

The spaMM package for mixed models

François Rousset

Dec. 2016

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With contributions from Jean-Baptiste Ferdy and Alex Courtiol.

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Outline

- 1 Motivations: spatial data and smoothers
 - Inference problems from spatial data
 - Smoothers
- 2 The GLMM approach
- 3 Effective software for inference in spatial GLMMs
- 4 Perspectives

Inference problems from spatial data

Typical question: does a genetic marker affect a trait? Hancock et al. Adaptation to climate across the *Arabidopsis thaliana* genome. Science (2011)

Fournier-Level et al. A map of local adaptation in *Arabidopsis thaliana*. Science (2011)

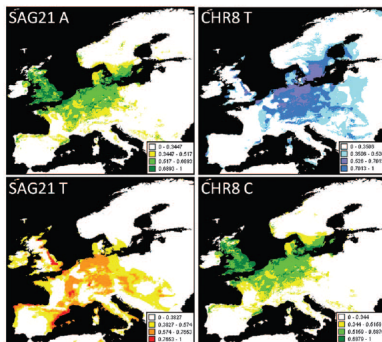


Fig. 3. Geographic distribution probability of the survival-associated alleles located within the *SAG21* gene (**left**) and the *CHR8* gene (**right**). Probabilities were calculated with MaxEnt models as described (16). For both genes, the minor allele is distributed at the species range margin following a particular climate space and shows signs of recent positive selection. They correspond to the best candidate genes for local adaptation reported in this study.

Inference problems from spatial data

Typical question: does environment affect a species presence/abundance?

Diggle et al. (2007)

Annals of Tropical Medicine & Parasitology 101 : 499–509 (2007) MODELLING *Loa* RISK 503

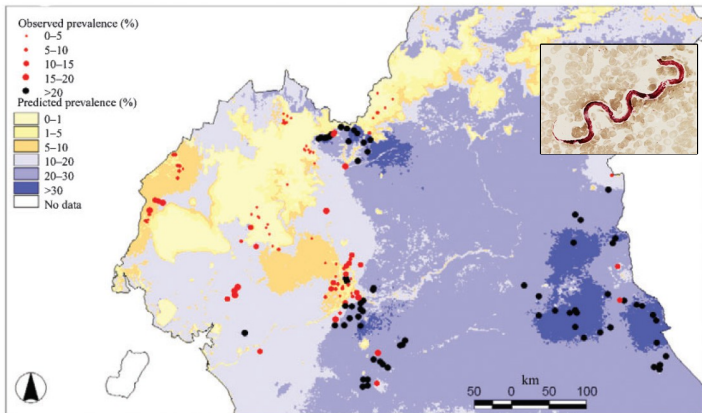
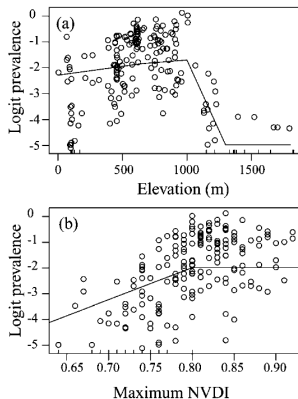


FIG. 2. Point estimates of the prevalence of *Loa loa* microfilaraemia, over-laid with the prevalences observed in field studies.

Inference problems from spatial data

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Diggle et al. develop MCMC algorithms to fit a binomial GLMM to these data.



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“takes into account the spatial structure in the data”

Criticized (Raufaste et Rousset 2001 *Evolution...* Guillot et Rousset 2013 *Meth. Ecol. Evol.*) and defended.

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... results of R & R 2001 imply that this is false.

The mirage of partial Mantel tests

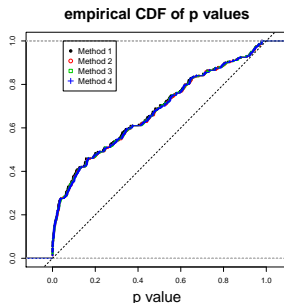
Legendre and Fortin further discuss 4 variants of PM tests.

- ▶ Example of their performance in simulations (Guillot & R., 2013)
 - Simulations under null hypothesis: no effect of some environmental variable
 - Spatial sampling design of the filariasis study
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Specifically “Kriging”

- Inference of likelihood surfaces in some population genetic inference problems (Migraine software)
- “Summary likelihood” alternative to Approximate Bayesian computation (ABC)

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Elements of a spatial GLMM

$$\text{LM: } y_i = \sum_k x_{ik} \beta_k + \epsilon_i$$

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Linear regression on 3 observations:

$$\mu_i = a + x_i b = \mathbf{X}\boldsymbol{\beta} \text{ for } \mathbf{X} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{pmatrix} \text{ and } \boldsymbol{\beta} = \begin{pmatrix} a \\ b \end{pmatrix}$$

Elements of a spatial GLMM

$$\text{LM: } \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

$$\text{LMM: } \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \underbrace{\mathbf{Z}\mathbf{v}}_{\text{Random effect}} + \boldsymbol{\epsilon}$$

Random effect $\mathbf{Z}\mathbf{v}$: unknown \mathbf{v} with given distribution, here independent Gaussian variables, so that correlations among elements of $\mathbf{Z}\mathbf{v}$ are given by correlation matrix $\mathbf{Z}\mathbf{Z}^\top$.

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Four observations in two blocks:

$$\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \mathbf{Z} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \text{ and correlation}$$

$$\mathbf{Z}\mathbf{Z}^\top = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}.$$

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$$\text{GLM: } \mathbf{y} = f(\mathbf{X}\boldsymbol{\beta}) + \underbrace{\boldsymbol{\epsilon}}_{\text{non-Gaussian}}$$

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Binomial GLM with logit link (f^{-1}):

$$\text{observed frequency} = \frac{1}{1 + e^{\mathbf{X}\boldsymbol{\beta}}} + \underbrace{\boldsymbol{\epsilon}}_{\text{Binomial}}$$

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spatial GLMM: Elements of the correlation matrix $\mathbf{Z}\mathbf{Z}^\top$ are larger when the observations are closer in space.

Parameters: $\boldsymbol{\beta}$

variance(s) $\text{Var}(v_i)$

(variance(s) $\text{Var}(\epsilon_i)$)

parameters defining the correlation matrix $\mathbf{Z}\mathbf{Z}^\top$.

Mixed models as smoothers

Prediction by mixed model:

$$\mathbf{y} = \underbrace{f(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{v})}_{\text{predictor}} + \boldsymbol{\epsilon}$$

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MODELLING *Loa* RISK

503

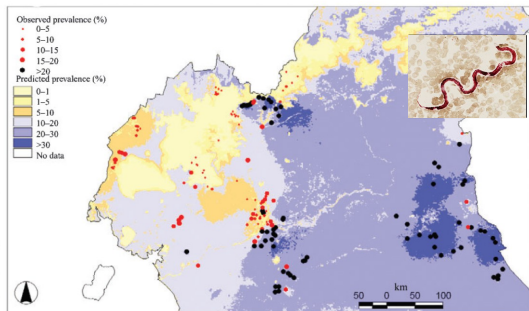


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Smoothers: estimated smooth predictor $f(\mathbf{X}\hat{\boldsymbol{\beta}} + \mathbf{Z}\hat{\mathbf{v}})$

Correlation models for spatial data

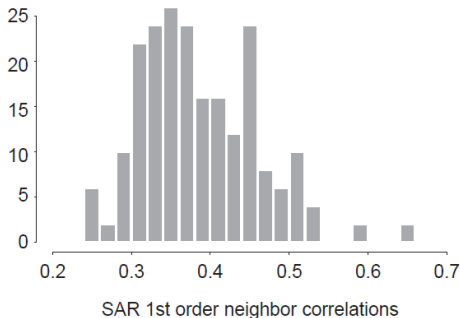
Autoregressive models

So-called **geostatistical** approach

Correlation models for spatial data

Autoregressive models

- Widely discussed (e.g. in econometry) because relatively easy to fit
- Derived from time series; can describe pedigree relationships
- Interpretation may be difficult for purely spatial processes



Wall (2004) *J. Stat. Planning & Inference*

- Do not provide smoothers

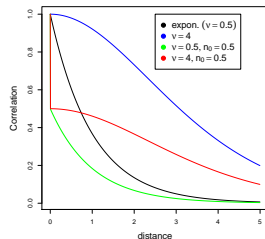
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So-called geostatistical approach

- Correlations are function of Euclidean (or of geodesic) distances
- Most useful is the so-called Matérn family of functions, which includes the exponential and squared exponential (e^x and e^{x^2}).



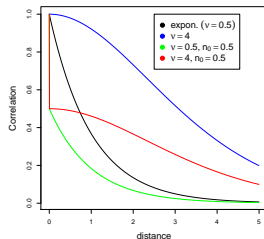
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- Scale parameter ρ ($x = \rho d$) or vector of parameters ($x = \sum_{\text{dims } i} \rho_i d_i^2$).



Approaches for fitting spatial GLMMs

Likelihood is an integral over the distribution of the random effects, usually a high-dimensional integral with no explicit analytical expression.

Numerical integration often not feasible

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Numerical integration often not feasible

MCMC

- “In general, a good choice of transition kernel is problem-specific, and in our experience involves considerable trial-and-error experimentation to achieve good results” (Diggle and Ribeiro, *Model-based geostatistics*, Springer, 2007)
- Often involve prior distributions, with the resulting problems for defining a “good” prior and validating the methods
- Distinct MC methods for binary (probit) models.

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Analytical approximations of the integrals (Laplace approximations, etc.)

lme4, glmmPQL, Lee and Nelder's Hierarchical GLM approach

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In practice, software failures and/or impenetrability and/or undocumented tricks advocated in the literature (lmer, glmmPQL)

Something easier and easily repeatable?

[illegible]

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spaMM R package for spatial Mixed Models

Models handled:

- Those previously described
- Basic set of GLMMs (Gaussian, Binomial, Poisson, Gamma) and link functions (identity, log, inverse, logit, probit, complementary log-log); + negative binomial, Conway-Maxwell-Poisson
- several random effects, non-spatial
- Some non-Gaussian distributions of random effects
- Heteroscedastic models

Cons: First implementation not fast

Validation: Type I error \Leftrightarrow coverage of likelihood ratio confidence intervals

The filaria prevalence data revisited

```

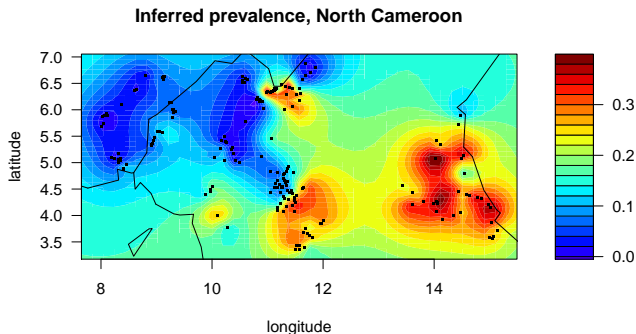
10 for p in 0, 1: prior gls normal(gls.parameters[0], length=1000) # mean var = 0.1
11 gls.data <- gls.data %>% filter(Year == 2000) # data = 2000
12 gls.model <- gls.normal(gls.prior ~ "NORM.Glm", data = loadedBMD.Glm, factor = loadedBMD, factor = loadedBMD, factor = loadedBMD)
13 run <- rstan::sample_large_hmc(model, prior = list(p, 0), num_iter = 100000, num_chains = 4)
14 ## Run MCMC
15
16 ## estimate parameters by QM first
17 gls.data <- cbind(loadedBMD, loadedBMD.loadedBMD)
18
19 gls <- gls.qm(gls ~ "NORM.Glm", data = loadedBMD.Glm, factor = loadedBMD, factor = loadedBMD, factor = loadedBMD, family = normal())
20 beta <- mcmc::mcmc(gls$coef[0:3])
21
22 num_iter <- mcmc::mcmc(loadedBMD ~ 1, n_iter = 100000, n_warm = 10000)
23
24 for m in 0, 1: gls.mcmc.normal.model <- family("normal")
25 beta.mcmc <- mcmc::mcmc(gls.mcmc.normal.model, num_iter = 100000, n_warm = 10000)
26 mcmc::mcmc(gls.mcmc.normal.model)
27
28 library(mcmc)
29
30 gls.mcmc <- apply(mcmc.model, list(m, 0), function(x) {
31   gls.mcmc <- gls.mcmc(gls.mcmc.model, num_iter = 100000, n_warm = 10000)
32   gls.mcmc
33 })
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222 mcmc::mcmc(gls.mcmc.normal.model)
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224 gls.mcmc <- prepare(list(gls.mcmc))
225
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The filaria prevalence data revisited

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corrHLfit(formula=cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4  
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family=binomial(),data=Loaloa)
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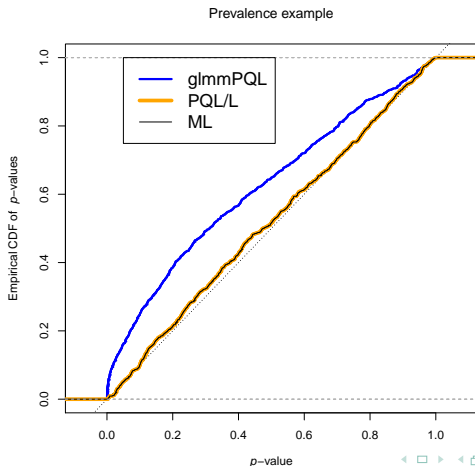


Comparison with a recommended alternative

A certain usage of `glmmPQL` which “produces the identical results as an official spatial GLMM in SAS (proc glimmix) and can hence be trusted.” (Dormann et al., 2007, *Ecography*, Appendix).

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Applications and perspectives

- “Summary likelihood” alternative to Approximate Bayesian computation (ABC): `Infusion` package
- Inference of origin of samples using isotopes: `IsoriX` package (A. Courtiol)
- Efficient implementation of autoregressive mixed models
- Monte Carlo EM techniques for binary probit models

Inference of origin of samples



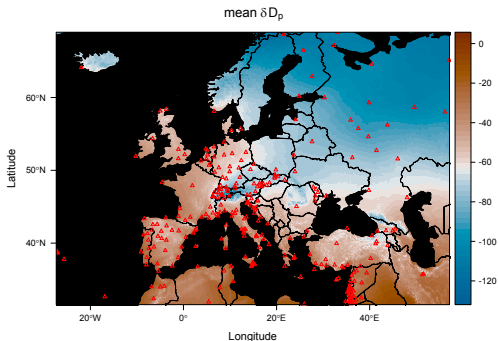
Myotis bechsteinii. Photo (C) Ján Svetlík

Inference of origin of samples



Myotis bechsteinii. Photo (C) Ján Svetlík

Variation in deuterium in rain samples

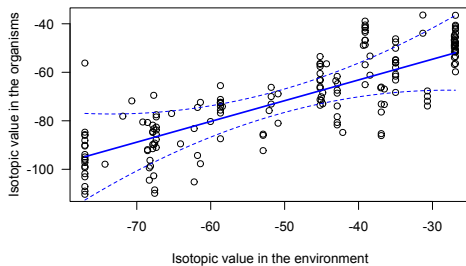


Inference of origin of samples



Myotis bechsteinii. Photo (C) Ján Svetlík

Calibration of deuterium in bats vs. deuterium in rain



Inference of origin of samples



Myotis bechsteinii. Photo (C) Ján Svetlík

Assignment by testing each location as possible origin

