Copula-basierte räumliche Interpolation

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Preliminary Remarks

Geostatistics

(much more than Kriging methodology!) has spread from traditional areas of application (mining and oil exploration) to nearly all branches of bio, earth and environmental sciences, medicine and technology

Recent Areas of Application:

- Public Health + Epidemiology
- Precision Farming
- Image Analysis (Gibbs/Markov-RF)
- Statistical Process Control (Semiconductor industry)
- Telecommunication network design

Partial Convergence with **Machine Learning** methodology

Geostatistics

= Statistical analysis of random phenomena distributed in space (and time) using the theory of Random Functions (Random Fields)

Milestone-Books

during the last 15 years:

- 1993: N. Cressie: Statistics for Spatial Data. Rev. ed., Wiley
- 1997: P. Goovaerts: Geostatistics for Natural Resources Evaluation. Oxford Univ. Press
- 1999: M.L. Stein: Interpolation of Spatial Data. Some Theory for Kriging. Springer

- 1999: J.-P. Chilès & P. Delfiner: Geostatistics: Modeling Spatial Uncertainty. Wiley
- 1999: R. Olea: Geostatistics for Engineers and Earth Scientists. Springer
- 2003: H. Wackernagel: Multivariate Geostatistics. 3rd ed., Springer
- 2003: S. Banerjee, B.P. Carlin & A. Gelfand: Hierarchical Modeling and Analysis for Spatial Data. CRC Chapman & Hall
- 2007: R. Webster & M. A. Oliver: Geostatistics for Environmental Scientists. 2nd ed., Wiley
- 2007: P.J. Diggle & P.J. Ribeiro, P.J.: Model-based Geostatistics. Springer

Most recent books:

- R. Bivand, E. Pebesma and V. Gomez-Rubio: Applied Spatial Data Analysis with R. Springer 2008
- J. Pilz (Ed.): Interfacing Geostatistics and GIS. Springer 2009

Current research issues:

- Non-Gaussianity
- Non-stationarity (Direct modeling via kernels, Grid deformation)
- Spatio-temporal extensions (Space-time covariance functions)
- Spatio-temporal monitoring network design/design of computer experiments

Spatial linear model/Kriging

$$\begin{array}{ccccccc} Z(x) & = & m(x) & + & \varepsilon(x); & x \in D \subset R^d, d > 1 \\ \text{Data} & = & \text{Trend} & + & \text{Error} & \end{array}$$

Linear trend model:

$$(1) m(x) = E\{Z(x)|\beta, \theta\} = f(x)^T \beta$$

Trend parameter covariance parameter

e.g. polynomials: $m(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$

$$(2) Cov\{(Z(x_1), Z(x_2))|\beta, \theta\} = C_\theta(x_1 - x_2)$$

covariance stationarity

$(1) + (2) =$ **universal kriging** setup

Given:

observations at points $x_1, \dots, x_n \in D$

$$\mathbf{Z} = (Z(x_1), \dots, Z(x_n))^T \text{ observation vector}$$

Goal:

Prediction of $Z(x_0)$ at $x_0 \in D$,
i.e. choose $\hat{Z}(x_0)$ such that

$$E\{\hat{Z}(x_0) - Z(x_0)\}^2 \longrightarrow \underset{\hat{Z}}{Min}$$

Spatial BLUP

$\hat{Z}_{UK}(x) = \lambda^T \mathbf{Z}$
takes the form

$$\hat{Z}_{UK}(x_0) = f(x_0)^T \underset{\substack{\downarrow \\ \text{GLS of } \beta}}{\hat{\beta}} + c(x_0)^T K^{-1} \underbrace{(\mathbf{Z} - F\hat{\beta})}_{\substack{\downarrow \\ \text{residual vector}}}$$

where

$$
\begin{aligned}
F &= (f(x_1), \ldots, f(x_n))^T = \text{design matrix} \\
c(x_0) &= (Cov(Z(x_0), Z(x_i)))_{i=1,\ldots,n} \\
K &= (Cov(Z(x_i), Z(x_j)))_{i,j=1,\ldots,n} \\
&= \text{covariance matrix of } \mathbf{Z}
\end{aligned}
$$

Usually,

further assumptions like

isotropy: $C_\theta(x_1 - x_2) = C_\theta(||x_1 - x_2||)$

sparse parametrization: $\theta = (\theta_1, \theta_2, \theta_3)$

$= (\text{nugget, sill, range})$

Statistical / numerical problem:

non-linearity in θ (esp. in range)

Weak point

of kriging: BLUP-optimality rests on exact knowledge of covariance function. In practice however: **plug-in-kriging** using empirical moment estimator of the cov. function, which is then fitted to some (conditionally) pos. semidefinite function

For sensible

predictions: further assumptions about the law of the R.F. are required. **Local** behaviour of the R.F. is critical

Essential Property:

Mean square differentiability
(defined as an L_2-limit)

Result:

Z is m-times m.s.d. iff $|C^{(2m)}(0)| < \infty$; $(m = 1, 2, \ldots)$
Local behaviour of W.R.F.'s is best studied using spectral methods

Bochner's Theorem:

$C(\cdot)$ is cov. function for a w.m.s.c. R.F. on $R^d \longleftrightarrow$

$$C(x) = \int_{R^d} \exp(i\omega^T x)\ F(d\omega)$$

$\downarrow$

positive finite measure
= **spectral measure**

$\Rightarrow$ Spectral density & Covariance function form a **Fourier pair**

Matérn class of covariance functions

Matérn class

of covariance functions widely popular over the last 10 years:

$C_\theta(h) = c * (\alpha|h|)^\nu \mathcal{K}_\nu(\alpha|h|)$

$\mathcal{K}_\nu$ = modified Bessel function of order ν
$\theta = (c, \alpha, \nu)$ = (sill, scale, smoothness) $\in (0, \infty)^3$

Spectral density: $f_M(\omega) = c(\alpha^2 + \omega^2)^{-\nu-d/2}$
valid for isotropic R.F.s in any dimension d!

Fitting procedures in: geoR, geoRglm (Diggle& Ribeiro, 2007)

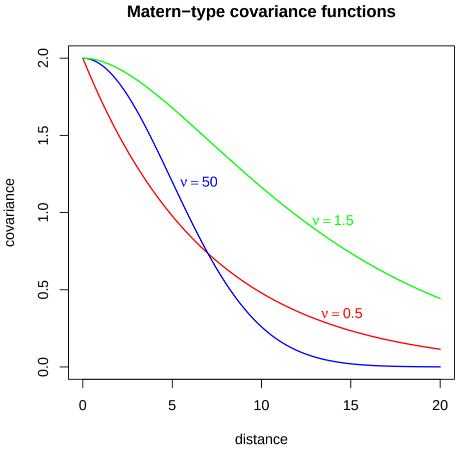


Figure: Matérn Covariance Functions

Prediction using likelihood methods

Assumption:

$Z(\cdot) \sim$ Gaussian R.F. on R^d

$$Z(x) = f(x)^T \beta + \varepsilon(x); \; E\varepsilon(x) = 0$$

with $\beta \in R^r$ = Trend parameter vector

Covariance function $C_\theta(h)$ = Matérn cov. function

$$\Longrightarrow \mathbf{Z} = (Z(x_1), \ldots, Z(x_n))^T = \text{ observation vector}$$

$$\sim \text{Multivariate Normal}$$

Log-Likelihood-Function

$$l(\beta,\theta) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log detK(\theta)$$
$$-\frac{1}{2}(\mathbf{Z}-F\beta)^T K(\theta)^{-1}(\mathbf{Z}-F\beta)$$

For any given θ, $l(\cdot,\theta)$ is maximized by

$$\hat{\beta}(\theta) = [F^T K(\theta)^{-1} F]^{-1} F^T K(\theta)^{-1}\mathbf{Z}$$

design matrix　　covariance matrix

Problem:

Maximize $l(\hat{\beta}(\theta),\theta)$ w.r.t. to θ

||

profile log-likelihood for θ

Disadvantage:

- MLE of θ tends to underestimate the variation
- Adjustments for the bias not available

Extension:

non-Gaussian R.F.s
Need models / computational methods for calculating likelihood functions
Diggle, Tawn & Moyeed (1998): MCMC methods

Key:

Model-based Geostatistics
$\Rightarrow$ serious computational issues!

Bayesian approach

Advantage:

provides a general methodology for taking into account the uncertainty about parameters on subsequent predictions.
Especially important for the Matérn class:
Large uncertainty about ν, it is impossible to obtain defensible MSE's from the data without incorporating prior information about ν!

First versions of Bayesian Kriging:
Kitanidis (1986), Omre (1987)

Bayesian solution:

For making inferences about $Z(x_0) =: Z_0$, use the **predictive density** $p(Z_0|Z)$ given the data $\mathbf{Z} = (Z(x_1), \ldots, Z(x_n))^T$,

$$p(Z_0|\mathbf{Z}) = \int_{\Theta}\int_{B} p(Z_0|\underset{\substack{\text{trend parameter}\\ \text{(1st order par.)}}}{\underset{\downarrow}{\beta}}, \theta, \mathbf{Z})\, p(\beta, \underset{\substack{\text{covariance par.}\\ \text{(2nd order par.)}}}{\underset{\downarrow}{\theta}}|\mathbf{Z})\, d\beta\, d\theta$$

where $p(\beta, \theta|\mathbf{Z})$ = posterior density

$$= \frac{p(\mathbf{Z}|\beta,\theta)p(\beta,\theta)}{\int_{\Theta}\int_{B} p(\mathbf{Z}|\beta,\theta)p(\beta,\theta)\,d\beta\, d\theta}$$

$\propto$ likelihood f. $*$ prior d.

Proposal:

conditional simulation

$$p(\beta,\theta|\mathbf{Z}) \quad \propto \quad \underbrace{p(\mathbf{Z}|\theta,\beta)}_{\text{likelihood f.}} * p(\beta) * \underbrace{p(\theta|\mathbf{Z})}_{\text{simulation}}$$

Empirical Bayes approach, see Pilz & Spöck, SERRA (2008)

Alternative way:

Objective Bayesian analysis:
determine non-informative priors
Berger, Sanso, DeOliveira 2001

Extension I: Bayesian trans-Gaussian Prediction

The transformed Gaussian Model

- Observations from random field $\{Z(x), x \in \mathbf{X} \subset \mathcal{R}^m\}$.
- Box-Cox family of power transformations (Box and Cox, 1964)

$$g_\lambda(z) = \begin{cases} \frac{z^\lambda - 1}{\lambda} & : \quad \lambda \neq 0 \\ \log(z) & : \quad \lambda = 0 \end{cases}$$

- transforms the random field $Z(x)$ for some unknown parameter λ to a Gaussian one with unknown trend and unknown covariance function $C_\theta(x_1, x_2)$.
- Definition of prior:

$$\Theta = (\lambda, \theta)$$
$$p(\beta, \Theta) = p(\beta, \lambda, \theta)$$

- Likelihood:

$$p(\mathbf{Z_0}, \mathbf{Z_{dat}}|\beta, \Theta) =$$

$$\underbrace{p(g_\lambda(Z_0, \mathbf{Z_{dat}})|\beta, \lambda, \theta, \sigma^2)}_{normal} * \underbrace{J_\lambda(Z_0, \mathbf{Z_{dat}})}_{Jacobian}$$

- Generalization:
  arbitrary monotone transformations $g(z)$, e.g. $g(z) = \log(-\log(1-z))$
- Posterior Predictive Distribution:

$$p(Z_0|\mathbf{Z_{dat}}) = \int_\Theta \underbrace{p(Z_0|\mathbf{Z_{dat}}, \Theta)}_{Gaussian} \underbrace{p(\Theta|\mathbf{Z_{dat}})}_{?} d\Theta,$$

Solution

- Instead of specifying the prior we specify the posterior $p(\Theta|\mathbf{Z_{dat}})$ by means of a *parametric bootstrap* of some estimator of Θ.

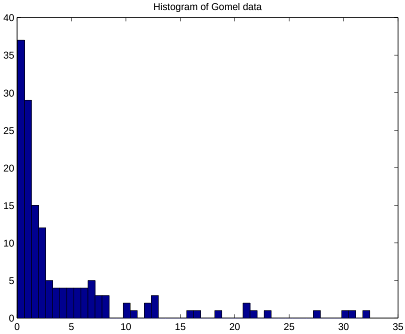


Figure: Histogram of Gomel data

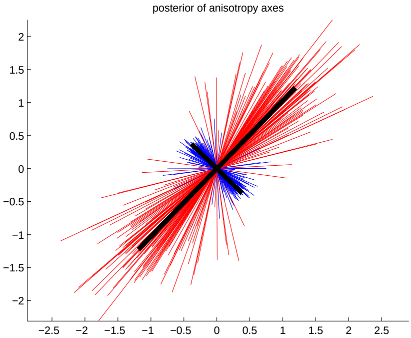


Figure: Bootstrapped anisotropy axes

Advantages

- Complete probability distribution (not only kriged values + variances)
- We have median, quantiles a.s.o.

  $\longrightarrow$ threshold values, confidence intervals a.s.o.
- "Automatic" Bayes procedure

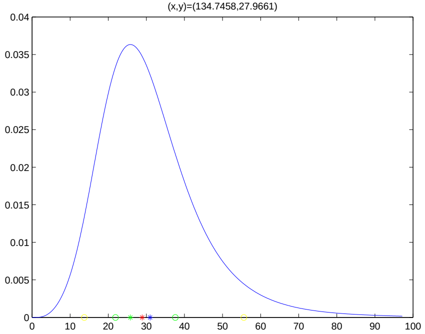


Figure: Posterior predictive distribution at (x,y)=(134.7,27.9)

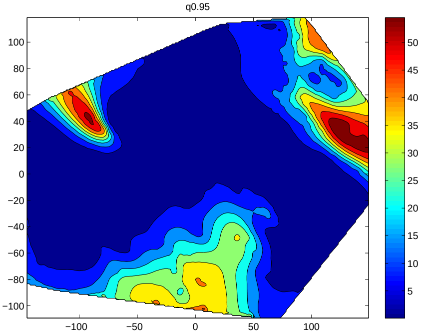


Figure: 95% posterior predictive quantile

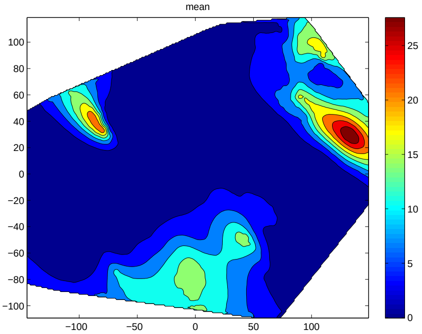


Figure: posterior predictive mean

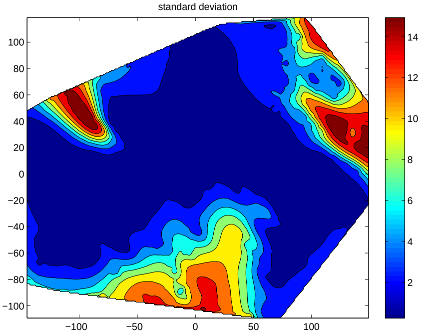


Figure: posterior predictive standard deviation

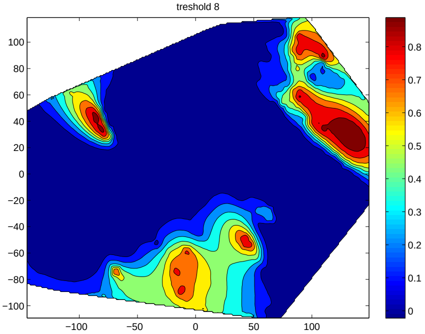


Figure: probability to be above threshold 8.0

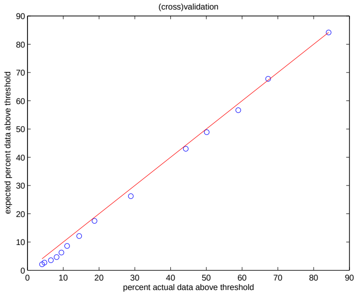


Figure: predicted percentage versus actual percentage of data above threshold

Extension II: Spatial Modelling Using Copulas

Problem:

What can we do if data are extreme, highly skewed?

Answer:

Copula-based spatial modeling

Copulas

are distribution functions on the unit cube $[0,1]^n$

Sklar's Theorem

Let H be an n-dimensional distribution function with margins $F_1,\dots,F_n$. Then there exists an n-dimensional copula C such that for all $\mathbf{x}=(x_1,\dots,x_n)\in\mathbf{R}^n$

$$H(x_1,\dots,x_n)=C\left(F_1(x_1),\dots,F_n(x_n)\right)$$

If $F_1,\dots,F_n$ are all continuous, then C is unique. Conversely, it holds:

$$C(u_1,\dots,u_n)=H\left(F_1^{-1}(u_1),\dots,F_n^{-1}(u_n)\right).$$

Properties of Copulas

- Copulas describe the dependence between the quantiles of random variables. They describe dependence without information about marginal distributions.
- Copulas are invariant under strictly increasing transformations of the random variables. Frequently applied data transformations do not change the copula.
- Random variables $X_1, \ldots, X_n$ are stochastically independent if and only if their copula is the product copula $\Pi^n(\mathbf{u}) = \prod_{i=1}^n u_i$.
- Bivariate copulas are directly related to the Spearman-ρ correlation coefficient:

$$\rho(X_1, X_2) = 12 \int_0^1 \int_0^1 C(u_1, u_2) du_1 du_2 - 3$$

Copulas in Geostatistics

How to incorporate copulas into the geostatistical framework?
The copula becomes a function of the separating vector $\mathbf{h}$ and does not depend on the location (due to the stationarity). The dependence of any two locations separated by the vector $\mathbf{h}$ is described by

$$P\left(Z\left(\mathbf{x}\right) \leq z_1, Z\left(\mathbf{x}+\mathbf{h}\right) \leq z_2\right) = C_{\mathbf{h}}\left(F_Z\left(z_1\right), F_Z\left(z_2\right)\right),$$

where F_Z is the univariate distribution of the random process and is assumed to be the same for each location $\mathbf{x}$. (Bardossy, 2006)

It is advantageous to work with copulas constructed from elliptical distributions since the correlation matrix explicitly appears in their analytical expression and can be parameterized by a correlation function model.

Examples

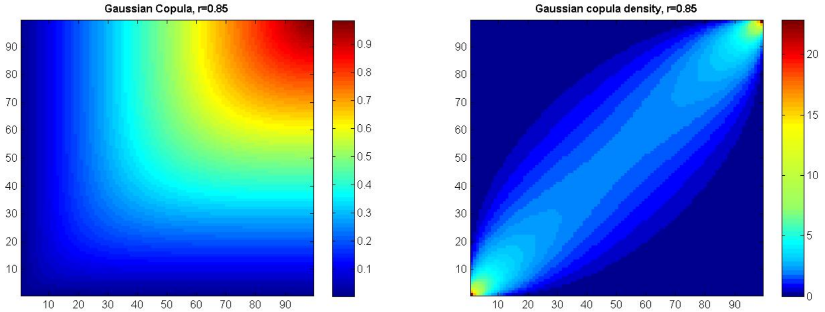
- Gaussian Copula: $C(u_1, \ldots, u_n) = \mathbf{\Phi}_{\mathbf{0},\mathbf{\Sigma}}\left(\Phi^{-1}(u_1), \ldots, \Phi^{-1}(u_n)\right)$.
- χ^2-copula (Bardossy)

The Gaussian Spatial Copula

Sklar's Theorem provides a simple way of constructing copulas from multivariate distributions. The Gaussian copula is

$$C_{\mathbf{\Sigma}}^{G}\left(u_1,\ldots,u_n\right) = \mathbf{\Phi}_{\mathbf{0},\mathbf{\Sigma}}\left(\Phi^{-1}\left(u_1\right),\ldots,\Phi^{-1}\left(u_n\right)\right).$$

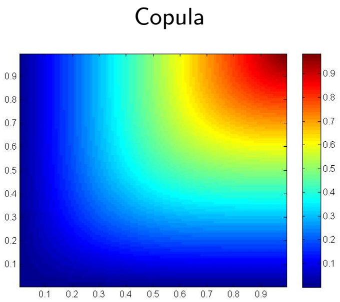
Parameterize the correlation matrix $\mathbf{\Sigma}$ by one of the well-known geostatistical correlation function models. The Gaussian copula is radially symmetric, which is quite restrictive: $c_{\mathbf{\Sigma}}^{G}\left(u_1,\ldots,u_n\right) = c_{\mathbf{\Sigma}}^{G}\left(1-u_1,\ldots,1-u_n\right)$.

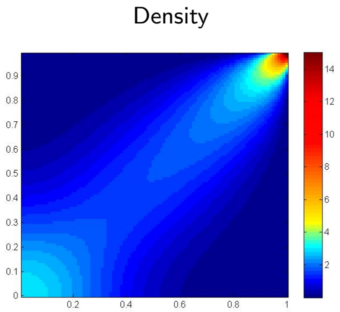


Non-central χ^2-Copula

Bivariate non-central χ^2-copula

Bivariate non-central χ^2-copula, where the underlying bivariate Gaussian random variable has correlation $r = 0.85$ and mean $m = 1$. Not radially symmetric but symmetric.





Parameter Estimation for Cont. Marginals

Maximum Likelihood

Let $\mathbf{\Theta} = (\boldsymbol{\theta}, \boldsymbol{\lambda})$ be the parameter vector, where $\boldsymbol{\theta}$ are the correlation function (and anisotropy) parameters and $\boldsymbol{\lambda}$ are the parameters of the known family of univariate distributions F.

$$l\left(\mathbf{\Theta}; Z\left(\mathbf{x}_1\right), \ldots, Z\left(\mathbf{x}_n\right)\right) =$$

$$c_{\theta}\left(F_{\lambda}\left(Z\left(\mathbf{x}_1\right)\right), \ldots, F_{\lambda}\left(Z\left(\mathbf{x}_n\right)\right)\right) \prod_{i=1}^{n} f_{\lambda}\left(Z\left(\mathbf{x}_i\right)\right)$$

Model-Based Approach

Plug-In Estimator

We use the predictive distribution in the **rank space**. Taking the ML-estimations, $\hat{\mathbf{\Theta}}$, as the true values we arrive at the plug-in estimator

$$\hat{z}(\mathbf{x}_0) = E\left(z(\mathbf{x}_0) \mid z(\mathbf{x}_1), \ldots, z(\mathbf{x}_n), \hat{\Theta}\right).$$

The estimator can therefore be obtained as

$$\hat{z}(\mathbf{x}_0) = \int_0^1 \underbrace{F_\lambda^{-1}(u(\mathbf{x}_0))}_{\text{Jacobian}} \underbrace{c_\theta(u(\mathbf{x}_0) \mid u(\mathbf{x}_1), \ldots, u(\mathbf{x}_n))}_{\text{conditional copula}} du(\mathbf{x}_0).$$

Not difficult with Gaussian copula

Equivalence

The trans-Gaussian kriging model using any strictly monotone transformation is equivalent to the Gaussian spatial copula model.

Proof follows from the invariance under strictly increasing transformations and the radial-symmetry of the Gaussian distribution.

Advantages of copula Kriging

- Any other copula different from the Gaussian copula can be used which leads to a generalization of trans-Gaussian kriging
- Even if we stay within the Gaussian framework, it is simpler to specify a family of marginal distributions than to determine a suitable transformation function, especially for multi-modal and extreme-value data
- Full predictive distribution is available and can be used to calculate predictive quantiles, confidence regions and prediction variance
- Easily extendable to a Bayesian approach
- Shares properties with kriging such as being exact at known locations
- Incorporating covariates is easy to do

EC-STREP "INTAMAP" (Interoperability and Automatic Mapping)

- Main objective of this project (IST, FP6): develop an interoperable framework for real time automatic mapping of critical environmental variables by extending spatial statistical methods and employing open, web-based, data exchange and visualisation tools.
- Project includes partners from Austria, Germany, Netherlands, Italy, Great Britain and Greece, for further information see
- `www.intamap.org`

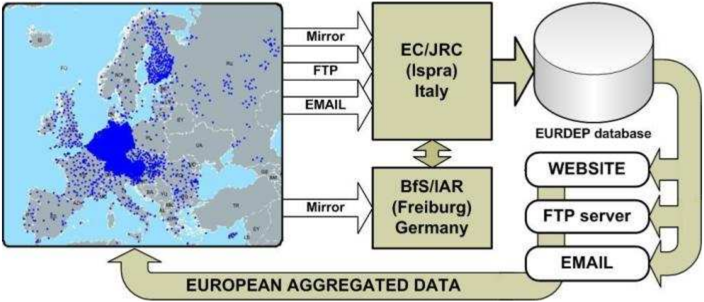
Main application:

System for automated mapping of radiation levels reported by 30 European countries participating in

EURDEP = European Radiological Data Exchange Platform

Data availability in nearly real-time (more and more on an hourly basis) currently: > 4200 stations

EURDEP Data Flow

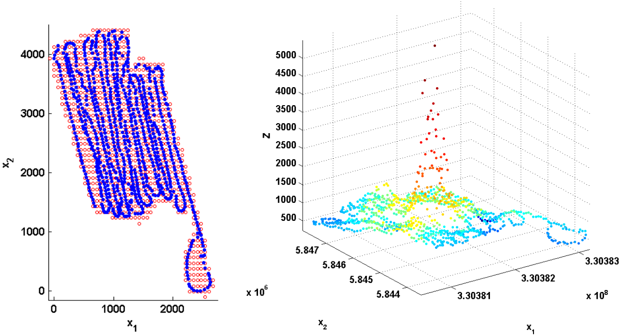


An overview

of the achievements of the INTAMAP-Project, including prototype demonstration + specific workshops by the project partners, was given at

Int. StatGIS 2009 Conference,
"Geoinformatics for Environmental Surveillance"
Milos, Greece, June 17-19, 2009

Helicopter Data Set



Helicopter data

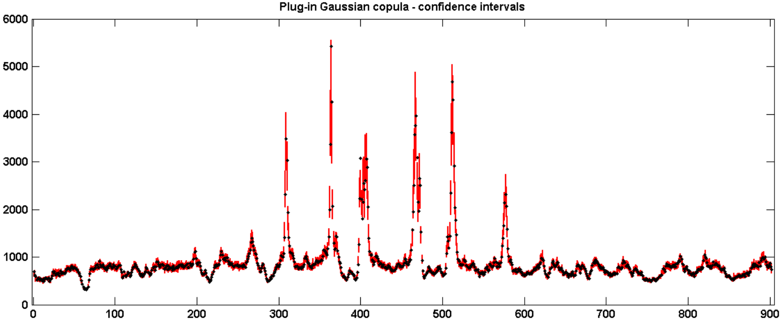
Measurements of gamma dose rates in Oranienburg, Germany. Log-normal marginals are not right-skewed enough to model the radioactivity hotspots. Therefore, use of the generalized extreme value distribution: $\boldsymbol{\lambda} = (\mu, \sigma, K)$.

	n	Min	Mean	Median	Max	Stand. dev.	Skewness
Heli	902	313	863.92	780.5	5420	482.06	4.74

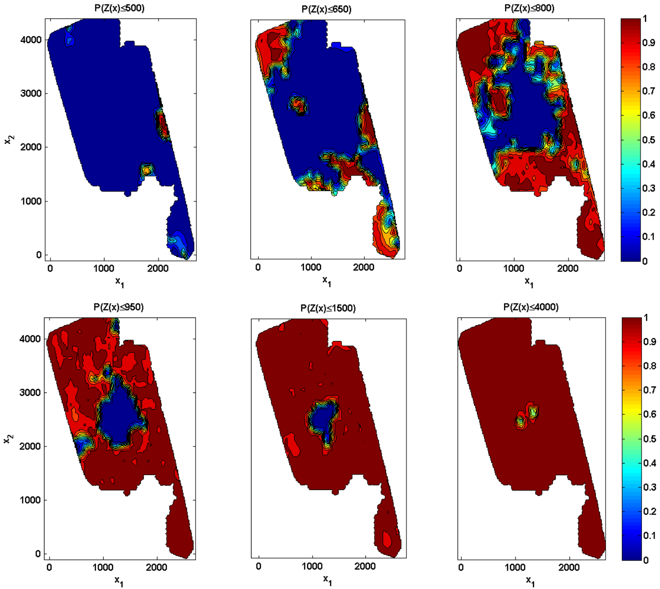
Analysis of Helicopter Data I

Analysis using the copula-based approach

- The Gaussian spatial copula is used
- Geometric anisotropy is considered
- Correlation function model is chosen to be a Matern model including a nugget effect: ϑ_1, ϑ_2, κ
- Parameter point estimates are obtained using maximum likelihood



Analysis of Helicopter Data II



Analysis of Helicopter Data III

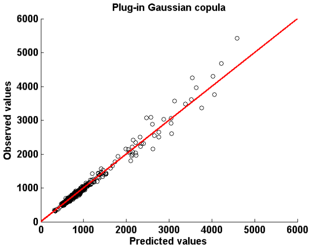
Cross-Validation

	GC	IDW	OK	PSGP	TGK
RMSE	72.38	167.15	149.57	104.07	85.90
MAE	34.74	63.19	55.95	41.73	37.69

The approaches using the Gaussian copula (GC) clearly outperform Inverse Distance Weighting (IDW), Ordinary kriging (OK), Projected Sequential Gaussian Processes (PSPG) and trans-Gaussian kriging (TGK) with the Box-Cox transformation.

Conclusion

Copulas can be used to flexibly describe spatial dependence and to perform spatial interpolation. Geostatistical methods using copulas are very much suited to model spatial extremes.



Software I

Main properties of the R-Software

- Code for estimation of parameters and prediction at unobserved locations in the case of the Gaussian spatial copula model and the non-central χ^2-copula model with continuous marginals is part of the `intamap` R-library. It is freely available from `https://sourceforge.net/projects/intamap`.
- Automatic choice of marginal distribution, correlation function model, anisotropy and starting values by using certain heuristics.
- Additionally, the `intamap` library performs
  - Inverse Distance Weighting (library `gstat`),
  - Ordinary Kriging (library `gstat`),
  - Projected Sequential Gaussian Processes (library `psgp`),
  - Trans-Gaussian Kriging (library `gstat`).
- The `intamap` package will be also available from CRAN soon.

Software II

Commands

There are two main functions, `estimateParameters.copula` and `spatialPredict.copula`, that perform parameter estimation and spatial prediction for an `intamapObject` of the class copula.

```
intamapObject<-createIntamapObject(observations=observations,
predictionLocations=predictionLocations,class="copula")
```

It is possible to work with trend surface models by setting the argument `formulaString` of the `intamapObject` accordingly. The requested prediction types are defined by the argument `outputWhat`:

```
outputWhat = list(mean = TRUE, variance = FALSE, excProb = 10,
excprob = 20, quantile = 0.025, quantile = 0.975)
```

The user has the choice to specify the correlation function model, anisotropy and starting values of the optimization himself or to let the program choose them.

Software III

The interpolate-Function

The `interpolate` function of the `intamap` R-package is designed for automatic spatial modeling and interpolation. The function decides which of the following three interpolation methods to apply: `automap` (ordinary kriging as implemented in the R-package `automap`), `psgp` and `copula`. If `copula` is chosen

1. the function `estimateAnisotropy` decides whether to include geometric anisotropy into the analysis or not,
2. `autofitVariogram` of the `automap` R-library is used to select a correlation model and starting parameters for the corresponding parameters,
3. the Gaussian, the log-Gaussian, the Student-t, the generalized extreme value (GEV) and the logistic distribution are tested and the best fitting one is chosen,
4. the Gaussian copula is used.

Software IV

Computation Time

Computation time is a major issue for the spatial copula algorithms. The following will influence the computational load:

- The number of observations.
- For the non-central χ^2-copula model computation will take much longer since a composite-likelihood approach is used.
- If the Matern model is chosen, the algorithm will be slower because the `besselk` function needs to be evaluated and there is one additional parameter.
- If the GEV distribution is chosen, the algorithm will be slower because there are three parameters to optimize instead of only two.
- Additionally accounting for covariates slows down the estimation process, since regression parameters are introduced and need to be optimized.
- Prediction is slower when quantiles of the predictive distribution are requested. This is because an integral equation is solved numerically.
- "Good" initial values for the optimization reduce the computational load since fewer iterations are needed to reach convergence.

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