Spatio-temporal modelling of environmental monitoring data

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October 1, 2015

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- Cocchi *et al.* (2007) **Hierarchical space-time modelling of PM_{10} pollution**, under the Bayesian framework, use data from 11 spatial locations collected over 1096 days
- Mitchell *et al.* (2005) **Testing for separability of space-time covariances**, aiming to study the effect of high levels of CO_2 on rice, use data from 13 spatial locations and 112 time points and test the separability of the proposed spatio-temporal model by rearranging the data as in the context of multivariate repeated measures
- Bruno *et al.* (2003) **Non-separability of space-time covariance models in environmental studies**, use a data set consisting of daily ozone measurements made at 32 monitoring locations, for the period 1998-2002, enabling the identification of the temporal variability which, when removed, leaves separable space and time correlation components

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There are cases, however, where data are collected over several locations but only few times, disabling the use of time series techniques.

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- Geostatistical models allow to interpolate the response variable at non-sampled locations, weighting values at nearby locations

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- Spatio-temporal geostatistical models take into account not only *where* data was collected, but also *when* they were collected
- Extending the spatial framework to the spatio-temporal framework is more than just the inclusion of one more dimension. It must reflect the diference in nature of the two dimensions involved

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- Developed in two stages
  - extending an existing model by including covariates
  - proposing a model suitable for studies with sparse time dimension

Application: environmental monitoring in mainland Portugal

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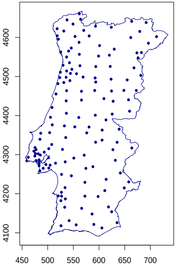

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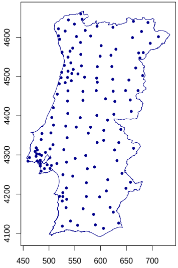

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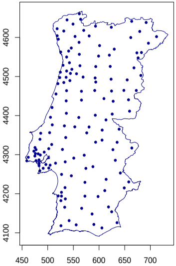

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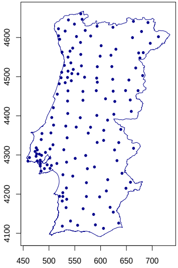

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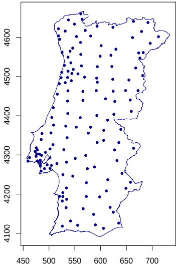

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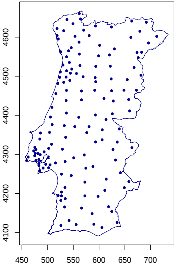

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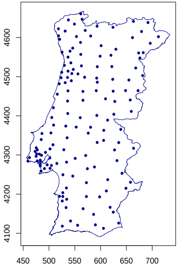

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  - spatial model with / without covariate included
  - spatio-temporal model with / without covariate included

Data summary of Mn concentration (observed and Box-Cox transformed values)

	Survey					
	1992		1996		2002	
	Observ.	Transf.	Observ.	Transf.	Observ.	Transf.
Min	16.00	3.39	4.03	1.54	23.14	3.96
Median	123.50	6.90	149.18	7.28	123.20	6.89
Max	970.00	11.63	685.55	10.73	503.11	9.97
Mean	161.62	6.88	178.62	7.13	147.12	6.85
St. dev.	147.97	1.69	136.01	1.65	99.28	1.41

Data summary of Pb concentration (observed and Box-Cox transformed values)

	Survey					
	1992		1996		2002	
	Observ.	Transf.	Observ.	Transf.	Observ.	Transf.
Min	0.50	-0.67	2.00	0.71	0.68	-0.38
Median	13.00	2.78	15.70	2.99	3.11	1.17
Max	172.00	6.04	191.17	6.18	109.93	5.44
Mean	16.40	2.75	21.72	3.03	5.40	1.29
St. dev.	16.91	0.86	24.05	0.92	10.39	0.90

One spatio-temporal model

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- Extending the model allowing for the inclusion of spatial covariates

$$M_1(\mathbf{s}) = \sum_{i=1}^{p} \beta_i f_i(\mathbf{s})$$

Summary of predicted concentration for the 2002 survey (with interpolation errors)

		Spatial model				Spatio-temporal model			
		without covar.		with covar.		without covar.		with covar	
Mn									
	Min	4.88	(1.04)	4.39	(1.03)	4.87	(0.92)	4.30	(0.80)
	Median	6.99	(1.26)	7.57	(1.25)	7.21	(1.16)	7.53	(1.07)
	Max	8.59	(1.47)	8.58	(1.37)	8.72	(1.45)	8.93	(1.18)
	Mean	6.97	(1.26)	7.40	(1.24)	7.03	(1.17)	7.37	(1.06)
	St. dev.	0.63	(0.12)	0.63	(0.09)	0.73	(0.14)	0.66	(0.12)
Pb									
	Min	0.19	(0.70)	0.13	(0.66)	0.67	(0.59)	0.61	(0.59)
	Median	1.19	(0.88)	0.89	(0.85)	1.15	(0.66)	0.87	(0.63)
	Max	3.01	(0.94)	3.25	(0.89)	2.16	(0.70)	2.00	(0.65)
	Mean	1.20	(0.86)	0.99	(0.83)	1.16	(0.66)	0.84	(0.63)
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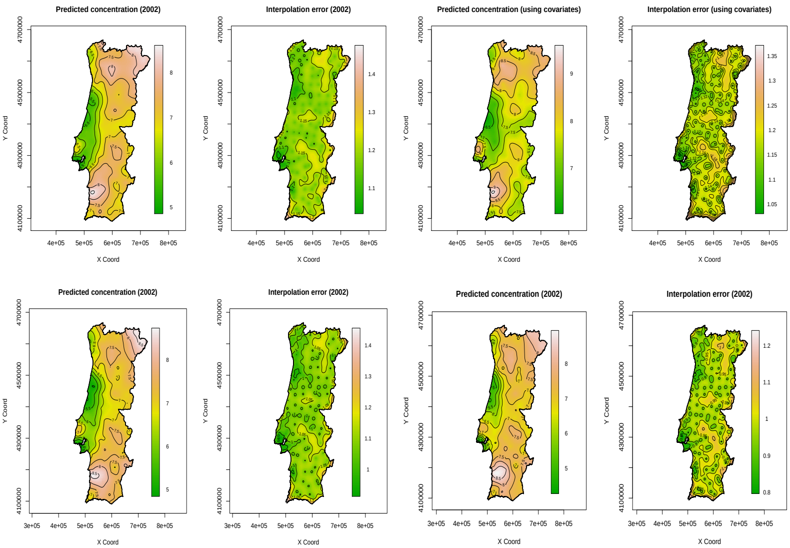
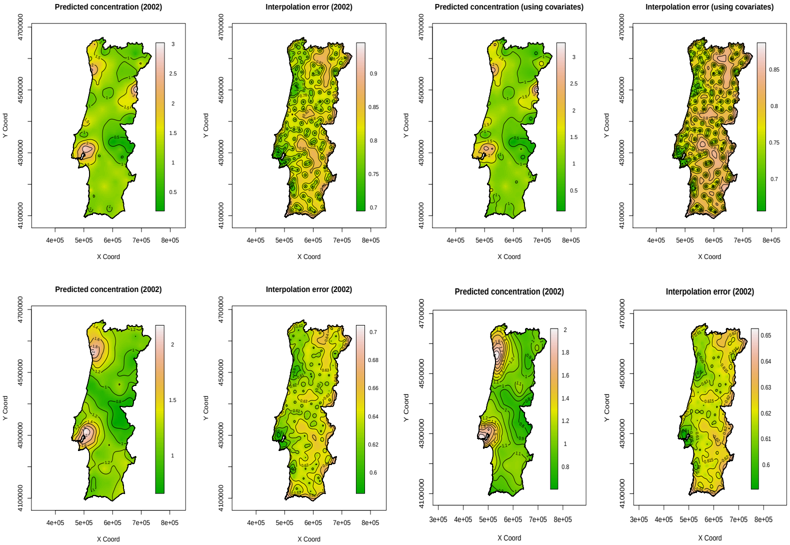
- The inclusion of covariate corrects underestimation of Mn and overestimation of Pb
- Lower amount of interpolation error attained by the most informative model



Prediction and interpolation error maps for Mn (top row: spatial models, bottom row: spatio-temporal models; 2 left panel: without covariates, 2 right panel: with covariates)



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Mean and standard deviation of the APE

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	MAPE	0.95	0.93	0.94	0.92
	Sd(APE)	0.65	0.65	0.64	0.65
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- Details in Margalho L., Menezes R., Sousa I. (2014). *Assessing interpolation error for space–time monitoring data*, Stochastic Environmental Research and Risk Assessment, 28:1307–1321

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- Gaussian space-time measurement errors,

$$\boldsymbol{\varepsilon} \sim MVN\left(\mathbf{0}, \tau^2 I_{NT}\right)$$

- Assuming a separable covariance structure,

$$
\begin{aligned}
\Sigma^{i,j,k,l} &= \mathrm{Cov}_{ST}\left[Z(\mathbf{s}_i, t_k), Z(\mathbf{s}_j, t_l)\right] \\
&= \mathrm{Cov}_S\left(\|\mathbf{s}_i - \mathbf{s}_j\|\right) \times \mathrm{Cov}_T\left(|t_k - t_l|\right) \\
&= \mathrm{Cov}_S\left(h_S\right) \times \mathrm{Cov}_T\left(h_T\right)
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- Two interpretations for Σ,
  - $\Sigma(h_{\boldsymbol{S}}, h_{\boldsymbol{T}}) = \sigma^{\mathbf{2}}_{\boldsymbol{total}} R_{\boldsymbol{S}}(h_{\boldsymbol{S}}) \otimes R_{\boldsymbol{T}}(h_{\boldsymbol{T}})$ (Rodriguez-Iturbe & Mejia (1974))

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- Number of temporal correlation parameters equals the number of temporal observations: saturated temporal correlation model.

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  - indexed in space: sampling locations intensity
  - indexed in time: specific contribution of a given survey

Predicted Mn concentration for the 2002 survey and interpolation error values

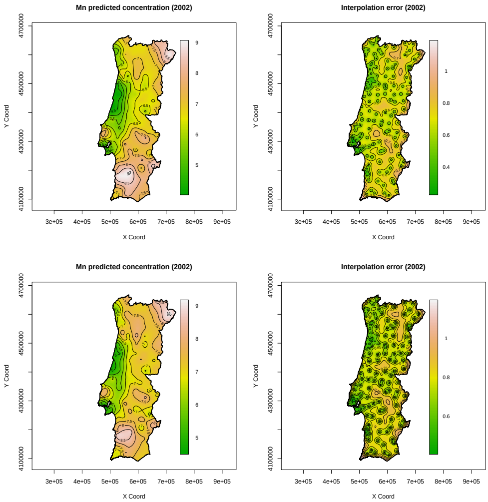
	Covariance as a function of σ^2_{total}		Covariance as a function of σ^2_S and σ^2_T	
	Predicted	Error	Predicted	Error
Min	4.05	0.23	4.53	0.41
Median	7.10	0.72	7.21	0.79
Max	9.05	1.19	9.16	1.19
Mean	6.92	0.78	7.09	0.85
St. dev.	0.92	0.23	0.74	0.19

- Better results in terms of interpolation error comparing with the previous model (Margalho *et al*, 2014)

Predicted Mn concentration for the 2002 survey and interpolation error values

	Covariance as a function of σ^2_{total}		Covariance as a function of σ^2_S and σ^2_T	
	Predicted	Error	Predicted	Error
Min	4.05	0.23	4.53	0.41
Median	7.10	0.72	7.21	0.79
Max	9.05	1.19	9.16	1.19
Mean	6.92	0.78	7.09	0.85
St. dev.	0.92	0.23	0.74	0.19

- Better results in terms of interpolation error comparing with the previous model (Margalho *et al*, 2014)
- Cross-validation study presents equal values of Mean Absolute Prediction Error for either interpretation of Σ



Prediction map for the 2002 survey (left) and the associated interpolation error map (right) for Mn transformed data, considering σ^2_{total} (top row), or σ^2_S and σ^2_T (bottom row)

R Code in the simulation study

- Finding locations

```
gera.locs<-function(num1,num2){
x1<-runif(num1,0,10)
y1<-runif(num1,0,10)
x2<-runif(num2,4.5,5.5)
y2<-runif(num2,4.5,5.5)
x<-c(x1,x2)
y<-c(y1,y2)
locs<-cbind(x,y)
return(locs)}
```

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x<-c(x1,x2)
y<-c(y1,y2)
locs<-cbind(x,y)
return(locs)}
```

- Design matrix

```
design.matrix<-function(intens){
c1<-rep(1,Num.Loc*Num.Temp)
c2<-rep(intens,Num.Temp)
c3<-c(rep(0,Num.Loc),rep(1,Num.Loc),rep(0,Num.Loc))
c4<-c(rep(0,Num.Loc),rep(0,Num.Loc),rep(1,Num.Loc))
M<-cbind(c1,c2,c3,c4)
return(M)}
```

- Spatial correlation matrix

```
mx.corr.spat<-function(locs,phi){
a<-as.matrix(dist(locs))
expon<-exp(-(1/exp(phi))*a)
return(expon) }
```

- Spatial correlation matrix

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mx.corr.spat<-function(locs,phi){
a<-as.matrix(dist(locs))
expon<-exp(-(1/exp(phi))*a)
return(expon) }
```

- Temporal correlation matrix

```
mx.corr.temp<-function(r12,r13,r23){
qsi<-matrix(c(1,r12,r13,r12,1,r23,r13,r23,1),ncol=3,byrow=T)
return(qsi) }
```

- Covariance matrix

```
matrix.cov<-function(sigma2s,sigma2t,tau2,spat,temp){
mx.sigma<-kronecker(spat,temp)
mx.cov<-exp(sigma2s+sigma2t)*mxsigma+exp(tau2)*diag(Num.Loc*Num.Temp)
return(mx.cov) }
```

- Covariance matrix

```
matrix.cov<-function(sigma2s,sigma2t,tau2,spat,temp){
mx.sigma<-kronecker(spat,temp)
mx.cov<-exp(sigma2s+sigma2t)*mxsigma+exp(tau2)*diag(Num.Loc*Num.Temp)
return(mx.cov) }
```

- Log-likelihood

```
log.lik<-function(ro12,ro13,ro23,sigma2s,sigma2t,tau2,phi,ygeodataST){
ydata<-ygeodataST$data
M<-design.matrix(int50-mean(int50))
corr.spat<-mx.corr.spat(locs.true,phi)
corr.temp<-mx.corr.temp(ro12,ro13,ro23)
V<-matrix.cov(sigma2s,sigma2t,tau2,corr.spat,corr.temp)
beta.hat<-solve(t(M)%*%solve(V)%*%M)%*%t(M)%*%solve(V)%*%ydata
LL<-((-Num.Loc*Num.Temp)/2)*log(2*pi)-(1/2)*log(det(V))-(1/2)*((t(ydata-
M%*%beta.hat))%*%solve(V)%*%(ydata-M%*%beta.hat))
return(LL)}
```

- Function to optimize

```
f.optim<-function(param){
load(file="ygeodataST.RData")
ro12<-param[1]
ro13<-param[2]
ro23<-param[3]
sigma2s<-param[4]
sigma2t<-param[5]
tau2<-param[6]
phi<-param[7]
valor<-log.lik(ro12,ro13,ro23,sigma2s,sigma2t,tau2,phi,ygeodataST)
return(-valor)}
```

- Function to optimize

```
f.optim<-function(param){
load(file="ygeodataST.RData")
ro12<-param[1]
ro13<-param[2]
ro23<-param[3]
sigma2s<-param[4]
sigma2t<-param[5]
tau2<-param[6]
phi<-param[7]
valor<-log.lik(ro12,ro13,ro23,sigma2s,sigma2t,tau2,phi,ygeodataST)
return(-valor)}
```

- Optimization

```
my.likfit<-function(ygeodataST,ini.pars){
save(ygeodataST,file="ygeodataST.RData")
opt<-optim(ini.pars,foptim,method="L-BFGS-
B",lower=lower.pars,upper=upper.pars,control=list(maxit=1000))
return(list(conv=optconvergence, params = optpar)) }
```