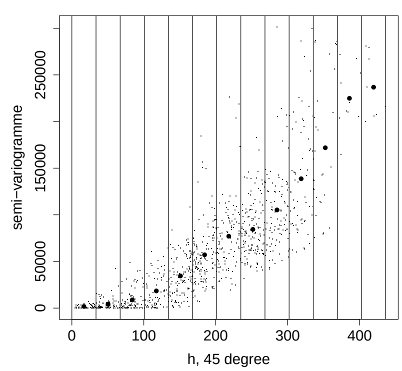
(B) Variogram cloud



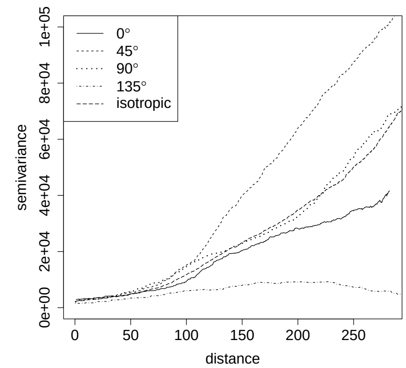
(C) Empirical estimate (isotropic)



(D) Empirical estimate (90°)



(E) Empirical estimate (45°)



(F) Empirical estimate (different directions)

FIGURE 13.2. Wolfcamp-aquifer dataset variogram estimations

Example 101. Fig. 13.1b and Fig. 13.2b show the variogram cloud plots (that is a point plot of the dissimilarities vs the distances) for the datasets Meuse and Wolfcamp-aquifer dataset. The red line is a smoother line of the cloud.

13.2. Non-parametric estimation of variogram.

Proposition 102. *Smoothed Matheron estimator* $\hat{\gamma}(\cdot)$ *of semi-variogram* $\gamma(\cdot)$ *is*

$$\hat{\gamma}_M(h) = \frac{1}{2\left|N_{r_1,r_2}(h)\right|} \sum_{\forall (s_i,s_j)\in N_{r_1,r_2}(h)} \left(Z(s_i) - Z(s_j)\right)^2 \tag{13.2}$$

where

$$N_{r_1,r_2}(h) = \left\{(s_i,s_j) \in \mathcal{S} : s_i - s_j \in B_{r_1,r_2}(h)\right\}$$

contains all the pairs of spatial points points whole difference is in a ball

$$B_{r_1,r_2}(h) = \left\{x : \left|\|x\| - \|h\|\right| < r_1, \text{ and } \left\|\frac{x}{\|x\|_2} - \frac{h}{\|h\|_2}\right\|_2 < r_2\right\} \tag{13.3}$$

centered at h with radius $r_1 > 0$ and $r_2 > 0$.

Note 103. Estimator 13.2 can be writen in matrix form as $\hat{\gamma}_{\mathrm{M}}(h) = Z^\top A(h) Z$, where $[A(h)]_{i,j} = 1(i \neq j) - 1/|N_{r_1,r_2}(h)|$ is a positive definite matrix.

Note 104. If we consider isotropic semi-variogram $\gamma(\cdot)$ then the ball may just considerate only the length of the distance as

$$B_{r_1}(h) = \{x : \left|\|x\| - \|h\|\right| < r_1\} \tag{13.4}$$

because the direction does not have any effect.

Note 105. The choice of r_1 , r_2 is an art, and a trade-off between variance and bias, similar to the bin length in histograms.

Note 106. In practice, we consider a finite number of k separations $\mathscr{H} = \{h_1, ..., h_k\}$, we estimate in such a way that each class contains at least 30 pairs of points. Then compute $\{\hat{\gamma}_{\mathrm{M}}(h); h \in \mathscr{H}\}$, and plot $\{(h_j, \hat{\gamma}_{\mathrm{M}}(h_j)); j = 1, ..., k\}$.

Example 107. Figs 13.1c and 13.2c, show the nonparametric estimator ignoring the direction for the datasets Meuse and Wolfcamp-aquifer dataset. The estimator is calculated by using the ball in (13.4).

Example 108. Figs 13.2dand 13.1e show the nonparametric estimator considering directions 90° and 45° for the dataset Meuse. Figs 13.2d and 13.2e do the same for the Wolfcamp-aquifer dataset. The estimator is calculated by using the ball (13.3).

Note 109. In practice anisotropies are detected by inspecting experimental variograms in different directions and are induced into the model by tuning predefined anisotropy parameters.

Example 110. Fig 13.1f and 13.2a show the nonparametric variogram estimator for different directions for the two datasets. We observe possible anisotropy due to the differences in the lines.

Proposition 111. *Assume a stationary Gaussian process $(Z_s \sim GP(0, c(\cdot,\cdot)))_{s\in\mathcal{S}}$ with semi-variogram $\gamma(\cdot) = c(0) - c(\cdot)$. The empirical semi-variogram $\hat{\gamma}_{\mathrm{M}}$* in *(13.2) is*

$$\hat{\gamma}_M(h) \sim \sum_{i=1}^{|N_{r_1,r_2}(h)|} \lambda_i \xi_i$$

where $\xi_i \overset{iid}{\sim} \chi^2_1$ and $\{\lambda_i\}$ are the non-zero eigen-values of $A(h)\,C$, $[C]_{i,j} = c(s_i, s_j)$.

Note 112. Estimation of the covariogram is done by

$$\hat{c}(h) = \frac{1}{2\,|N_{r_1,r_2}(h)|} \sum_{\forall (s_i,s_j)\in N_{r_1,r_2}(h)} \left(Z(s_i) - \bar{Z}\right)\left(Z(s_j) - \bar{Z}\right) \tag{13.5}$$

where $\bar{Z} = \frac{1}{n}\sum_{i=1}^{n} Z(s_i)$. It's sampling distribution etc. can be computed in a similar manner.

13.3. **Parametric estimation.**

Note 113. Smoothed Matheron estimator (13.2) does not necessarily satisfies semi-variogram properties, such as negative definiteness. To address this we use a parametric family of appropriate semi-variogram functions and tune them against data.

Note 114. Popular parametrized isotopic semi-variogrames/covariogrames are those Sec 9.1. Anisotropic semi-variogrames/covariogrames can be specified by using isotropic ones and applying a rotation and dilation as in Ex 68.

Proposition 115. *(Criteria checking variogram's validity.) A continuous function $2\gamma(\cdot)$ with $\gamma(0) = 0$ is a valid variogram iff: any of the following is satisfied:*

1. $\lim_{\|h\|\to\infty} \frac{\gamma(h)}{\|h\|^2} = 0$ *, or*
2. $\exp(-a\gamma(\cdot))$ *is positive definite for any $a > 0$.*

Example 116. Gaussian semi-variogram in Ex 41, it is

$$\lim_{\|h\|\to\infty} \frac{\gamma(h)}{\|h\|^2} = \lim_{\|h\|\to\infty} \frac{\sigma^2\left(1 - \exp\left(-\beta\,\|h\|_2^2\right)\right)}{\|h\|^2} = -\lim_{\|h\|\to\infty} \frac{\exp\left(-\beta\,\|h\|_2^2\right)}{\|h\|^2} = 0.$$

Yet $\gamma(h) = \|h\|^2$ is variogram as well because $\exp\left(-\beta\,\|h\|_2^2\right)$ is a c.f. and hence positive definite.

13.3.1. *Least Square Errors training methods for semi-variogram.*

Proposition 117. *(Least Square Errors) Consider that the empirical semivariogram $\hat{\gamma}$ (e.g., Matheron (13.2)) of γ have been computed at k classes, i.e. it is available $\{h_j, \hat{\gamma}(h_j)\}_{j=1}^{k}$. The Least Square Errors (LSE) estimator of $\gamma_\theta(h)$ parametrised by the unknown θ for all h is $\hat{\gamma}_{LSE}(h) = \gamma\left(h; \hat{\theta}_{LSE}\right)$, where*

$$\hat{\theta}_{LSE} = \arg\min_{\theta} \left(\hat{\gamma} - \gamma(h;\theta)\right)^\top V(\theta)\left(\hat{\gamma} - \gamma(h;\theta)\right), \tag{13.6}$$

$V(\theta)$ is a user specific positive definite matrix $V(\theta)$ serving as a weight, $\hat{\gamma} = (\hat{\gamma}(h_1), ..., \hat{\gamma}(h_k))^\top$, and $\gamma(h;\theta) = (\gamma(h_1;\theta), ..., \gamma(h_k;\theta))^\top$.

Proposition 118. *(Ordinary least squares) If use $V(\theta) = I$ in (13.6), we get the OLS $\hat{\gamma}_{OLS}(h) = \gamma\left(h; \hat{\theta}_{OLS}\right)$*

$$\hat{\theta}_{OLS} = \arg\min_{\theta} \left(\sum_{j} \left(\hat{\gamma}(h_j) - (h; \theta) \right)^2 \right)$$

Proposition 119. *(Weighted least squares) If use $V(\theta) = diag(\varpi_1(\theta), ..., \varpi_k(\theta))$ for some weight function $\{\varpi_j(\theta)\}$, we get the WLE $\hat{\gamma}_{WLE}(h) = \gamma\left(h; \hat{\theta}_{WLE}\right)$*

$$\hat{\theta}_{WLE} = \arg\min_{\theta} \left(\sum_{j} \varpi_j(\theta) \left(\hat{\gamma}(h_j) - \gamma_\theta(h_j) \right)^2 \right)$$

For instance $\varpi_j(\theta) = |N_r(h_j)|$ or $\varpi_j(\theta) = |N_r(h_j)| / (\gamma_\theta(h_j))^2$.

13.3.2. *Training methods for semi-variogram with trend.*

Note 120. Assume a stochastic process model (Z_s) decomposed as

$$Z(s) = \mu(s; \beta) + \delta(s; \theta)$$

where the trend $\mu(s; \beta)$ is parameterized by unknown β (e.g. $\mu(s; \beta) = s^\top \beta$), and the zero mean intrinsic process $\delta(s; \theta)$ has a semi-variogram $\gamma(h; \theta)$ parameterised by unknown θ.

Proposition 121. *(Least square errors with trend) Do the following:*

(1) Compute estimates $\hat{\beta}$ via LSE (or equivalent)

$$\hat{\beta}_{LSE} = \arg\min_{\theta} \left(\sum_{i} \left(Z(s_i) - \mu(s_i; \beta) \right)^2 \right)$$

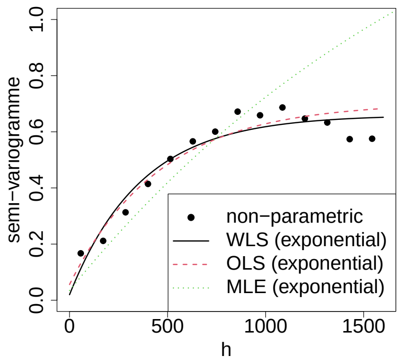
(2) Compute the residuals $\hat{\delta} := \hat{\delta}(s_i)$ from

$$\hat{\delta}(s_i) = Z(s_i) - \mu\left(s_i; \hat{\beta}_{LSE}\right)$$

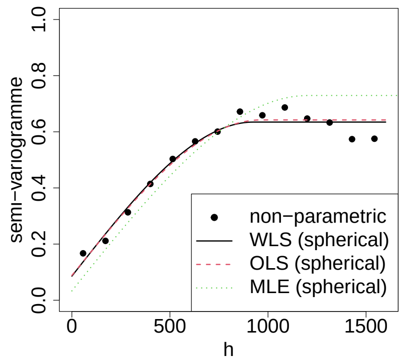
(3) Estimate the empirical variogram for $\hat{\delta}$ on $\mathscr{H}$ according to Prop 102, and estimate θ according to Prop 117.

Example 122. Fig 13.3a and 13.3b fit an exponential c.f. and a spherical c.f. in the data of Meuse dataset (assuming constant mean); we cannot eyeball any big difference. Fig 13.3c fit an exponential c.f. in the data of Wolfcamp dataset (assuming constant mean); the fit looks really bad, possibly we should consider a non-constant mean and remove the trend.

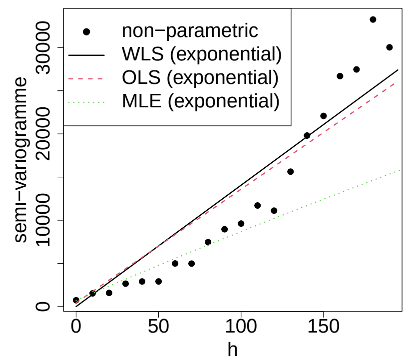
Example 123. Fig 13.3d fits an exponential c.f. in the residuals $\delta(s) = Z(s) - \mu(s)$ where $\mu(s) = \mu(s) = \beta_0 + \beta_1 s_1 + \beta_2 s_2$ and $\hat{\beta}_{\text{OLS}} = (-42.8, -9.5 \cdot 10^{-4}, -6.6 \cdot 10^{-4})^\top$in Meuse dataset. Possibly inference would suggest a constant mean function. Fig 13.3e fits an



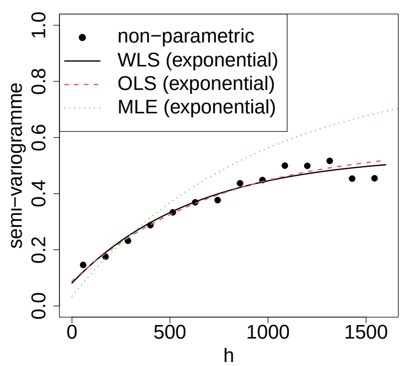
(A) Exponential c.f. with constant mean (Meuse dataset)



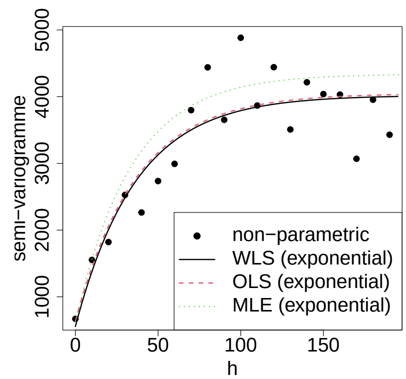
(B) Spherical c.f. with constant mean (Meuse dataset)



(C) Exponential c.f. with constant mean (Wolfcamp dataset)



(D) Exponential c.f. with linear trend (Meuse dataset)



(E) Exponential c.f. with linear trend (Wolfcamp dataset)

FIGURE 13.3. Parametric training

exponential c.f. in the residuals $\delta(s) = Z(s) - \mu(s)$ where $\mu(s) = \mu(s) = \beta_0 + \beta_1 s_1 + \beta_2 s_2$ and $\hat{\beta}_{\text{OLS}} = (-607, -1.12, -1.13)^{\top}$ in Wolfcamp dataset; we see an improvement in fit compared to Fig 13.3c.

13.4. **Training via Maximum likelihood estimation.**

Note 124. Given that a probability distribution has been specified for the stochastic process $(Z_s)_{s \in \mathcal{S}}$, the MLE involves the derivation of the associated n-dimensional pdf $\Pr(Z_1, ..., Z_n | \beta, \theta)$ of the sampling distribution, and the computation of the associated likelihood function

$L(z_1, ..., z_n|\beta, \theta)$ given the data $\{(s_i, Z_i)\}_{i=1}^n$. The MLE of β, and θ are

$$\left(\hat{\beta}_{\text{MLE}}, \hat{\theta}_{\text{MLE}}\right) = \arg\min_{\beta,\theta} \left(-2\log\left(L\left(z_1, ..., z_n|\beta, \theta\right)\right)\right)$$

Example 125. If $(Z_s)_{s\in\mathcal{S}}$ is specified as $Z(\cdot) \sim \text{GP}(\mu(\cdot;\beta), c(\cdot,\cdot;\theta))$, with $\mu(s;\beta) = \beta_0 + s_1\beta_1 + s_2\beta_2$ then MLE of (β, θ) is

$$\left(\hat{\beta}_{\text{MLE}}, \hat{\theta}_{\text{MLE}}\right) = \arg\min_{\beta,\theta} \left(-2\log\left(\text{N}\left(Z|\mu_\beta, C_\theta\right)\right)\right)$$

where $\text{N}(Z|\mu_\beta, C_\theta)$ is the Gaussian pdf at $Z = (Z(s_1), ..., Z(s_n))^\top$, with mean $[\mu_\beta]_i = \mu(s_i;\beta) = \beta_0 + s_{1,i}\beta_1 + s_{2,i}\beta_2$ and covariance matrix $[C_\theta]_{i,j} = c_\theta(s_i, s_j)$.

13.5. **Training via Bayesian statistics.**

Note 126. Given that a probability distribution has been specified for the stochastic process $(Z_s)_{s\in\mathcal{S}}$, the Bayesian training involves (1) the derivation of the associated n-dimensional pdf $\Pr(Z_1, ..., Z_n|\beta, \theta)$ of the sampling distribution, and the computation of the associated likelihood function $L(z_1, ..., z_n|\beta, \theta)$ given the data $\{(s_i, Z_i)\}_{i=1}^n$; and the specification of the prior model $(\beta, \theta) \sim \Pr(\beta, \theta)$, leading to the Bayesian hierarchical model

$$\begin{cases} Z|\beta, \theta \sim \Pr(Z|\beta, \theta) & \text{sampling distr.} \\ \beta, \theta \sim \Pr(\beta, \theta) & \text{priors} \end{cases}$$

Posterior moments can be derived from the posterior distribution of β, θ given is given the data by using the Bayes theorem as

$$\Pr(\beta, \theta|Z) = \frac{\Pr(Z|\beta, \theta)\Pr(\beta, \theta)}{\int \Pr(Z|\beta, \theta)\Pr(\beta, \theta)\,\text{d}(\beta, \theta)}.$$

(See Handout 1, Sec 3)

Note 127. If the stochastic model is $Z(\cdot) \sim \text{GP}(\mu(\cdot;\beta), c(\cdot,\cdot;\theta))$, and specify priors $(\beta, \theta) \sim \Pr(\beta, \theta)$, the Bayesian hierarchical model is

$$\begin{cases} Z|\beta, \theta \sim \text{N}(Z|\mu_\beta, C_\theta) & \text{sampling distr.} \\ \beta, \theta \sim \Pr(\beta, \theta) & \text{priors} \end{cases}$$

and the posterior is given by the Bayes theorem as

$$\Pr(\beta, \theta|Z) = \frac{\text{N}(Z|\mu_\beta, C_\theta)\Pr(\beta, \theta)}{\int \text{N}(Z|\mu_\beta, C_\theta)\Pr(\beta, \theta)\,\text{d}(\beta, \theta)}.$$

The parametric variogram can be estimated via

$$\hat{\gamma}(h) = \text{E}_{\Pr(\theta|Z)}(\gamma(h;\theta)) = \int \gamma(h;\theta)\Pr(\theta|Z)\,\text{d}\theta$$

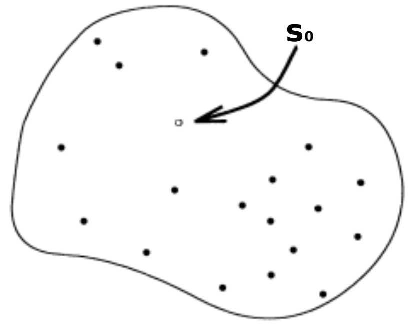


FIGURE 14.1. Kriging area

14. KRIGING THE MEAN

Note 128. We are interesting in learning the mean value of samples from a geographical (spatial) space using observations (dataset) and theoretical knowledge about that space. (Fig 14.1)

Note 129. Let $(Z_s)_{s\in\mathcal{S}}$ be a specified statistical model and assume that it is weakly stationary, with unknown constant mean $\mu = \mathrm{E}(Z(s))$ and known covariogram $c(\cdot)$. Consider there is available a dataset $\{(s_i, Z_i := Z(s_i))\}_{i=1}^n$ and assume they are realizations of $(Z_s)_{s\in\mathcal{S}}$.

Note 130. "Kriging the mean" is the technique which considers learning/estimating the mean value of samples from a spatial domain by constructing a weighted average of $\{(s_i, Z_i)\}_{i=1}^n$ and hence integrating the knowledge of the spatial correlation of those samples.

Note 131. Consider the Kriging estimator μ_{KM} of μ as

$$\mu_{\mathrm{KM}} = \sum_{i=1}^n w_i Z(s_i), \tag{14.1}$$

where $\{w_i\}$ is a set of unknown weights to be learned.

Note 132. For 14.1, it is reasonable to assume zero systematic error (unbiasness), hence

$$\mathrm{E}(\mu_{\mathrm{KM}} - \mu) = \mathrm{E}\left(\sum_{i=1}^n w_i Z(s_i) - \mu\right) = \sum_{i=1}^n w_i \overset{=1}{\cancel{\mathrm{E}(Z(s_i))}} - \mu$$

which is satisfied given the assumption

$$\sum_{i=1}^n w_i = 1 \quad \text{(ASSUMPTION)} \tag{14.2}$$

Note 133. We define the standard error as $\sigma_{\text{KM}}=\sqrt{\text{E}\left(\mu_{\text{KM}}-\mu\right)^{2}}$. Given (14.2), it is

$$\sigma_{\text{KM}}^{2}=\text{E}\left(\mu_{\text{KM}}-\mu\right)^{2}=\text{E}\left(\mu_{\text{KM}}^{2}+\mu^{2}-2\mu_{\text{KM}}\mu\right)=\sum_{i=1}^{n}\sum_{j=1}^{n}w_{i}w_{j}\text{E}\left(Z\left(s_{i}\right)Z\left(s_{j}\right)\right)$$

$$=\sum_{i=1}^{n}\sum_{j=1}^{n}w_{i}w_{j}c\left(s_{i}-s_{j}\right) \tag{14.3}$$

Note 134. For 14.1, it is reasonable to tune the unknown weights $\{w_i\}$ as

$$w^{\text{KM}}=\arg\min_{w}\text{E}\left(\mu_{\text{KM}}-\mu\right)^{2},\ \text{ subject to }\ \sum_{i=1}^{n}w_{i}=1$$

The Lagrange function is

$$\mathfrak{L}\left(w,\lambda\right)=\sum_{i=1}^{n}\sum_{j=1}^{n}w_{i}w_{j}c\left(s_{i}-s_{j}\right)-\lambda\left(\sum_{i=1}^{n}w_{i}-1\right)$$

The Kriging to mean equations are $0=\nabla_{w,\lambda}\mathfrak{L}\left(w,\lambda\right)$ producing

$$\begin{cases}0=2\sum_{j=1}^{n}w_{j}^{\text{KM}}c\left(s_{i}-s_{j}\right)-\lambda & \forall i=1,...,n\\ 1=\sum_{i=1}^{n}w_{i}^{\text{KM}}\end{cases} \tag{14.4}$$

The associated KM standard error (14.3) is the Lagrange multiplier

$$\sigma_{\text{KM}}=\sqrt{\sum_{i=1}^{n}w_{i}^{\text{KM}}\sum_{j=1}^{n}w_{j}^{\text{KM}}c\left(s_{i}-s_{j}\right)}=\sqrt{\lambda/2}$$

15. Ordinary Kriging

16. Universal Kriging

17. Bayesian Kriging (Gaussian process regression)