

# Project2

## Gaussian random field with application of INLA

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## Part I Multivariate normal distribution

Let  $\mathbf{x} = (x_1, \dots, x_n), n = 100$  be multivariate normal distributed with  $E(x_i) = 0, Var(x_i) = 1$ , and  $Corr(x_i, x_j) = e^{-0.1|i-j|}$

- a) Compute and image the covariance matrix  $\Sigma$  of  $\mathbf{x}$
  - b) Find the lower Cholesky factor  $\mathbf{L}$ , such that  $\mathbf{L}\mathbf{L}^T = \Sigma$ , of this covariance matrix, and image.
  - c) Sample  $\mathbf{x} = \mathbf{L}\mathbf{z}$ , where  $\mathbf{z}$  is a length n random vector of independent standard normal variables. Plot the sample.
  - d) Find the precision matrix  $\mathbf{Q}$  of the covariance matrix, and compute the lower Cholesky factor  $\mathbf{L}_Q$ , such that  $\mathbf{L}_Q\mathbf{L}_Q^T = \mathbf{Q}$ , of this matrix. Image these matrices and compare them to the images obtained in a) and b)
  - e) Sample  $\mathbf{x}$  by solving  $\mathbf{L}_Q^T\mathbf{x} = \mathbf{z}$ , where  $\mathbf{z}$  is a length n random vector of independent standard normal variables. Plot the sample.
  - f) Permute the ordering of variables in  $\mathbf{x}$ , and redo the exercises.
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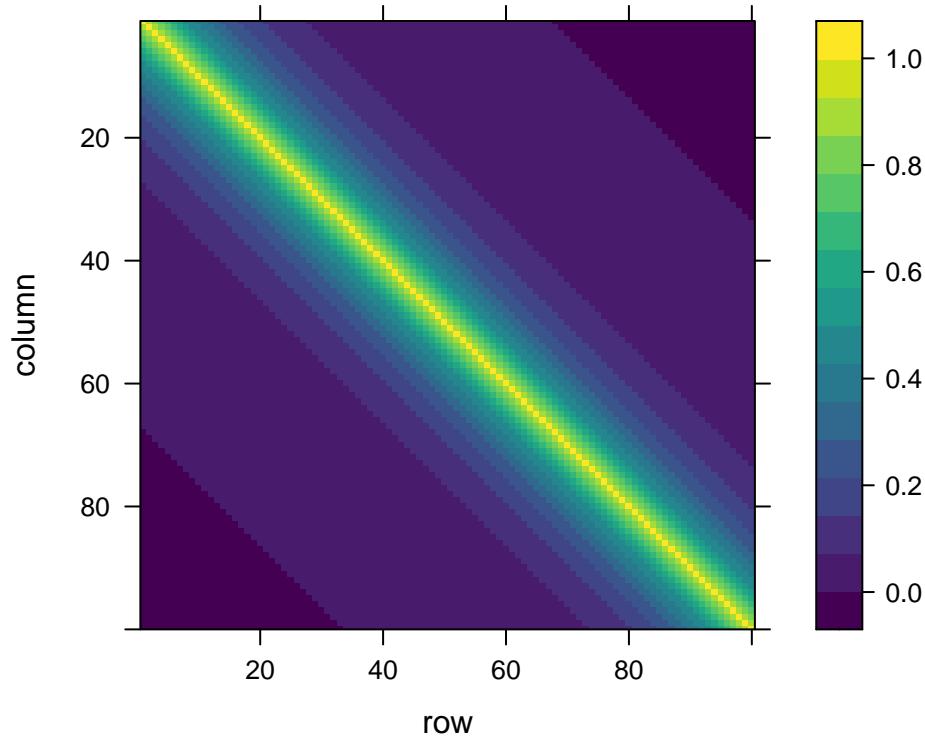
## Solution to Part I

a)

Given that  $\Sigma = e^{-0.1|i-j|}$ . The covariance matrix can be expressed as follows:

$$\Sigma = \begin{pmatrix} 1 & e^{-0.1h_{12}} & \dots & e^{-0.1h_{1n}} \\ e^{-0.1h_{21}} & 1 & \dots & e^{-0.1h_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-0.1h_{n1}} & e^{-0.1h_{n2}} & \dots & 1 \end{pmatrix}$$

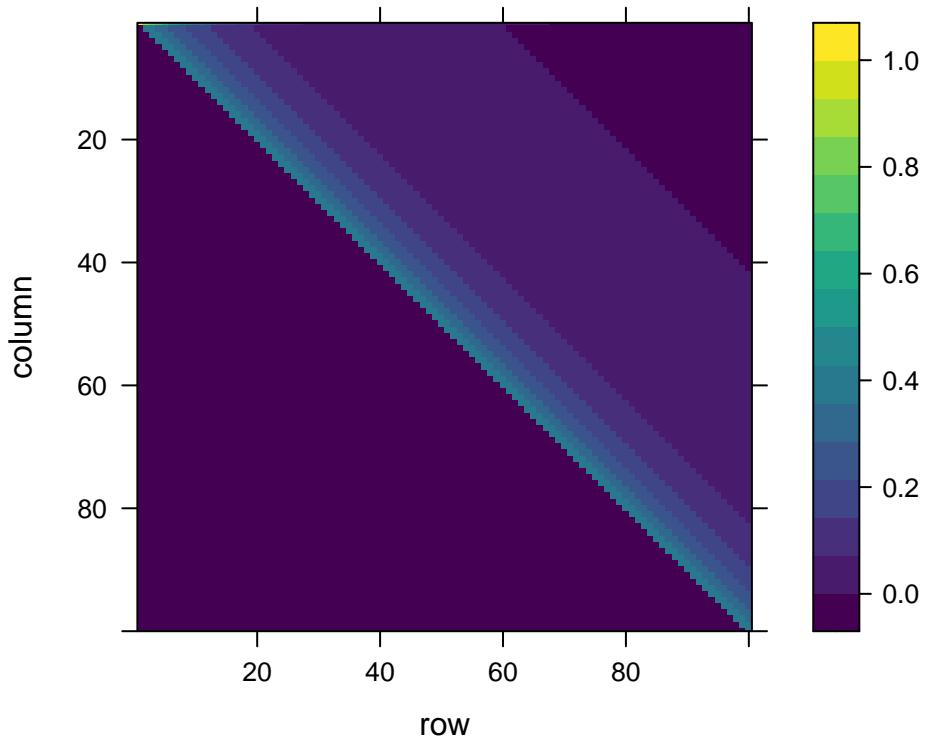
**Covariance matrix**



b)

According to the cholesky decomposition rule,  $\mathbf{L}$  is the lower triangular matrix for  $\Sigma$ , it can be easily computed from R using `L = chol(Sigma)`. It is then plotted as below.

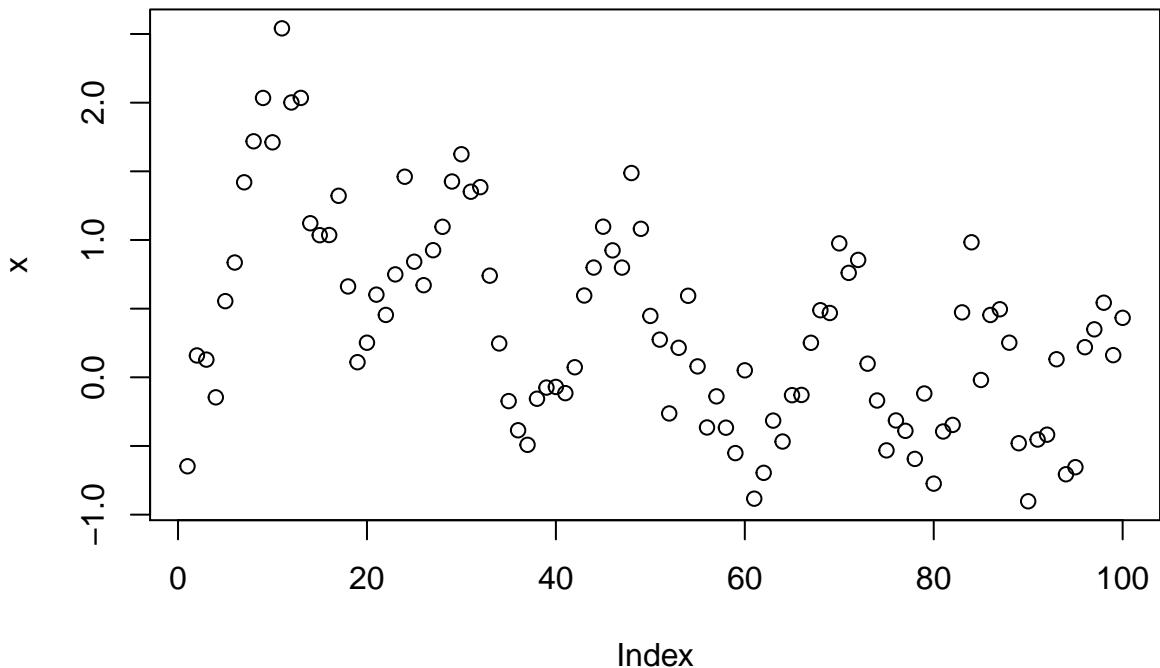
### Lower triangular matrix



c)

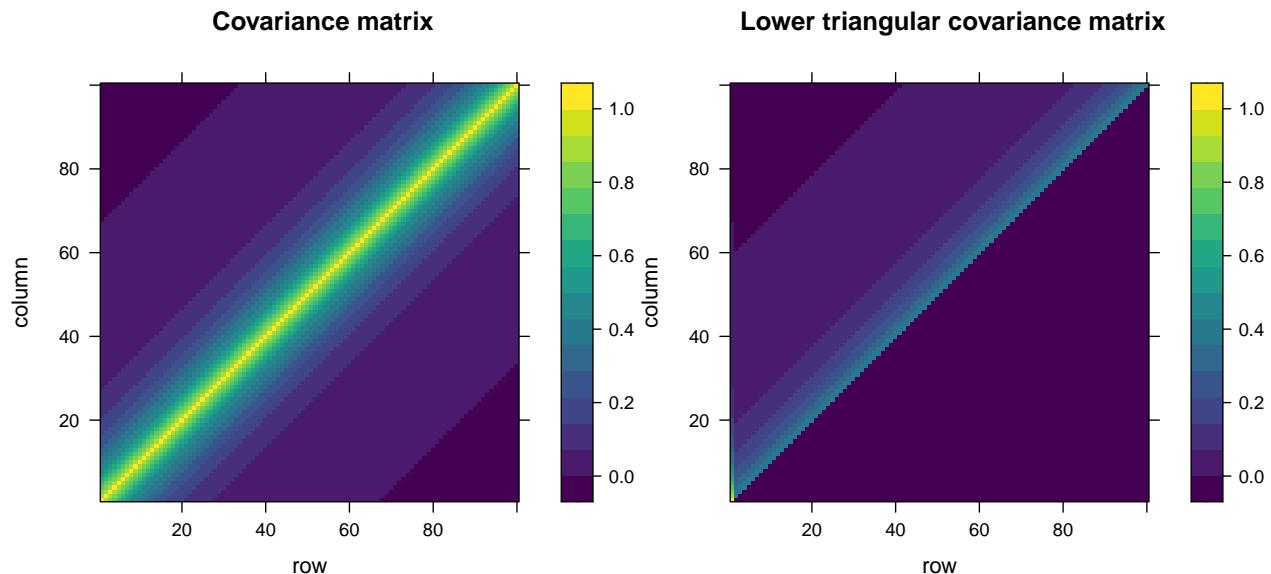
Sample using  $\mathbf{x} = \mathbf{L}\mathbf{z}$  transforms the zero-mean, standard normal random variables to the random variables with the desired covariance matrix.

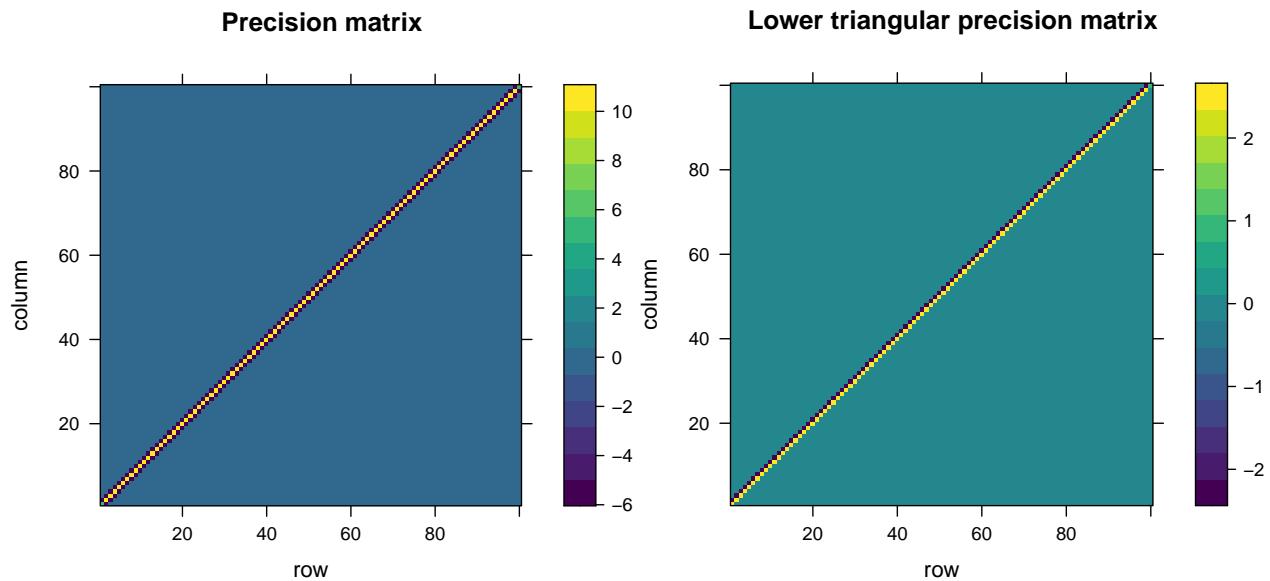
## Random samples given the covariance



d)

The precision matrix  $\mathbf{Q}$  is the inverse of the covariance matrix  $\Sigma$ , it is computed using `Q = solve(Sigma)` in R. The three matrices are thereby depicted as follows. Since the covariance matrix is not singular, given that it belongs to the Matern family, thus it is analytically guaranteed to have positive definite property. Therefore, both precision matrix and the lower triangular precision matrix exist.

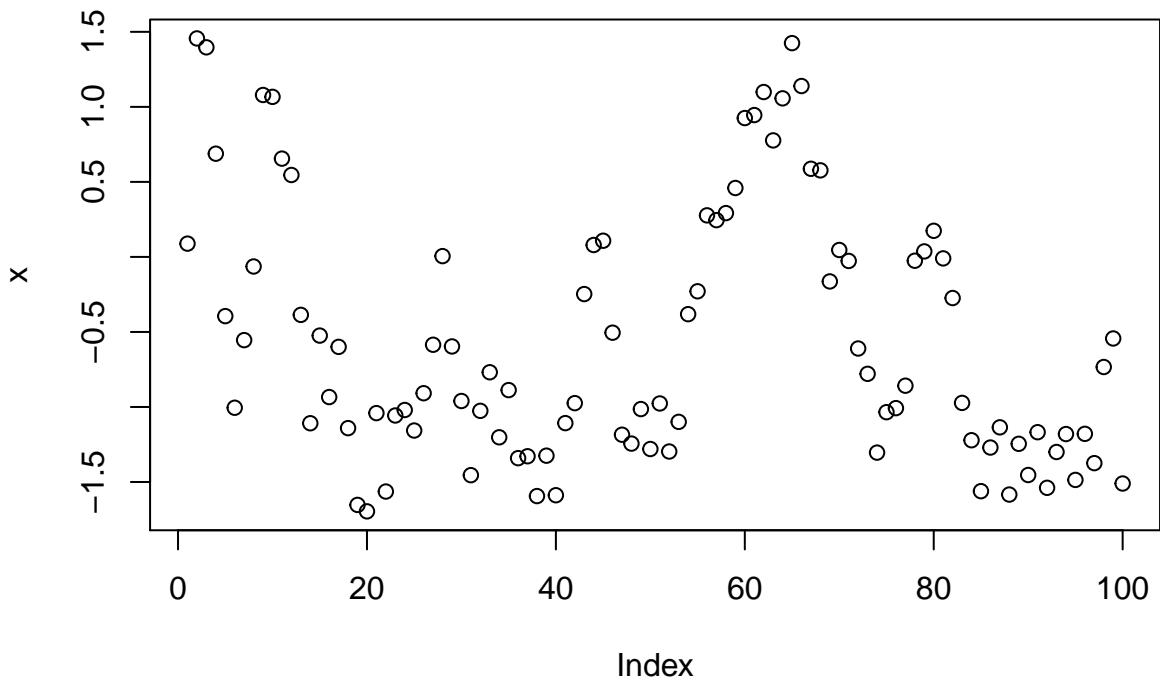




e)

Similarly, the expected random samples can be generated using the inversion of the above formula, thus  
 $\mathbf{L}_Q^T \mathbf{x} = \mathbf{z}$

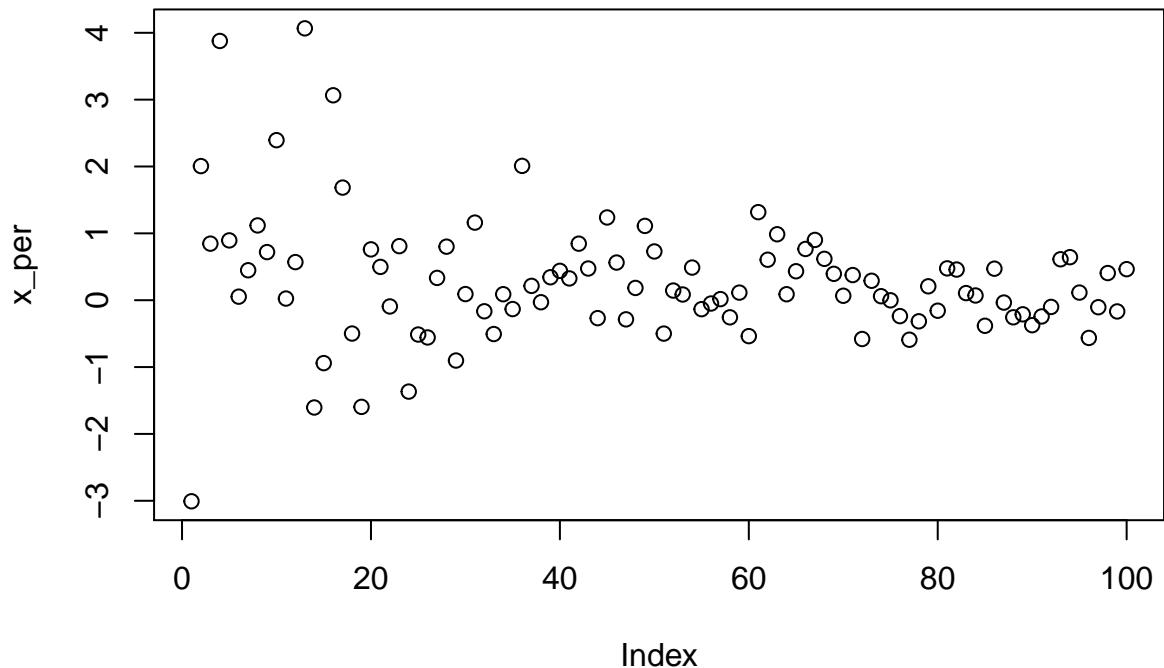
### Random samples using inversion rule



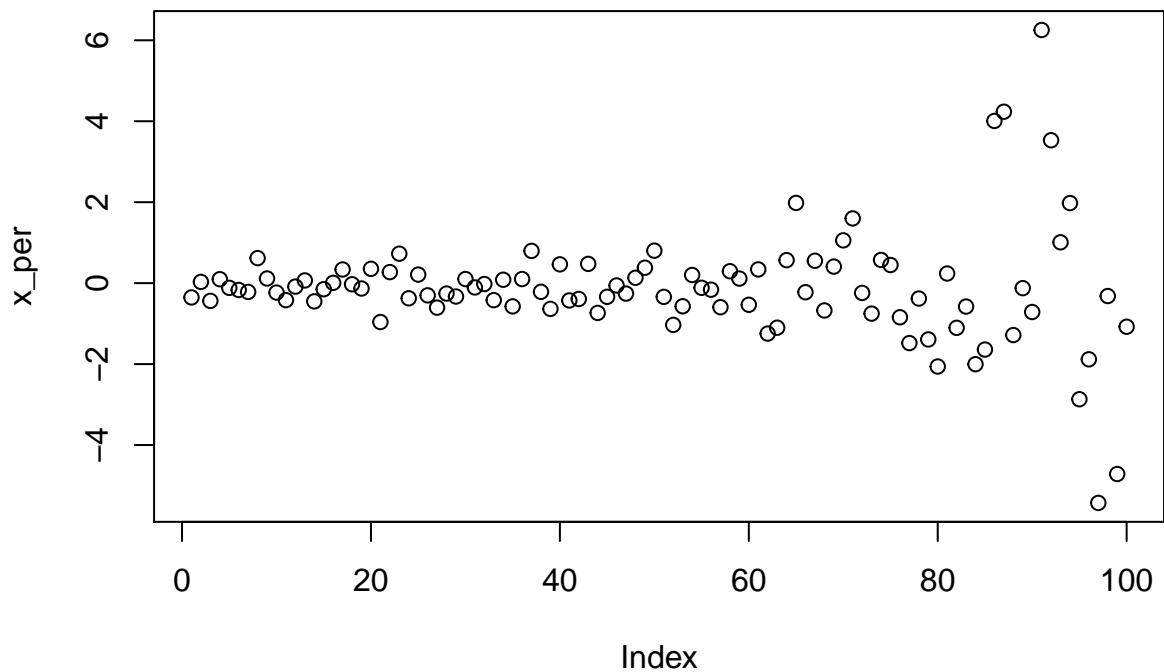
f)

Permute  $\mathbf{x}$  to make randomise the ordering of the grid, the associated covariance matrix can be thereby modified in a sparse way.

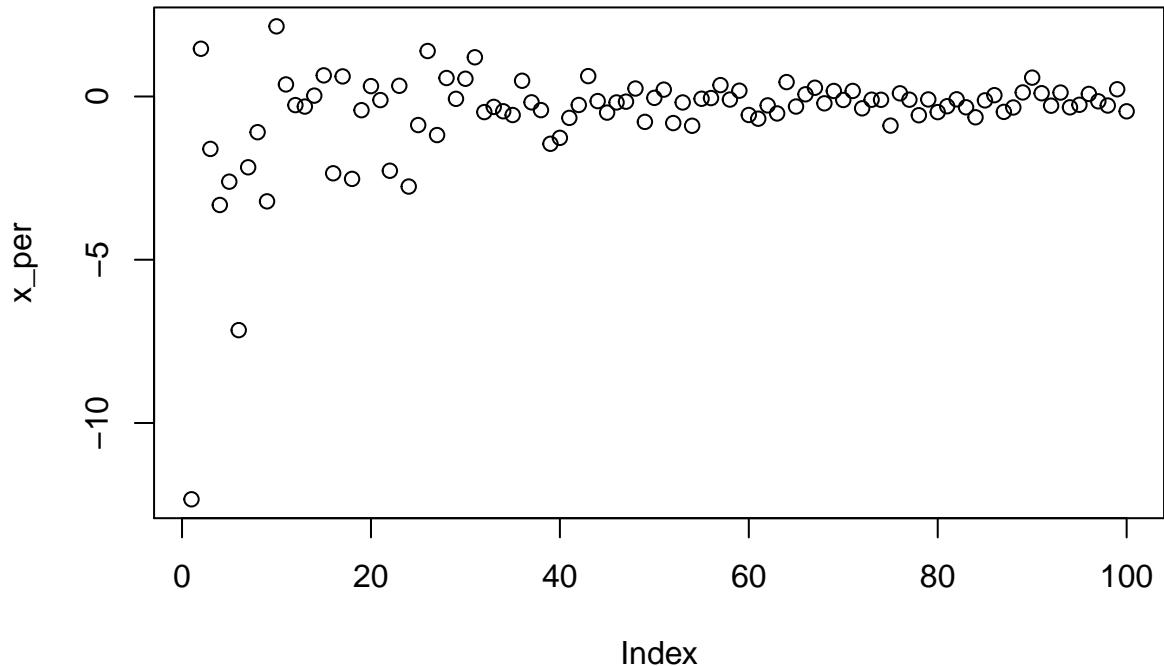
### **1 Permuted random samples given the covariance**



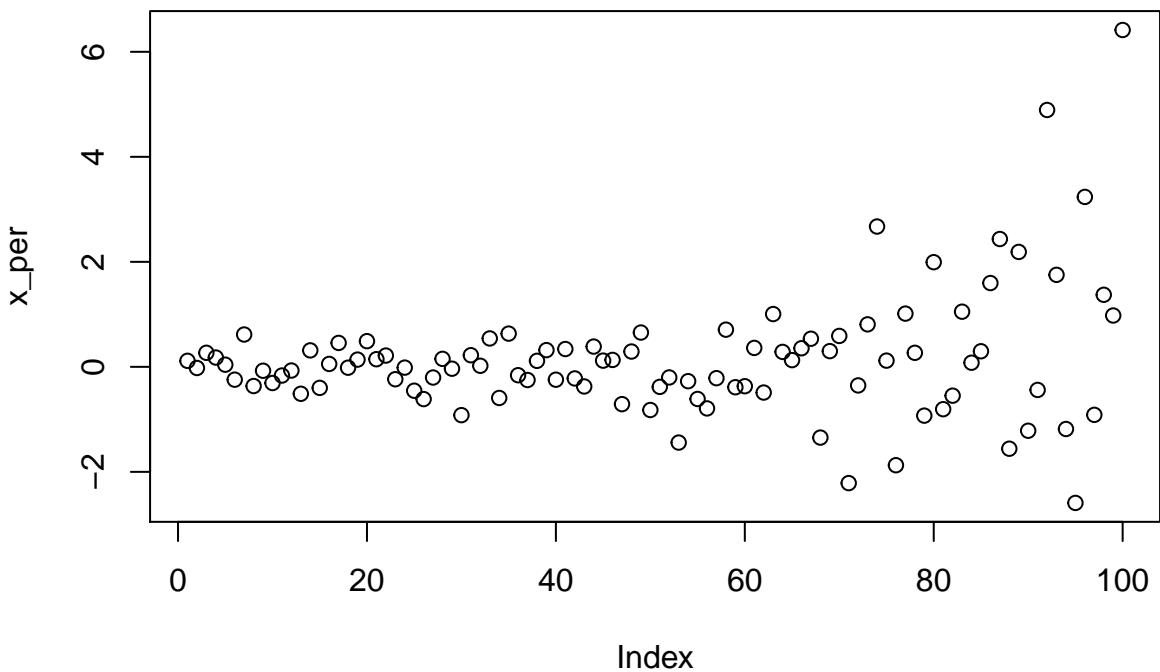
### **1 Permuted random samples using inversion rule**



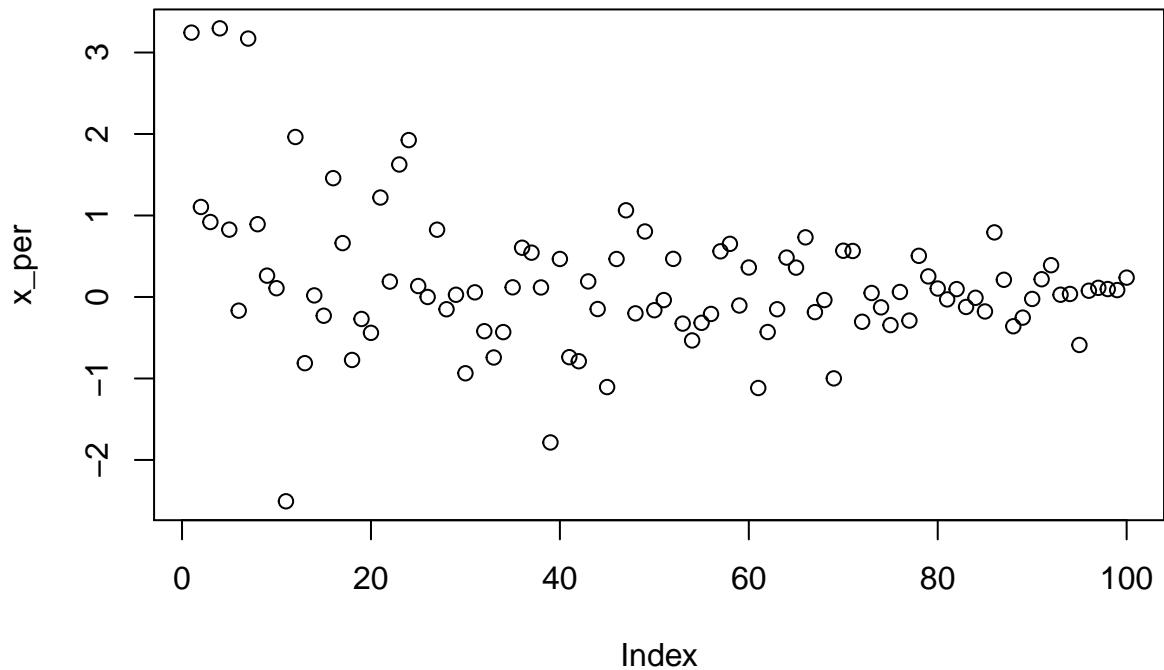
**2 Permutated random samples given the covariance**



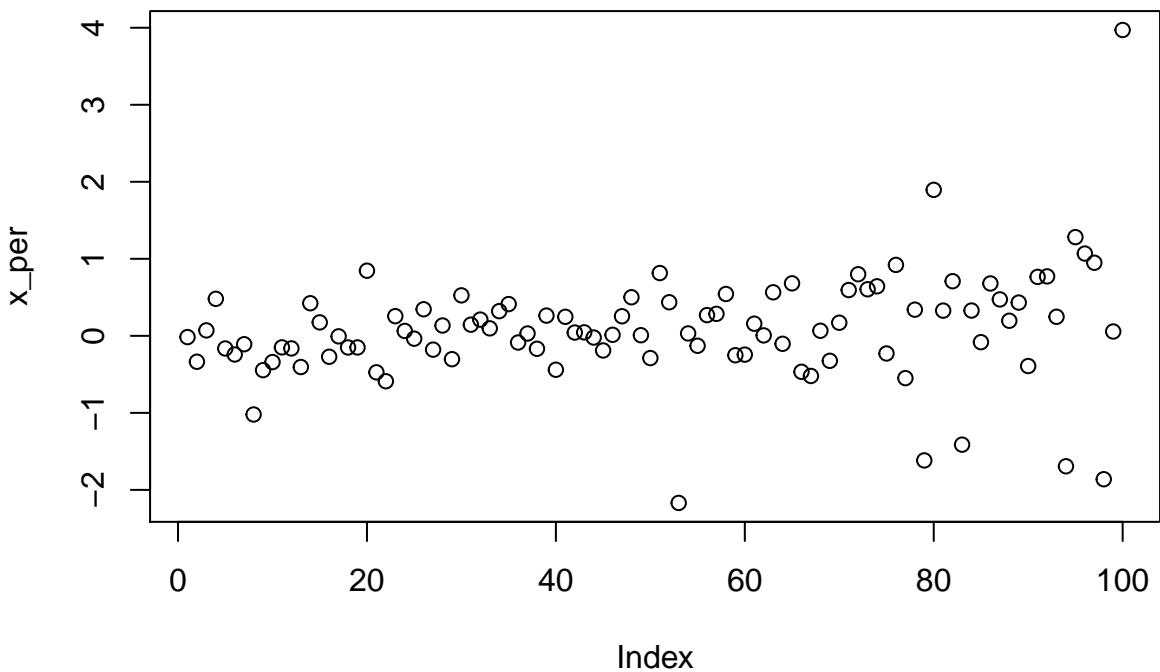
**2 Permutated random samples using inversion rule**

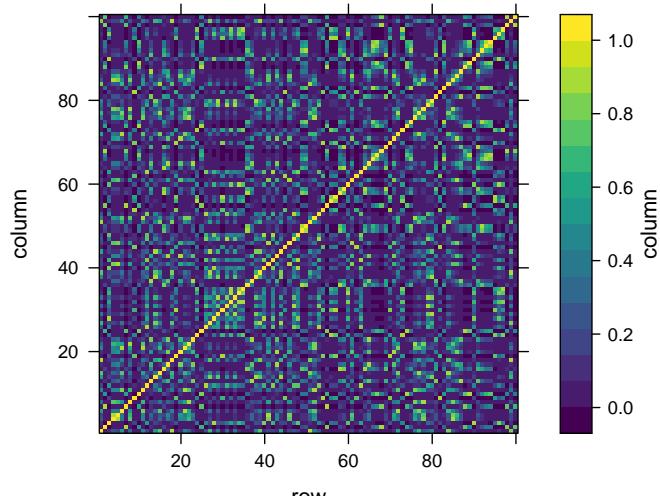
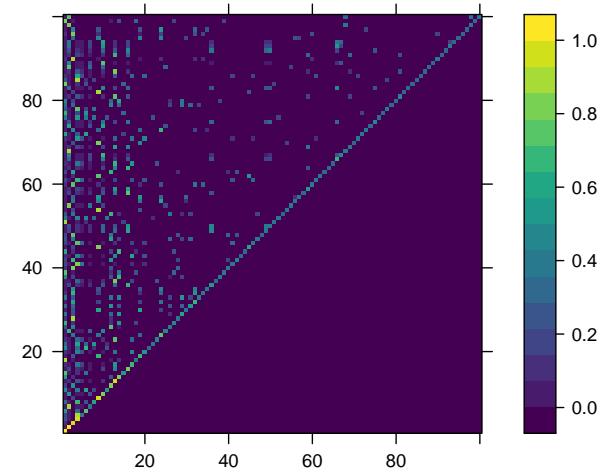
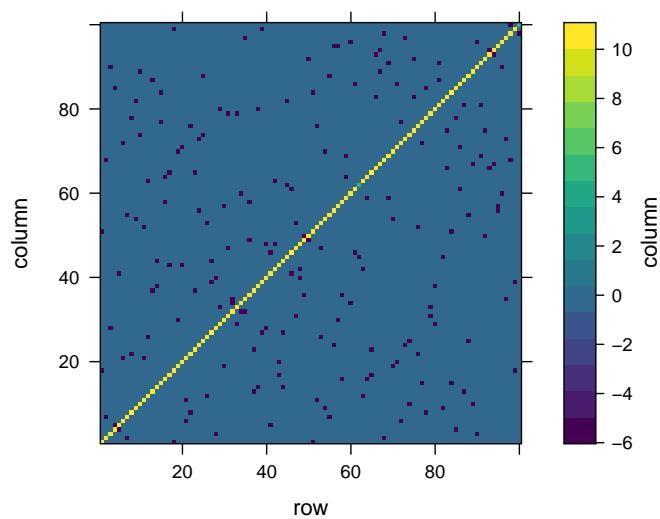
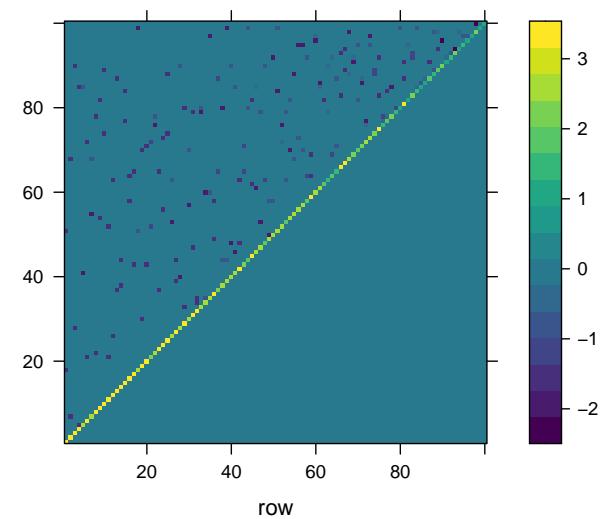
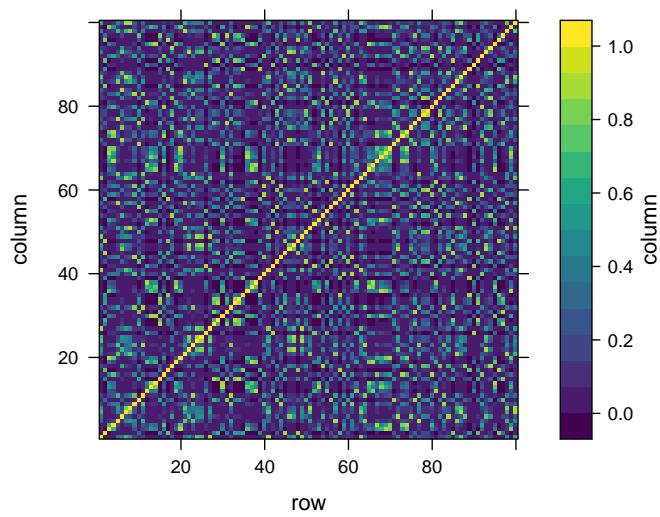
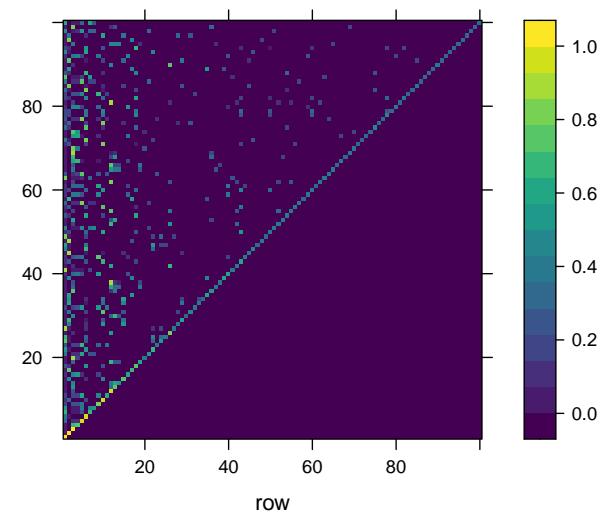


**3 Permutated random samples given the covariance**

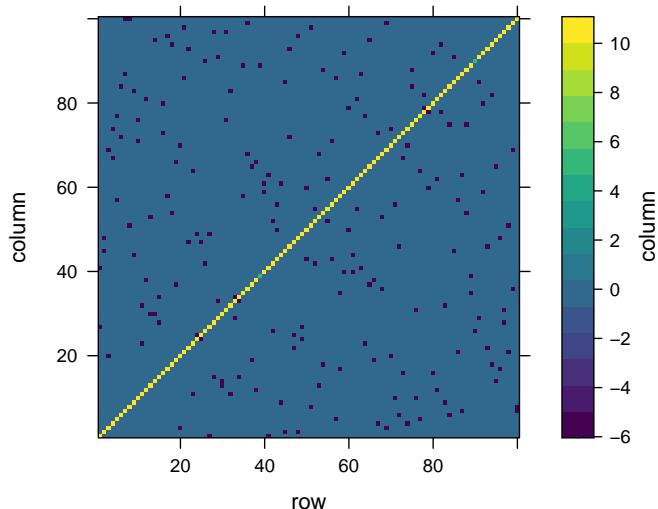


**3 Permutated random samples using inversion rule**

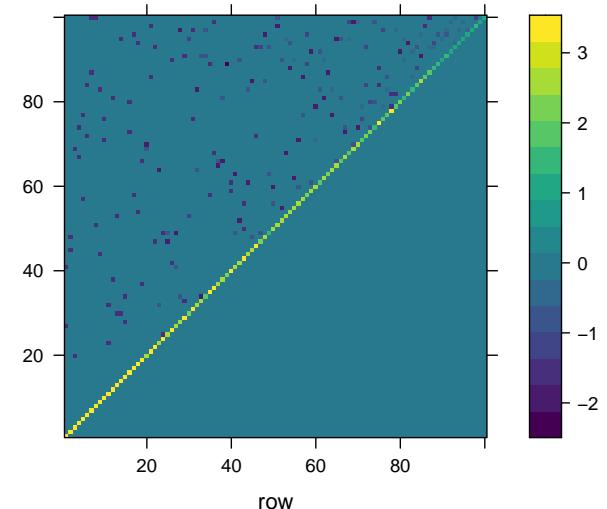


**1 Permuted covariance matrix****1 Permuted lower triangular covariance matrix****1 Permuted precision matrix****1 Permuted lower triangular precision matrix****2 Permuted covariance matrix****2 Permuted lower triangular covariance matrix**

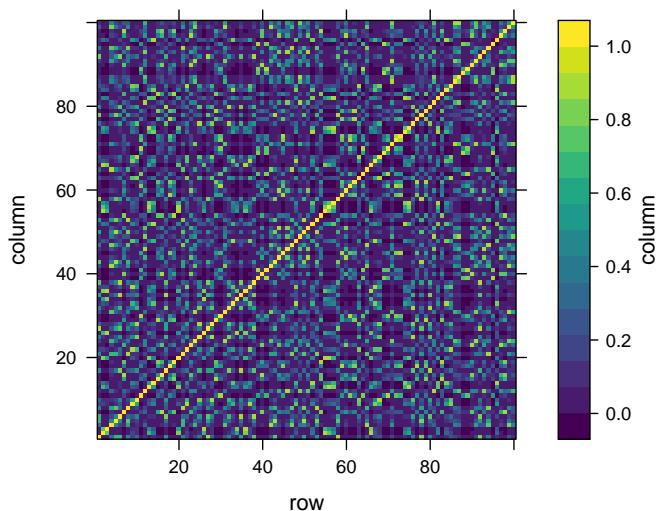
**2 Permuted precision matrix**



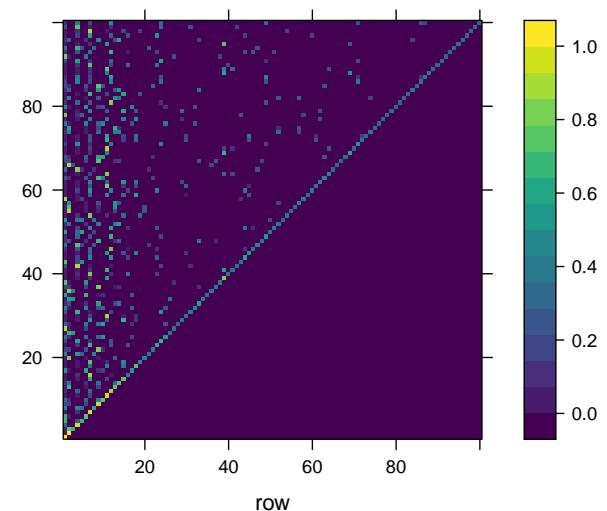
**2 Permuted lower triangular precision matrix**



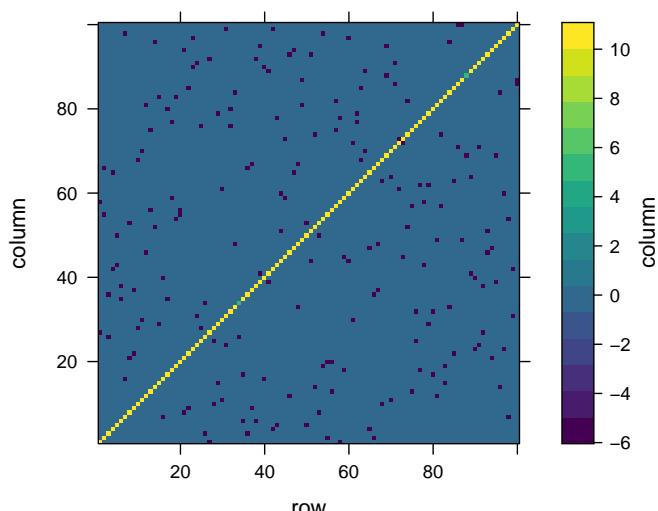
**3 Permuted covariance matrix**



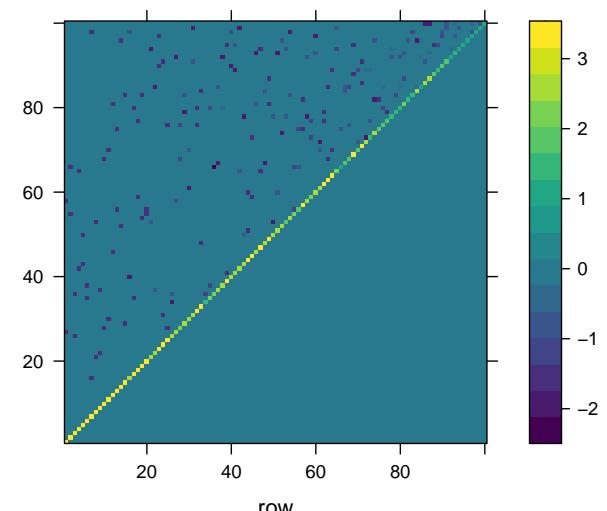
**3 Permuted lower triangular covariance matrix**



**3 Permuted precision matrix**



**3 Permuted lower triangular precision matrix**



## Part II Gaussian random fields and Kriging

The purpose of this computer exercise is to give an introduction to parameter estimation and kriging for Gaussian random field models for spatial data.

We assume the following observation model on the unit square:

$$y(\mathbf{s}_j) = x(\mathbf{s}_j) + \epsilon_j, \quad j = 1, \dots, N,$$

where  $\epsilon_j \sim N(0, \tau^2)$  are independent measurement noise terms. Further, consider a Matérn covariance function for the Gaussian random field  $x(\mathbf{s})$ :

$$\text{Cov}(x(\mathbf{s}_i), x(\mathbf{s}_j)) = \Sigma_{i,j} = \sigma^2(1 + \phi h) \exp(-\phi h),$$

where  $h$  denotes the Euclidean distance between the two sites  $\mathbf{s}_i$  and  $\mathbf{s}_j$ .

We assume the mean increases with east and north coordinates as follows:  $\mu_j = \alpha((s_{j1} - 0.5) + (s_{j2} - 0.5))$ , for site  $\mathbf{s}_j = (s_{j1}, s_{j2})$  on the unit square.

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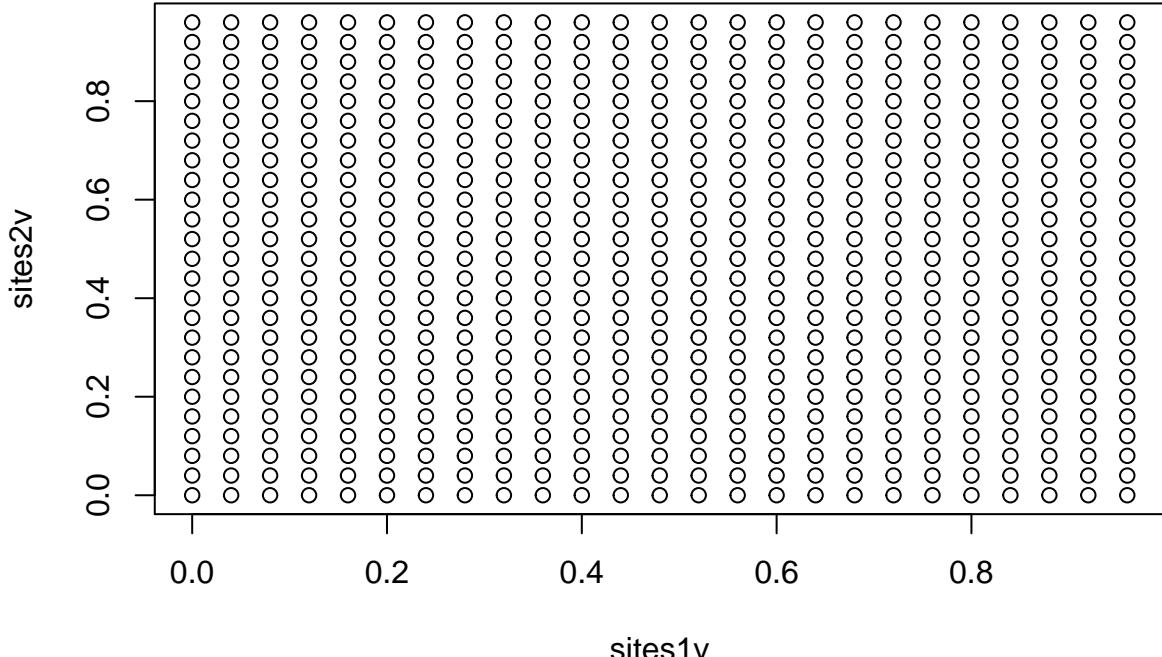
### 2.1 Simulation

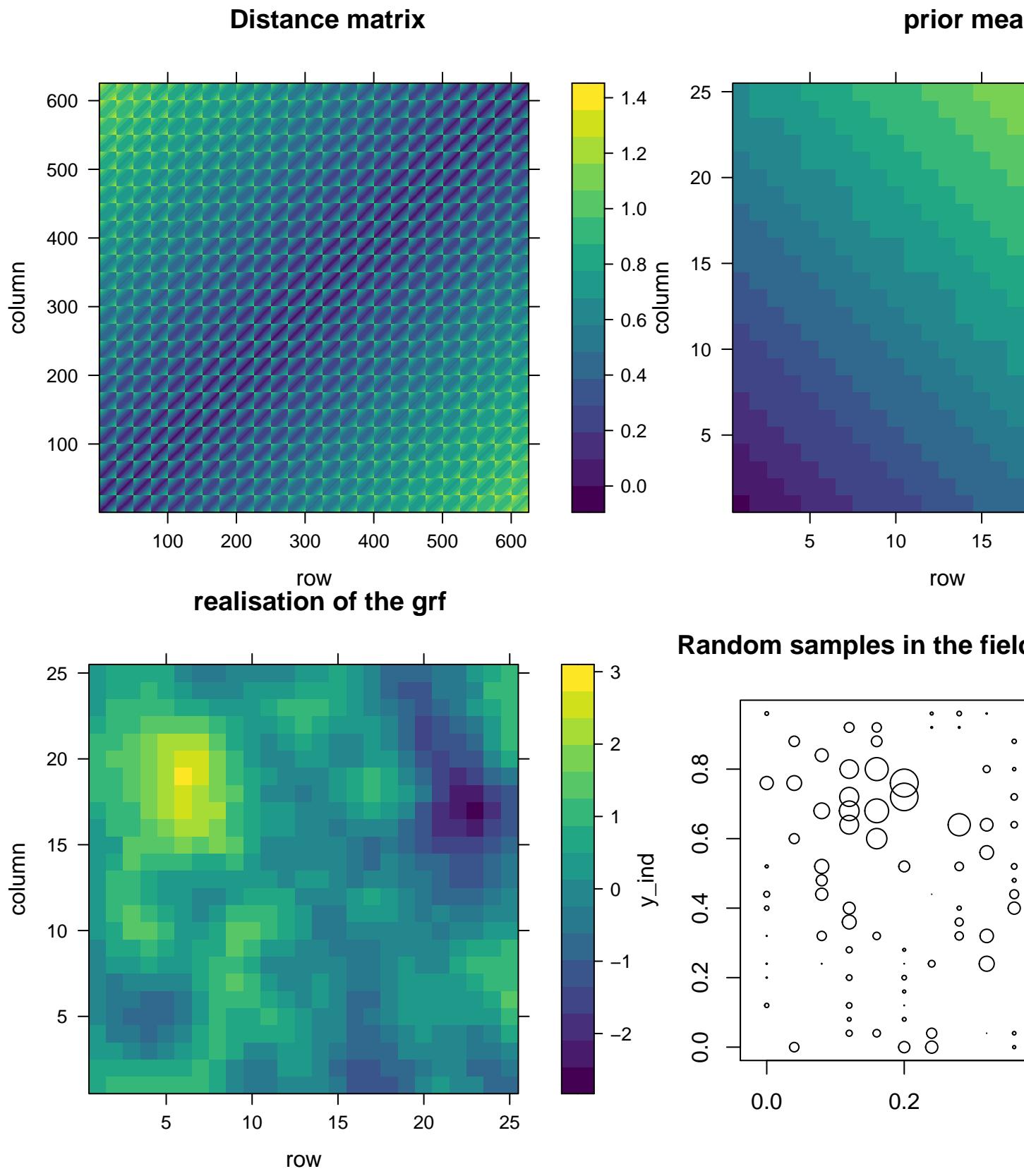
Simulate  $N = 200$  random sites in the unit square and plot them. Form the covariance matrix using  $\sigma = 1, \phi = 10, \tau = 0.05$ . Take its Cholesky decomposition and simulate dependent zero-mean Gaussian data variables, then add the mean using  $\alpha = 1$ . Plot your observations.

The true mean of the field is expressed as

$$\mu_i = \alpha((s_{i1} - 0.5) + (s_{i2} - 0.5)) = -\alpha + \alpha s_{i1} + \alpha s_{i2} = \underbrace{\begin{bmatrix} 1 & s_{i1} & s_{i2} \end{bmatrix}}_{\mathbf{h}^T(\mathbf{s}_i)} \underbrace{\begin{bmatrix} -\alpha \\ \alpha \\ \alpha \end{bmatrix}}_{\boldsymbol{\beta}}$$

where  $s_{i1}, s_{i2}$  are the location from east and north direction in the grid.





## 2.2 Parameter estimation

We will now use the simulated data to estimate the model parameters  $\alpha, \sigma^2, \tau^2, \phi$  using maximum likelihood estimation. Iterate between the update for the mean parameter, and updating the covariance parameters. Monitor the likelihood function at each step of the algorithm to check convergence.

The mean of the field is modelled by  $p(\mathbf{x})$  and the imperfect information  $\mathbf{y} = (y_1, \dots, y_m)$  conditional on  $\mathbf{x}$  can be modelled by  $p(\mathbf{y}|\mathbf{x})$ , which can be expressed as follows:

$$p(\mathbf{x}) = N(\mathbf{H}\beta, \Sigma), \quad p(\mathbf{y}|\mathbf{x}) = N(\mathbf{F}\mathbf{x}, \mathbf{T})$$

Therefore, the marginal likelihood of the data is

$$p(\mathbf{y}) = N(\mathbf{G}\beta, \mathbf{C}), \quad \mathbf{G} = \mathbf{F}\mathbf{H}, \quad \mathbf{C} = \mathbf{F}\Sigma\mathbf{F}^T + \mathbf{T}$$

The log-likelihood as a function of  $\beta$  and unknown fixed nuisance parameters  $\theta$  in the prior covariance matrix  $\Sigma = \Sigma(\theta)$ , and/or the likelihood noise matrix  $\mathbf{T} = \mathbf{T}(\theta)$  becomes

$$l(\theta, \beta) = -\frac{m}{2} \log(2\pi) - \frac{1}{2} \log |\mathbf{C}| - \frac{1}{2} (\mathbf{y} - \mathbf{G}\beta)^T \mathbf{C}^{-1} (\mathbf{y} - \mathbf{G}\beta)$$

The MLEs of  $\beta$  and  $\theta$  are obtained by

$$(\hat{\beta}, \hat{\theta}) = \arg \max_{\beta, \theta} \{l(\beta, \theta)\}$$

For fixed  $\theta$ , the MLEs of  $\beta$  can be determined analytically.

$$\frac{dl}{d\beta} = \mathbf{G}^T \mathbf{C}^{-1} \mathbf{y} - \mathbf{G}^T \mathbf{C}^{-1} \mathbf{G}\beta = \mathbf{0}, \quad \hat{\beta} = (\mathbf{G}^T \mathbf{C}^{-1} \mathbf{G})^{-1} \mathbf{G}^T \mathbf{C}^{-1} \mathbf{y}$$

Whereas for fixed  $\beta$ , the MLE of nuisance parameters  $\theta$  can be obtained by numerical maximization. Let  $\mathbf{z} = \mathbf{y} - \mathbf{G}\beta$ , and  $\mathbf{Q} = \mathbf{C}^{-1}$ . For each component of  $\theta_r$ ,  $r = 1, \dots, d$ , in this case,  $\theta$  has 3 components  $(\sigma^2, \eta, \tau^2)$ . The score of the log-likelihood becomes

$$\frac{dl}{d\theta_r} = -\frac{1}{2} \text{trace}(\mathbf{Q} \frac{d\mathbf{C}}{d\theta_r}) + \frac{1}{2} \mathbf{z}^T \mathbf{Q} \frac{d\mathbf{C}}{d\theta_r} \mathbf{Q} \mathbf{z}$$

The above mentioned score can be solved iteratively using Fisher scoring algorithm. To achieve the numerical stability, the expected Hessian is applied, which is

$$E\left(\frac{d^2 l}{d\theta_r d\theta_{\bar{r}}}\right) = -\frac{1}{2} \text{trace}(\mathbf{Q} \frac{d\mathbf{C}}{d\theta_r} \mathbf{Q} \frac{d\mathbf{C}}{d\theta_{\bar{r}}})$$

The pseudo code for the Fisher scoring algorithm can then be expressed as follows:

**Data:** initial  $\beta_0, \theta_0$

**Result:** Converged  $\hat{\beta}, \hat{\theta}$

**while** not converged **do**

```

     $C = C(\theta^b);$ 
     $\beta^{b+1} = [\mathbf{G}^T \mathbf{C}^{-1} \mathbf{G}]^{-1} \mathbf{G}^T \mathbf{C}^{-1} \mathbf{y};$ 
     $\mathbf{z} = \mathbf{y} - \mathbf{G}\beta^{b+1};$ 
     $\mathbf{Q} = \mathbf{C}^{-1};$ 
     $C_r^* = \frac{dC(\theta^b)}{d\theta_r}, \quad r = 1, \dots, d;$ 
     $u_r = \frac{dl}{d\theta_r} = -\frac{1}{2} \text{trace}(\mathbf{Q} C_r^*) + \frac{1}{2} \mathbf{z}^T \mathbf{Q} C_r^* \mathbf{Q} \mathbf{z};$ 
     $V_{rr} = E\left(\frac{d^2 l}{d\theta_r d\theta_{\bar{r}}}\right) = -\frac{1}{2} \text{trace}(\mathbf{Q} C_r^* \mathbf{Q} C_{\bar{r}}^*);$ 
     $\theta^{b+1} = \theta^b + V^{-1} u;$ 
     $b = b + 1$ 

```

**end**

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## [1] "1.67144672777389 , iter no is 901"
## [1] "1.63521090368874 , iter no is 902"
## [1] "1.67144672777387 , iter no is 903"
## [1] "1.63521090368879 , iter no is 904"
## [1] "1.671446727774 , iter no is 905"
## [1] "1.63521090368887 , iter no is 906"
## [1] "1.6714467277741 , iter no is 907"
## [1] "1.63521090368896 , iter no is 908"
## [1] "1.67144672777404 , iter no is 909"
## [1] "1.63521090368891 , iter no is 910"
## [1] "1.67144672777407 , iter no is 911"
## [1] "1.63521090368893 , iter no is 912"
## [1] "1.67144672777406 , iter no is 913"
## [1] "1.63521090368892 , iter no is 914"
## [1] "1.6714467277741 , iter no is 915"
## [1] "1.63521090368887 , iter no is 916"
## [1] "1.67144672777391 , iter no is 917"

```

```

## [1] "1.63521090368872 , iter no is 918"
## [1] "1.67144672777395 , iter no is 919"
## [1] "1.6352109036888 , iter no is 920"
## [1] "1.67144672777406 , iter no is 921"
## [1] "1.63521090368893 , iter no is 922"
## [1] "1.67144672777415 , iter no is 923"
## [1] "1.63521090368893 , iter no is 924"
## [1] "1.67144672777414 , iter no is 925"
## [1] "1.63521090368891 , iter no is 926"
## [1] "1.67144672777399 , iter no is 927"
## [1] "1.63521090368887 , iter no is 928"
## [1] "1.67144672777392 , iter no is 929"
## [1] "1.63521090368874 , iter no is 930"
## [1] "1.67144672777405 , iter no is 931"
## [1] "1.63521090368885 , iter no is 932"
## [1] "1.67144672777407 , iter no is 933"
## [1] "1.63521090368893 , iter no is 934"
## [1] "1.67144672777411 , iter no is 935"
## [1] "1.63521090368894 , iter no is 936"
## [1] "1.67144672777416 , iter no is 937"
## [1] "1.63521090368892 , iter no is 938"
## [1] "1.67144672777405 , iter no is 939"
## [1] "1.63521090368894 , iter no is 940"
## [1] "1.67144672777413 , iter no is 941"
## [1] "1.63521090368892 , iter no is 942"
## [1] "1.67144672777404 , iter no is 943"
## [1] "1.63521090368888 , iter no is 944"
## [1] "1.67144672777391 , iter no is 945"
## [1] "1.63521090368874 , iter no is 946"
## [1] "1.67144672777408 , iter no is 947"
## [1] "1.63521090368896 , iter no is 948"
## [1] "1.67144672777405 , iter no is 949"
## [1] "1.63521090368896 , iter no is 950"
## [1] "1.67144672777415 , iter no is 951"
## [1] "1.63521090368896 , iter no is 952"
## [1] "1.67144672777403 , iter no is 953"
## [1] "1.63521090368886 , iter no is 954"
## [1] "1.67144672777397 , iter no is 955"
## [1] "1.63521090368887 , iter no is 956"
## [1] "1.67144672777404 , iter no is 957"
## [1] "1.63521090368882 , iter no is 958"
## [1] "1.67144672777403 , iter no is 959"
## [1] "1.63521090368879 , iter no is 960"
## [1] "1.67144672777407 , iter no is 961"
## [1] "1.63521090368879 , iter no is 962"
## [1] "1.67144672777385 , iter no is 963"
## [1] "1.63521090368863 , iter no is 964"
## [1] "1.67144672777386 , iter no is 965"
## [1] "1.63521090368867 , iter no is 966"
## [1] "1.67144672777393 , iter no is 967"
## [1] "1.63521090368876 , iter no is 968"
## [1] "1.67144672777396 , iter no is 969"
## [1] "1.63521090368882 , iter no is 970"
## [1] "1.67144672777399 , iter no is 971"

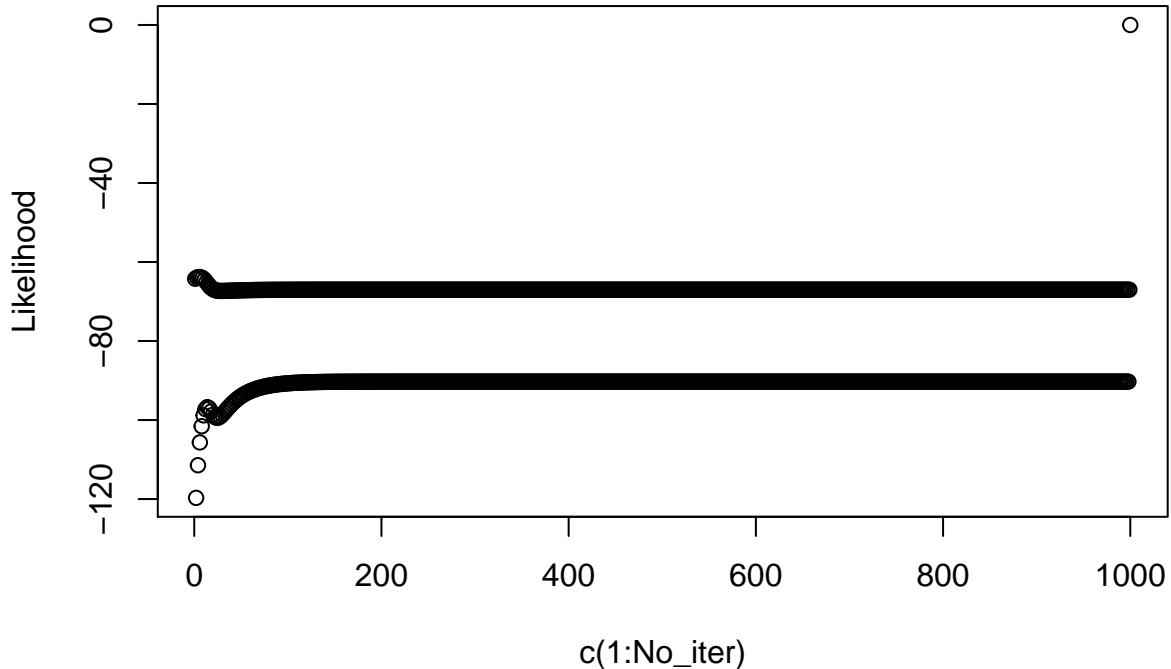
```

```

## [1] "1.63521090368878 , iter no is 972"
## [1] "1.67144672777401 , iter no is 973"
## [1] "1.63521090368888 , iter no is 974"
## [1] "1.671446727774 , iter no is 975"
## [1] "1.63521090368886 , iter no is 976"
## [1] "1.67144672777405 , iter no is 977"
## [1] "1.63521090368892 , iter no is 978"
## [1] "1.67144672777399 , iter no is 979"
## [1] "1.63521090368882 , iter no is 980"
## [1] "1.67144672777388 , iter no is 981"
## [1] "1.63521090368884 , iter no is 982"
## [1] "1.67144672777397 , iter no is 983"
## [1] "1.63521090368888 , iter no is 984"
## [1] "1.67144672777395 , iter no is 985"
## [1] "1.63521090368879 , iter no is 986"
## [1] "1.67144672777397 , iter no is 987"
## [1] "1.63521090368879 , iter no is 988"
## [1] "1.67144672777387 , iter no is 989"
## [1] "1.63521090368874 , iter no is 990"
## [1] "1.67144672777381 , iter no is 991"
## [1] "1.63521090368863 , iter no is 992"
## [1] "1.67144672777386 , iter no is 993"
## [1] "1.63521090368879 , iter no is 994"
## [1] "1.67144672777402 , iter no is 995"
## [1] "1.63521090368889 , iter no is 996"
## [1] "1.67144672777407 , iter no is 997"
## [1] "1.63521090368878 , iter no is 998"
## [1] "1.67144672777402 , iter no is 999"

```

### likelihood function



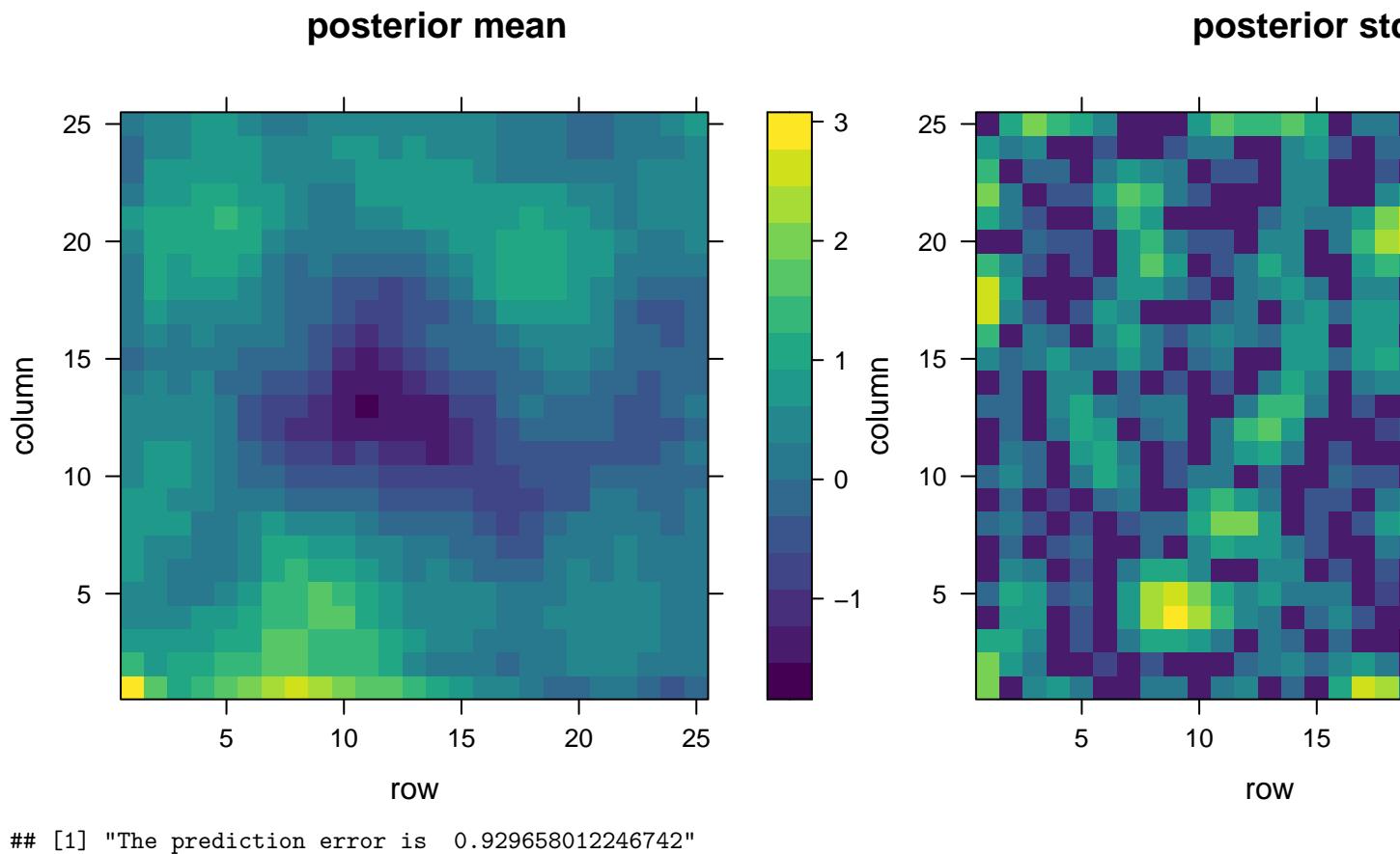
```

## [1] "\nEstimated sigma is 0.689 ; True sigma is 1 \nEstimated phi is 9.53 ; True phi is 10 \nEsti"

```

## 2.3 Kriging

We will now use the estimated model parameters to perform kriging prediction. Predict variables  $x(s)$ , where predictions sites lie on a regular grid of size 25x25 for the unit square. Visualize the Kriging surface and the prediction standard error. Compare with the true field.



## Part III Integrated nested Laplace Approximations (INLA)

In the last part of this exercise, we explore the R-INLA package along two examples.

### 3.1 Simple Linear Regression

First, we analyse the ski jumping data set using a linear regression model, which can be phrased as Latent Gaussian model suitable for INLA. Therefore, we start with loading the INLA package and exploring the dataset.

The ski jumping data set contains 26 observations of measured lengths in ski jumping competitions (in meters) between the years 1961 and 2011.

In Figure 1 we depict the 26 observations given their year. We observe a clear (almost linear) trend in the measured jumping lengths to increase with the years.

## Ski jumping data

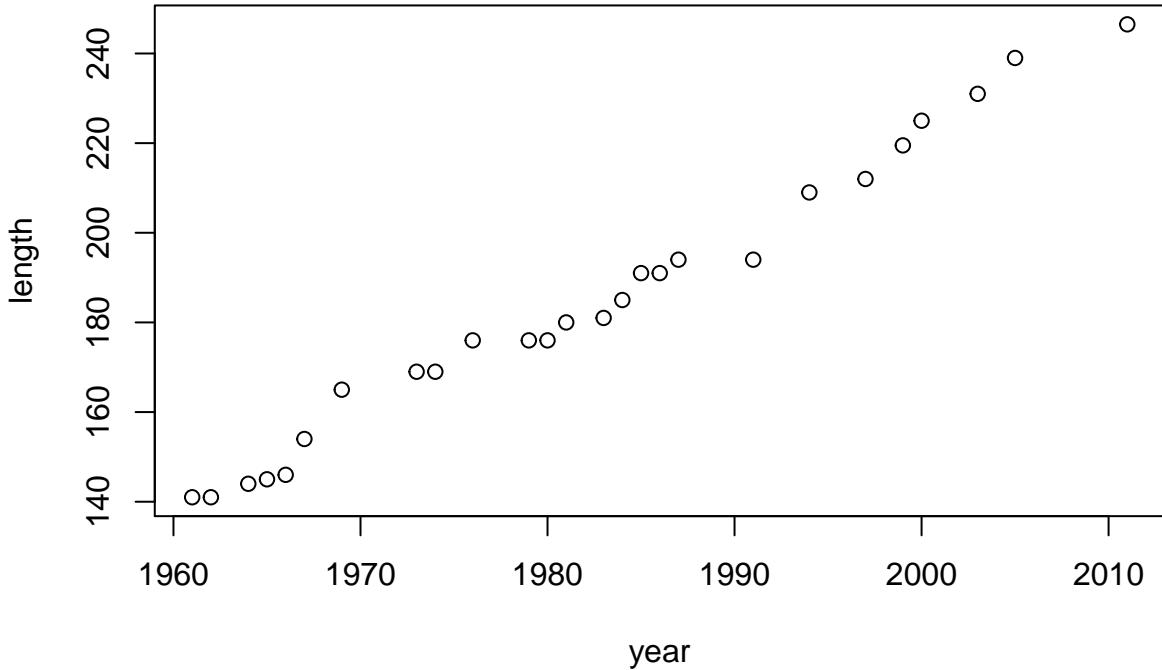


Figure 1: Visualisation of the ski jumping data set

Suitable for this model assumption on the data, we use linear regression approach for the statistical modelling of this data, where the years  $x_i$  are the covariates and the lengths  $y_i$  are the responses for  $i = 1, \dots, 26$ :

$$\mathbb{E}[y_i] = \mu + \beta x_i, \quad \mathbb{V}\mathcal{D}\backslash[y_i] = \tau^{-1}.$$

This can be posed as a latent Gaussian model suited for the INLA framework.

1. The response depends on the linear predictors  $\eta$  as  $y|x, \theta = \Pi\pi(y_i|\eta_i, \tau)$  with Gaussian likelihood  $\pi(y_i|\eta_i, \tau) \sim \mathcal{N}(\eta_i, \tau^{-2})$
2. The parameters  $\mu$  and  $\beta$  of the linear predictor  $eta_i = \mu + x_i\beta$  are independent Gaussian with a fixed huge variance and mean zero. Note that no additional hyperparameter is introduced here.
3. The model's hyperparameter  $\tau$  is only one-dimensional and is equipped with a Gaussian prior by default with out specification.

The distributions which are not specified in detail here use default settings in the R-INLA package, which are naturally compatible with the LGM construction.

```
## 
## Call:
##   "inla(formula = Length ~ Year, data = skiData, control.predictor =
##     list(compute = TRUE))"
## Time used:
##   Pre = 3.65, Running = 4.29, Post = 0.236, Total = 8.18
## Fixed effects:
##               mean      sd 0.025quant 0.5quant 0.975quant      mode kld
## (Intercept) -4029.646 106.615 -4240.649 -4029.650 -3818.934 -4029.646  0
## Year        2.126  0.054      2.019     2.126      2.232     2.126  0
## 
```

```

## Model hyperparameters:
##                                     mean    sd 0.025quant 0.5quant
## Precision for the Gaussian observations 0.072 0.02      0.038     0.07
##                                     0.975quant mode
## Precision for the Gaussian observations      0.116 0.066
##
## Expected number of effective parameters(stdev): 2.00(0.00)
## Number of equivalent replicates : 13.00
##
## Marginal log-Likelihood: -89.58
## Posterior marginals for the linear predictor and
## the fitted values are computed

```

The INLA run generates posterior estimates for the fixed effects  $\mu$  and  $\beta$ , which will be investigated below. In the summary, we read the precision of the distribution for the hyperparameter  $\tau$  which is rather small, meaning that the variance will be rather big. However, in a ski jumping competition we can expect a variance of several meters such that this is reasonable.

## Prediction for the data

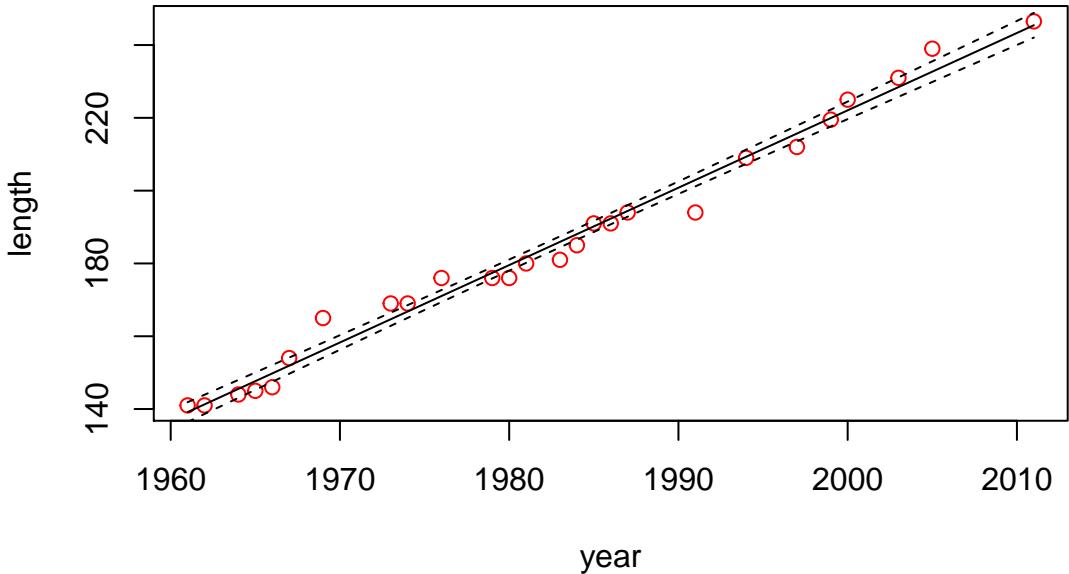


Figure 2: Linear regression with INLA

In Figure 2 we see that the linear trend is really well captured by the model (black line), whereas the 95% credibility interval (dashed line) does not cover all data points.

```

## [1] "Estimates for sigma:"
## Mean          3.83993
## Stdev         0.552976
## Quantile 0.025 2.93482
## Quantile 0.25  3.44617
## Quantile 0.5   3.77761
## Quantile 0.75  4.16357
## Quantile 0.975 5.09958

```

In Figure 3, we depict the marginal posterior distributions for all variables of interest. In particular, the

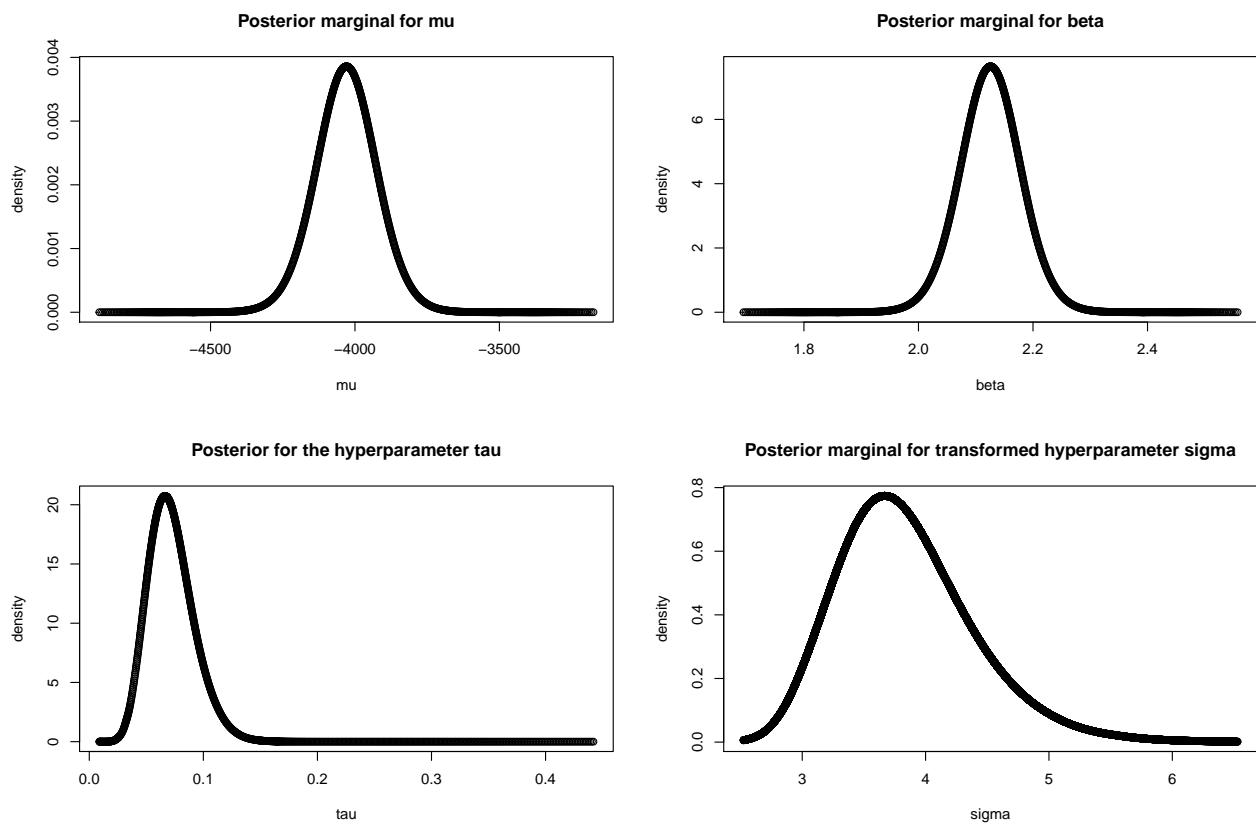


Figure 3: Posterior marginals for selected effects

transformed marginal analysis confirms our interpretation that the variance in the magnitude of several meters (roughly around 4 meters), but again this is very reasonable for this application.

### 3.2 GLMM with random effects

Last, we use INLA to analyse the “Seeds” data set. This data concerns the portion of seeds that germinated on a sample set of 21 plates. The plates are equipped with one of two types of seeds and one of two types of extracts. The characteristics of plate  $i$  are described by the covariates  $x_{1,i}$  which is the type of seed and  $x_{2,i}$  which is the type of root extract - these covariates are either 0 or 1 for the different possibilities. Then the number of germinated seeds  $r_i$  on plate  $i$  is counted in contrast to the number of total seeds  $n_i$  on that plate. Having  $p_i$  as the probability of germination on plate  $i$ , a binomial model for this example is

$$r_i \sim \text{Binomial}(p_i, n_i)$$

$$\text{logit}(p_i) = a_0 + a_1 x_{1,i} + a_2 x_{2,i} + \varepsilon_i$$

where  $\varepsilon_i$  is some iid noise. As above non-specified prior- and hyperparameter-distributions use the default of R-INLA. This model is then again implemented in R-INLA.

```
## [1] "The x1 covariate:"
## [1] 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1
## [1] "The x2 covariate:"
## [1] 0 0 0 0 0 1 1 1 1 1 1 0 0 0 0 0 1 1 1 1 1 1 1
##
## Call:
##   c("inla(formula = formula, family = \"binomial\", data = data, Ntrials
##     = n, ", " control.predictor = list(compute = TRUE), control.family =
##     list(link = \"logit\"))" )
## Time used:
##   Pre = 4.56, Running = 0.484, Post = 0.217, Total = 5.26
## Fixed effects:
##           mean      sd 0.025quant 0.5quant 0.975quant    mode kld
## (Intercept) -0.429  0.115     -0.656   -0.429     -0.204 -0.428    0
## x1          -0.272  0.156     -0.580   -0.272      0.033 -0.271    0
## x2          1.066  0.146      0.782   1.066      1.353  1.065    0
##
## Random effects:
##   Name      Model
##   plate IID model
##
## Model hyperparameters:
##           mean      sd 0.025quant 0.5quant 0.975quant mode
## Precision for plate 18930.69 20071.40      30.63 12701.76 73765.97 7.83
##
## Expected number of effective parameters(stdev): 3.25(1.16)
## Number of equivalent replicates : 6.46
##
## Marginal log-Likelihood: -73.75
## Posterior marginals for the linear predictor and
## the fitted values are computed
```

Remark the structured pattern in the covariates. Furthermore, here the precision is rather higher yielding a small variance in the estimate.

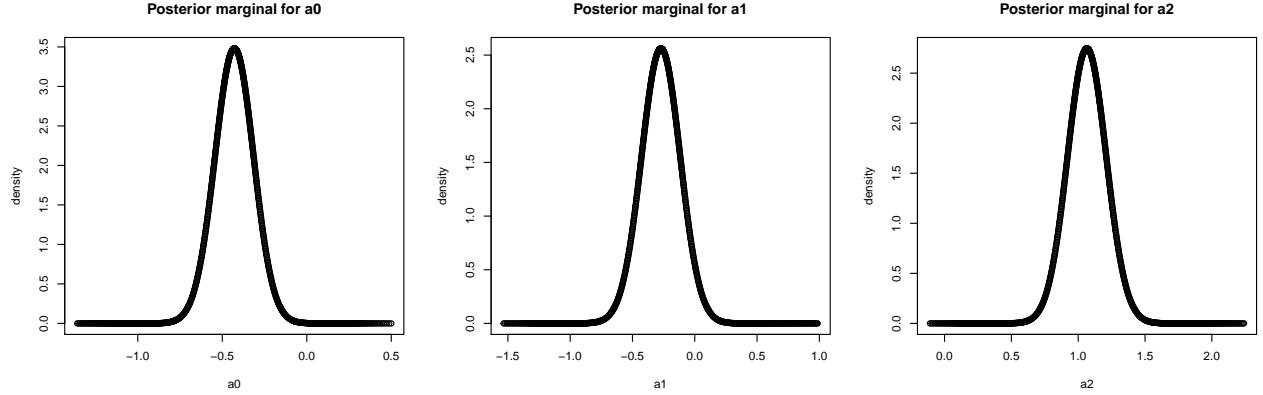


Figure 4: Posterior marginals for selected effects

In Figure 4, we see rather confident estimates for the fixed effects of the model. In particular, we note that the effect  $a_2$  will dominate the model since we only have 0 and 1 values for the covariates. The effect  $a_0$  is common for all plates and the absolute value of  $a_1$  for the seed type is a way smaller than the one for the root extract.

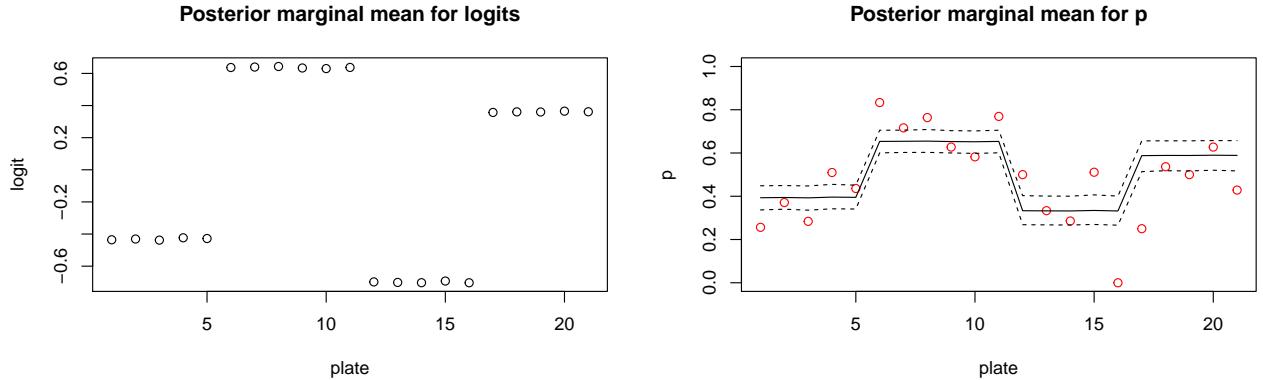


Figure 5: GLMM with INLA

In Figure 5, we recognize a clear pattern with high values when the root extract with value 1 is chosen. The choice of the seed only has minor influence on the prediction. Moreover, the variance of this model cannot cover all data points, which is a common issue in binomial models with few data though.