#### RGEOSTATS TUTORIAL

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GeoENV 1 / 63

#### **ORGANIZATION**

- 4 main tutorials
  - Variography
  - Estimation (kriging)
  - Multivariate Geostatistics
  - Simulations (part I-II-III)

GeoENV 2 / 63

#### ORGANIZATION

- 4 main tutorials
  - Variography
  - Estimation (kriging)
  - Multivariate Geostatistics
  - Simulations (part I-II-III)
- For each tutorial
  - An ascii (text) file is available
  - Preamble
  - Several independent parts
  - Copy-Paste each line
  - You should run the preamble before each part!
  - Some parts are indicated as "see also"
  - You can also play by yourself

GeoENV 2 / 63

#### SCOTLAND JANUARY TEMPERATURES

- The data set contains temperatures of January measured on 151 stations and averaged over twenty years (1961-1980)<sup>1</sup>
- The data set will be used for the first three parts

Geoenv 3 / 63

<sup>&</sup>lt;sup>1</sup>Hudson, G. and Wackernagel, H. (1994) Mapping temperature using kriging with external drift: theory and example from Scotland. International Journal of Climatology 14, 77-91.

#### INTRODUCTION

- Preamble: load and prepare the data
- Exploratory data analysis
- Compute and plot an omnidirectional experimental variogram
- Fit a model
- Several directions
- Variogram map
- Variogram for data on a grid

GEOENV 5 / 63

1. Preamble

```
# Load the data
# Change the name (to have a shorter name)
# Make the variable 4 (Elevation) inactive
data(Exdemo_Scotland_Temperatures)
dat=Exdemo_Scotland_Temperatures
dat=db.locate(dat,4)
```

GEOENV 6 / 63

# Load the data

1. Preamble

```
# Change the name (to have a shorter name)
# Make the variable 4 (Elevation) inactive
data(Exdemo_Scotland_Temperatures)
dat=Exdemo_Scotland_Temperatures
dat=db.locate(dat,4)
#Last line equivalent to
dat=db.locate(dat,4,"NA")
dat=db.locate(dat, "Elevation", "NA")
# . . .
```

GeoENV 6 / 63

2. Exploratory data analysis

```
?db.plot
dat
dat[]
hist(dat[,5])
db.stat(dat,fun="maxi",name=5)
plot(dat)
plot(dat,scalefactor=1)
plot(dat,scale=1)
plot(dat,scale=1,name.post=5)
```

GEOENV 7 / 63

3. Experimental variogram

#For documentation on vario-class class?vario

3. Experimental variogram

#For documentation on vario-class class?vario

vario=vario.calc(dat,lag=10,nlag=40)

3. Experimental variogram

```
#For documentation on vario-class
class?vario
vario=vario.calc(dat,lag=10,nlag=40)
?vario.plot
```

3. Experimental variogram

```
#For documentation on vario-class
class?vario
vario=vario.calc(dat,lag=10,nlag=40)
?vario.plot
plot(vario)
plot(vario,npairdw=TRUE)
plot(vario,npairdw=TRUE,npairpt=TRUE)
```

GEOENV 8 / 63

4. Fitting

#For documentation on model-class class?model

GeoENV 9 / 63

4. Fitting

#For documentation on model-class class?model

model=model.auto(vario)

GeoENV 9 / 63

4. Fitting

```
#For documentation on model-class
class?model
model=model.auto(vario)
melem.name()
melem.name(c(1,2,3))
```

4. Fitting

```
#For documentation on model-class
class?model
model=model.auto(vario)
melem.name()
melem.name(c(1,2,3))
model.auto(vario,struct=melem.name(c(1,2,3)))
model.auto(vario,struct=melem.name(c(1,3,2)))
```

GeoENV 9 / 63

4. Fitting

```
#For documentation on model-class
class?model
model=model.auto(vario)
melem.name()
melem.name(c(1,2,3))
model.auto(vario,struct=melem.name(c(1,2,3)))
model.auto(vario,struct=melem.name(c(1,3,2)))
model.auto(vario,struct=melem.name(c(1,3,2)),
           maxiter=0)
```

GEOENV 9 / 63

4. FITTING (WITH CONSTRAINTS)

GeoENV 10 / 63

4. FITTING (WITH CONSTRAINTS)

GeoENV 10 / 63

4. FITTING (WITH CONSTRAINTS)

```
model.auto(vario,struct=melem.name(c(1,2,3)),
           flag.noreduce=T)
model.auto(vario,struct=melem.name(c(1,2,3)),
           flag.noreduce=T, verbose=T)
model.auto(vario,struct=melem.name(c(1,2,3)),
           flag.noreduce=T,
           lower=c(0.02,NA,NA,NA,NA),
           upper=c(0.02,NA,NA,NA,400)
```

GeoENV 10 / 63

5. Several directions

GEOENV 11 / 63

5. Several directions

```
#Display results
```

```
plot(vario_4dir,npairdw=TRUE)
plot(m4dir,add=T,vario=vario_4dir)
```

GEOENV 12 / 63

6. Variogram map

GeoENV 13 / 63

6. Variogram map

GeoENV 13 / 63

6. Variogram map

```
plot(vario_4dir)
plot(model,vario=vario_4dir,add=T)
```

GeoENV 14 / 63

7. Variogram for grid

data(Exdemo\_Scotland\_Elevations)
grid=Exdemo\_Scotland\_Elevations

GeoENV 15 / 63

7. Variogram for grid

GEOENV 15 / 63

#### 7. Variogram for grid

GeoENV 15 / 63

7. Variogram for grid

model.auto(vario,struct=melem.name(c(1,3,2)))

GeoENV 16 / 63

#### 7. Variogram for grid

GeoENV 16 / 63

## 2) Estimation

#### Introduction

- Preamble
  - Load and prepare the data
  - Create the variogram model
  - Create a neighborhood
- Perform kriging
- Cross-validation
- Moving neighborhood

GeoENV 17 / 63

# 2) Estimation

Preamble (1)

```
#1) Prepare the data
```

```
data(Exdemo_Scotland_Temperatures)
data(Exdemo_Scotland_Elevations)
dat=Exdemo_Scotland_Temperatures
grid=Exdemo_Scotland_Elevations
dat=db.locate(dat,4)
```

GEOENV 18 / 63

# ESTIMATION

Preamble (2)

```
vario=vario.calc(dat,lag=10,nlag=40)
model=model.auto(vario,
                 struct=melem.name(c(1,3,2)))
```

# We could have used model.create (script) or # model.input (interface)

to create a model.

#2) Define the model

19 / 63 GeoENV

# 2) Estimation

Preamble (3)

```
#3) Define the neighborhood
unique.neigh=neigh.init(type=0,ndim=2)
#Equivalent to
unique.neigh=neigh.input(ndim=2)
#answer 0
```

GeoENV 20 / 63

### 2) Estimation

2. Kriging

GeoENV 21 / 63

2. Kriging

GeoENV 21 / 63

2. Kriging

```
result0=kriging(dat,grid,model=model,
                neigh=unique.neigh)
plot(result0, scale=1,
     col=topo.colors(100),pos.legend=5)
plot(dat,add=T)
plot(result0, name=7, scale=1,
     col=topo.colors(100),pos.legend=5)
plot(dat,add=T)
```

GEOENV 21 / 63

3. Cross-validation

```
res.xv = xvalid(dat,model,neigh=unique.neigh)
hist(res.xv[,6],breaks=20)
hist(res.xv[,7],breaks=20)
mean(res.xv[,7]^2,na.rm=T)
plot(res.xv,scale=1)
```

GeoENV 22 / 63

3. Cross-validation

```
res.xv = xvalid(dat, model, neigh=unique.neigh)
hist(res.xv[,6],breaks=20)
hist(res.xv[,7],breaks=20)
mean(res.xv[,7]^2,na.rm=T)
plot(res.xv,scale=1)
plot(result0, scale=1,
     col=topo.colors(100),pos.legend=5)
plot(res.xv,scale=1,add=T,
     col=1+as.numeric(res.xv[,6]>0))
```

GeoENV

4. Moving neighborhood

```
moving.neigh=neigh.input()
#answers 2, 5, 200, n, n, 50
```

GEOENV 23 / 63

4. Moving neighborhood

moving.neigh=neigh.input()

```
#answers 2, 5, 200, n, n, 50
result1=kriging(dat,grid,
```

GeoENV 23 / 63

model=model,neigh=moving.neigh)

4. Moving neighborhood

GeoENV 23 / 63

4. Moving neighborhood

abline(0,1,col=2)

```
moving.neigh=neigh.input()
#answers 2, 5, 200, n, n, 50
result1=kriging(dat,grid,
                model=model,neigh=moving.neigh)
plot(result1,scale=1,
     col=topo.colors(100),pos.legend=5)
plot(result0[,6],result1[,6],cex=.2)
```

GEOENV 23 / 63

#### INTRODUCTION

- The temperature stations are not located at high elevations
- The temperature depends on the altitude
- We know the elevation of the stations (and some other elevations)
- We want to use this auxiliary information to improve the prediction
- In a second step, we will use the full Digital Terrain Model (DTM)

GEOENV 24 / 63

#### INTRODUCTION

- Preamble
- Exploratory data analysis (bivariate)
- Cross-variogram model
- Co-kriging
- Collocated co-kriging
- External drift

GEOENV 25 / 63

1. Preamble

The results of ordinary kriging are stocked in result0.

GEOENV 26 / 63

#### 1. Preamble

The results of ordinary kriging are stocked in result0.

data(Exdemo\_Scotland\_Temperatures)
data(Exdemo\_Scotland\_Elevations)
dat=Exdemo\_Scotland\_Temperatures
grid=Exdemo\_Scotland\_Elevations

#### 1. Preamble

```
The results of ordinary kriging are stocked in result0.
data(Exdemo_Scotland_Temperatures)
data(Exdemo_Scotland_Elevations)
dat=Exdemo_Scotland_Temperatures
grid=Exdemo_Scotland_Elevations
Creation of the variable indicating if the temperature is
available or if there is only the elevation.
dat=db.add(dat,
             "Available_Temp"=(!is.na(dat[,5])),
             loctype="NA")
```

GEOENV 26 / 63

#### 1. Preamble

```
The results of ordinary kriging are stocked in result0.
```

```
data(Exdemo_Scotland_Temperatures)
data(Exdemo_Scotland_Elevations)
dat=Exdemo_Scotland_Temperatures
grid=Exdemo_Scotland_Elevations
```

Creation of the variable indicating if the temperature is available or if there is only the elevation.

unique.neigh=neigh.init(type=0,ndim=2)

2. Exploratory data analysis (bivariate)

```
dat=db.locate(dat,6,"sel")
plot(dat)
db.stat(dat,fun="maxi",names=4)
```

GEOENV 27 / 63

2. Exploratory data analysis (bivariate)

```
dat=db.locate(dat,6,"sel")
plot(dat)
db.stat(dat,fun="maxi",names=4)
dat[,6]=!dat[,6]
plot(dat,add=T,col=3)
db.stat(dat,fun="maxi",names=4)
```

GEOENV 27 / 63

2. Exploratory data analysis (bivariate)

```
dat=db.locate(dat,6,"sel")
plot(dat)
db.stat(dat,fun="maxi",names=4)
dat[,6]=!dat[,6]
plot(dat,add=T,col=3)
db.stat(dat,fun="maxi",names=4)
dat[,6]=!dat[,6]
correlation(dat,icol1=4,icol2=5,col=c(2,3),
            pos.legend=1)
```

GeoENV 27 / 63

2. Exploratory data analysis (bivariate)

```
dat=db.locate(dat,6,"sel")
plot(dat)
db.stat(dat,fun="maxi",names=4)
dat[,6]=!dat[,6]
plot(dat,add=T,col=3)
db.stat(dat,fun="maxi",names=4)
dat[.6]=!dat[.6]
correlation(dat,icol1=4,icol2=5,col=c(2,3),
            pos.legend=1)
regression(dat,icol1=4,icol2=5,flag.draw=T,
           save.coeff= T)
```

GEOENV 27 / 63

3. Cross-variogram model

GeoENV 28 / 63

4. Co-kriging (isotopic)

#### Isotopic

dat=db.locate(dat,6,"sel")

4. Co-kriging (isotopic)

## Isotopic

GeoENV 29 / 63

4. Co-Kriging (heterotopic)

#### Heterotopic

dat=db.locate(dat,6)

GeoENV 30 / 63

4. Co-Kriging (heterotopic)

#### Heterotopic

GeoENV 30 / 63

4. Co-Kriging (collocated)

```
moving.neigh=neigh.input(ndim=2)
#Answers 2, 5, 20, n, n, 50
```

GEOENV 31 / 63

4. Co-Kriging (collocated)

4. Co-Kriging (collocated)

GEOENV 31 / 63

5. Kriging with external drift

```
dat=db.locate(dat,4,"f")
grid=db.locate(grid,4,"f")
```

5. Kriging with external drift

GeoENV 32 / 63

5. Kriging with external drift

5. Kriging with external drift

GEOENV 33 / 63

First steps

```
grid=db.create(nx=c(100,100))
model=model.create(vartype= "Gaussian",range=30)
```

GeoENV 34 / 63

First steps

```
grid=db.create(nx=c(100,100))
model=model.create(vartype= "Gaussian",range=30)
grid = simtub(,grid,model=model,nbtuba=1,seed=0)
plot(grid,scale=1,col=topo.colors(100))
```

Try several times the last two commands.

nbtuba = 1000

GEOENV

FIRST STEPS

```
grid=db.create(nx=c(100,100))
model=model.create(vartype= "Gaussian",range=30)
grid = simtub(,grid,model=model,nbtuba=1,seed=0)
plot(grid,scale=1,col=topo.colors(100))
Try several times the last two commands.
Try with
 nbtuba = 2
and
 nbtuba = 10
and
 nbtuba = 100
and
```

#### STATISTICAL FLUCTUATIONS

A stationary Gaussian random function  $Y = (Y(x), x \in \mathbb{R}^d)$  with

- mean m
- variance  $\sigma^2$
- correlation function  $\rho(h)$
- variogram  $\gamma(h) = \sigma^2(1 \rho(h))$

is simulated on a domain V.

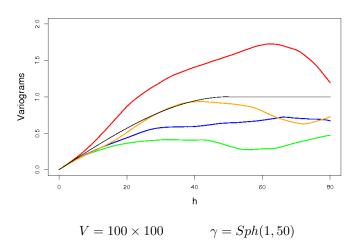
 $(y(x), x \in V)$  is the realization

#### STATISTICAL FLUCTUATIONS

From the simulation  $(y(x), x \in V)$  some  $\mbox{ experimental quantities can be computed:}$ 

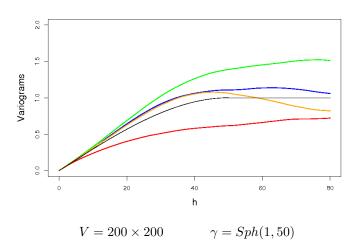
- the mean  ${\color{red} y_{\scriptscriptstyle V}} = \frac{1}{|V|} \int_{V} y(x) dx$
- $\bullet$  the dispersion variance  $s^2(0\,|V) = \frac{1}{|V|} \int_V (y(x)-y_{\scriptscriptstyle V})^2 dx$
- ullet the regional variogram  $\gamma_V(h)=rac{1}{2|V\cap V_{-h}|}\int_{V\cap V_{-h}}(y(x)-y(x+h))^2dx$
- ullet some proportions  $\displaystyle {m p(a)} = rac{1}{|V|} \int_V 1_{y(x) < a} dx$

#### STATISTICAL FLUCTUATIONS



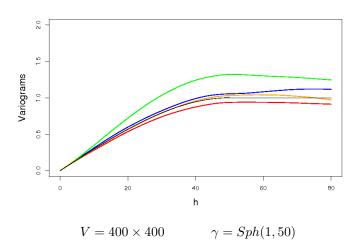
GeoENV 37 / 63

#### STATISTICAL FLUCTUATIONS



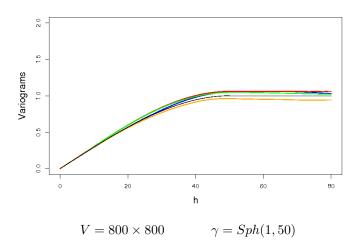
GEOENV 38 / 63

#### STATISTICAL FLUCTUATIONS



GEOENV 39 / 63

#### STATISTICAL FLUCTUATIONS



GEOENV 40 / 63

#### STATISTICAL FLUCTUATIONS

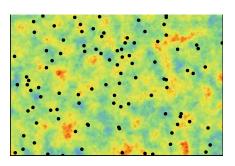
The experimental quantities are not equal to their corresponding quantities in the model:

- $y_v \neq m$
- $s^2(0|V) \neq \sigma^2$
- $\gamma_V(h) \neq \gamma(h)$
- $p(a) \neq G\left(\frac{a-m}{\sigma}\right)$  (G is the Gaussian cumulative distribution function)
- they differ from one simulation to another (statistical fluctuations)
- ullet the experimental statistics tends to their corresponding quantities in the model when the size of V increases (ergodicity)

GEOENV 41 / 63

#### CONDITIONAL SIMULATIONS

How to simulate a realization  $\{y(x), x \in \mathbb{R}^d\}$  of a second order Gaussian random function  $\{Y(x), x \in \mathbb{R}^d\}$  with mean m and covariance function C with respect to the data  $\{Y(x_i) = y_i, i = 1, \dots, n\}$ ?



GEOENV 42 / 63

Principe

Let

$$Y(x) = Y^{SK}(x) + Y(x) - Y^{SK}(x)$$

where

$$Y^{SK}(x) = m + \sum_{j=1}^n \lambda_j(x) [Y(x_j) - m]$$
 simple kriging

$$Y(x) - Y^{SK}(x)$$
 kriging residuals

 ${\cal Y}^{SK}$  et  ${\cal Y}-{\cal Y}^{SK}$  are to independant Gaussian random functions

#### Algorithm

- (i) make an unconditional simulation  $\{s(x), x \in \mathbb{R}^d\}$  and set  $s_i = s(x_i)$ .
- (ii) for all  $x \in \mathbb{R}^d$ , compute the kriging weights  $(\lambda_i(x), j = 1, \dots, n)$
- (iii) set

$$y^{CS}(x) = y^{SK}(x) + s(x) - s^{SK}(x)$$
$$= s(x) + \sum_{j=1}^{n} \lambda_j(x)(y_j - s_j)$$

GEOENV 44 / 63

CHECKING

• If  $x = x_i$ , then  $y^{CS}(x_i) = y_i + s(x_i) - s(x_i) = y_i$ 

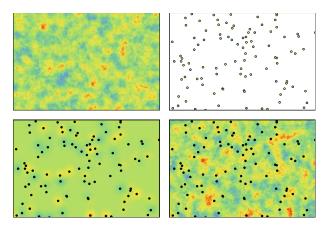
The conditioning data are honored

• If  $C(x-x_{\alpha}) \simeq 0$  for all  $i=1,\ldots,n$ , then  $y^{CS}(x) \simeq m+s(x)-m=s(x)$ 

For points distant from the data, the simulation is unconditional

GEOENV 45 / 63

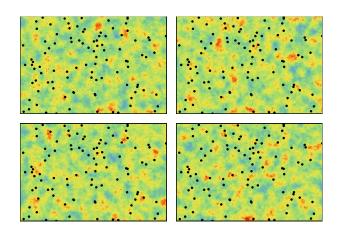
#### ILLUSTRATION



Simulation (TL), Synthetic data (TR), Simple kriging (BL), a conditional simulation (BR)

GEOENV 46 / 63

4 CONDITIONAL SIMULATIONS



GEOENV 47 / 63

#### Gaussian Transform

- Limitation of the Gaussian model:
  - Symetrical distribution
  - Inadapted to model data with heavy tail histogram
  - Conditional variance does not depend on the data (homoscedasticity)
- ullet Anamorphosis: bijective function  $\Phi$  defined on  $\mathbb R$
- $\bullet$  Model: data are a realization of a second order stationary Gaussian random function transformed by  $\Phi$
- Example : The log-normal model

$$\Phi(Y) = \exp(\mu + \sigma Y)$$

GeoENV 48 / 63

#### CONDITIONAL SIMULATION OF A TRANSFORMED GAUSSIAN RANDOM FUNCTION

#### MODEL

 $(z(x_1),\ldots,z(x_n))$  is a realization of  $(Z(x),x\in\mathbb{R}^d)$ , a transformed Gaussian random function:

- $\bullet \ Z(x) = \Phi(Y(x)) \ \text{for all} \ x \in \mathbb{R}^d$
- $(Y(x), x \in \mathbb{R}^d)$  a second order stationary Gaussian random function with correlation function C

How to simulate a realization  $(z(x),x\in\mathbb{R}^d)$  from  $(Z(x),x\in\mathbb{R}^d)$  such as  $Z(x_i)=z(x_i)$  for  $i=1,\ldots,n$ ?

#### ALGORITHM

(i) transform the data in the Gaussian scale

$$y_i = \Phi^{-1}(z(x_i))$$

(ii) Perform a conditional simulation  $\{y(x), x \in \mathbb{R}^d\}$  from the Gaussian random function  $(Y(x), x \in \mathbb{R}^d)$  which honors the data in the Gaussian case

$$Y(x_i) = y_i$$

(iii) transform back the simulation for all  $x \in \mathbb{R}^d$ 

$$z(x) = \Phi(y(x))$$

GeoENV 50 / 63

CONDITIONAL SIMULATIONS

```
data(Exdemo_Scotland_Temperatures)
data(Exdemo Scotland Elevations)
dat=Exdemo_Scotland_Temperatures
grid=Exdemo_Scotland_Elevations
dat=db.locate(dat,4)
vario=vario.calc(dat,lag=10,nlag=40)
model=model.auto(vario, flag.noreduce=T,
                 struct=melem.name(c(1,2,3)),
                 lower=c(0.02,NA,NA,NA,NA),
                 upper=c(0.02,NA,NA,NA,NA))
unique.neigh=neigh.init(type=0,ndim=2)
```

GEOENV 51 / 63

CONDITIONAL SIMULATIONS

GEOENV 52 / 63

CONDITIONAL SIMULATIONS

```
m=mean(dat[,5],na.rm=T)
simu = simtub(dat,grid,model=model,mean=m,
              neigh=unique.neigh,uc="",
              nbtuba=1000,nbsimu=100)
plot(simu, scale=1, col=topo.colors(100),
     name=6,zlim=c(-2,5),pos.legend=5)
result=db.compare(simu,fun="mean",name=6:105)
```

GeoENV 52 / 63

Comparison with simple kriging

GeoENV 53 / 63

Comparison with simple kriging

Comparison with simple kriging

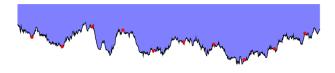
```
result0=kriging(dat,grid,uc="",mean=m,
                model=model, neigh=unique.neigh)
plot(result[,106],result0[,6],cex=.2)
abline(0.1,col=2)
result=db.compare(simu,fun="stdv",name=6:105)
plot(result[,107],result0[,7],cex=.2)
abline(0,1,col=2)
```

GeoENV 53 / 63

#### OPTIMAL PREDICTOR

**Example:** a submarine cable has to be set on the seabed between Lisbonne and New-York.

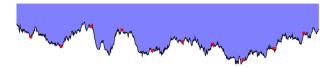
How to predict its length from the bathymetry z sampled every 200m. Uncertainty?



$$l = \int_{a}^{b} \sqrt{1 + [z(x)']^{2}} dx$$

GEOENV 54 / 63

#### NATURAL IDEA

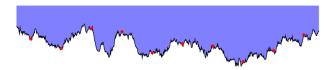


Measuring the length of the predicted (kriged) bathymetry  $\hat{z}$ 

$$\hat{l} = \int_{a}^{b} \sqrt{1 + [\hat{z}(x)']^2} dx$$

GEOENV 55 / 63

#### NATURAL IDEA



Measuring the length of the predicted (kriged) bathymetry  $\hat{z}$ 

$$\hat{l} = \int_{a}^{b} \sqrt{1 + [\hat{z}(x)']^2} dx$$



Systematic under-estimation: predicted trajectory is much smoother than the actual one

GeoENV 55 / 63

#### OPTIMAL PREDICTOR

- $(X_0, X_1, \dots, X_n)$  is a random vector with finite variance.
- The regression of  $X_0$  on  $(X_1,\ldots,X_n)$  is the function r such as the mean squared error

$$E[(X_0-r(X_1,\ldots,X_n))^2]$$

is minimal

#### OPTIMAL PREDICTOR

- $(X_0, X_1, \dots, X_n)$  is a random vector with finite variance.
- The regression of  $X_0$  on  $(X_1,\ldots,X_n)$  is the function r such as the mean squared error

$$E[(X_0 - r(X_1, \dots, X_n))^2]$$

is minimal

• It is given by the conditional expectation of  $X_0$  knowing  $X_1, \ldots, X_n$ :

$$r(x_1,\ldots,x_n) = E[X_0|X_1 = x_1,\ldots,X_n = x_n].$$

GEOENV 56 / 63

#### OPTIMAL PREDICTOR

- $(X_0, X_1, \dots, X_n)$  is a random vector with finite variance.
- The regression of  $X_0$  on  $(X_1,\ldots,X_n)$  is the function r such as the mean squared error

$$E[(X_0 - r(X_1, \dots, X_n))^2]$$

is minimal

• It is given by the conditional expectation of  $X_0$  knowing  $X_1, \ldots, X_n$ :

$$r(x_1, \dots, x_n) = E[X_0 | X_1 = x_1, \dots, X_n = x_n].$$

 In the multi-Gaussian case, the regression is linear In other words, simple kriging is optimal

GeoENV 56 / 63

#### OPTIMAL PREDICTOR

• In other cases, we can compute  $r(x_1, \ldots, x_n)$  by averaging conditional simulations of  $X_0$  knowing  $X_1 = x_1, \dots, X_n = x_n$ :

$$E[X_0|X_1 = x_1, \dots, X_n = x_n] \simeq \frac{1}{N} \sum_{i=1}^N X_0^{(i)}$$

where  $X_0^{(i)}$  is the  $i^{th}$  conditional simulation of  $X_0$  knowing  $X_1 = x_1, \ldots, X_n = x_n$ 

GeoENV

#### OPTIMAL PREDICTOR

• In other cases, we can compute  $r(x_1, \ldots, x_n)$  by averaging conditional simulations of  $X_0$  knowing  $X_1 = x_1, \dots, X_n = x_n$ :

$$E[X_0|X_1 = x_1, \dots, X_n = x_n] \simeq \frac{1}{N} \sum_{i=1}^N X_0^{(i)}$$

where  $X_0^{(i)}$  is the  $i^{th}$  conditional simulation of  $X_0$  knowing  $X_1 = x_1, \ldots, X_n = x_n$ 

• For the submarine cable  $X_0 \equiv \text{Length}$ .

PREAMBLE

```
data(Exdemo_bathymetry_1D)
dat=Exdemo_bathymetry_1D
v=vario.calc(dat,lag=1,nlag=50)
model=model.auto(v,melem.name(c(5,2)).
                 flag.noreduce=T)
neigh=neigh.init(ndim=1,type=0)
```

GEOENV 58 / 63

FUNCTION TO COMPUTE THE LENGTH OF THE CABLE

GeoENV 59 / 63

LENGTH OF THE KRIGING

GeoENV 60 / 63

CONDITIONAL SIMULATIONS

GEOENV 61 / 63

CONDITIONAL SIMULATIONS

GeoENV 61 / 63

Display the results

```
hist(res,prob=T,xlim=range(c(resk,res)))
abline(v= calcul_length(db_krig),col=3)
abline(v= mean(res),col=4)
```

GeoENV 62 / 63

Display the results

```
hist(res,prob=T,xlim=range(c(resk,res)))
abline(v= calcul_length(db_krig),col=3)
abline(v= mean(res),col=4)

plot(dat,xlim=c(0,1000),type="p",cex=.5,col=2)
plot(db_krig,add=T,lwd=2,col=3)
plot(db_simu,add=T,col=4,name=3,lty=2)
```

GeoENV 62 / 63

Compare with the reality

```
data(Exdemo_bathymetry_1D_full)
grid=Exdemo_bathymetry_1D_full
plot(grid,add=T,col=2)
```

Compare with the reality

```
data(Exdemo_bathymetry_1D_full)
grid=Exdemo_bathymetry_1D_full
plot(grid,add=T,col=2)
true_length=calcul_length(grid)
```

Compare with the reality

```
data(Exdemo_bathymetry_1D_full)
grid=Exdemo_bathymetry_1D_full
plot(grid,add=T,col=2)
true_length=calcul_length(grid)
hist(res,prob=T,xlim=range(c(resk,res)))
abline(v= calcul_length(db_krig),col=3)
abline(v= mean(res),col=4)
abline(v=true_length,col=2)
```

GEOENV 63 / 63