The (un)reliability of contour curves

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Joint work with David Bolin

and also
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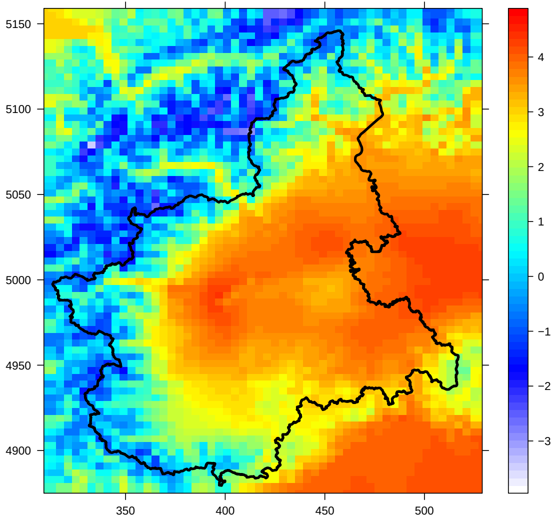
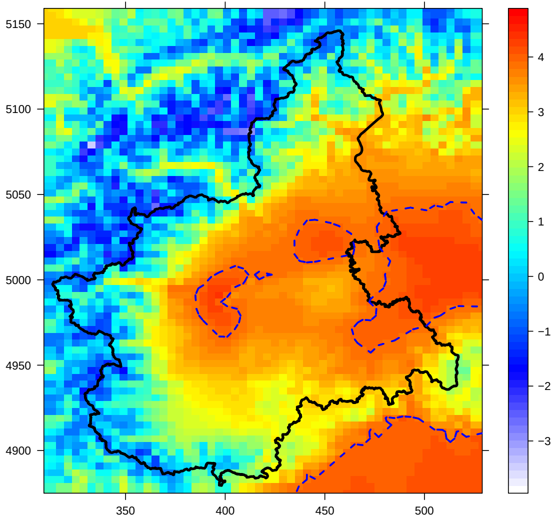
Outline

PM_{10} in Piemonte: Where is $PM_{10} > 50$?



PM_{10} in Piemonte: Where is $PM_{10} > 50$? Uncertainty?



Contours and excursions

- Lindgren, Rychlik (1995): *How reliable are contour curves? Confidence sets for level contours*, Bernoulli
  Regions with a single expected crossing
- Polfeldt (1999) *On the quality of contour maps*, Environmetrics
  How many contour curves should one use?
- A countour curve of a reconstructed field can (almost) be found from the pointwise marginal distributions.
- The *uncertainty* depends on the full joint distribution.
- A credible contour region is a region where the field transitions from being clearly below, to being clearly above.
- Solving the problem for excursions solves it for contours.

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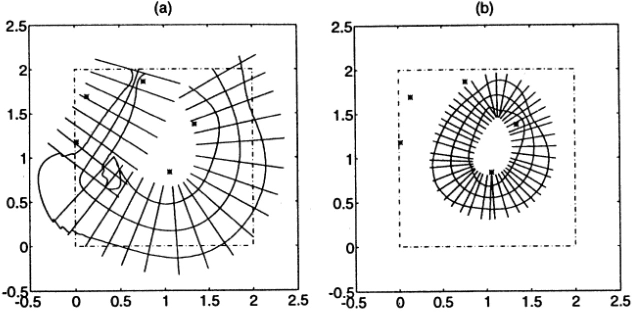
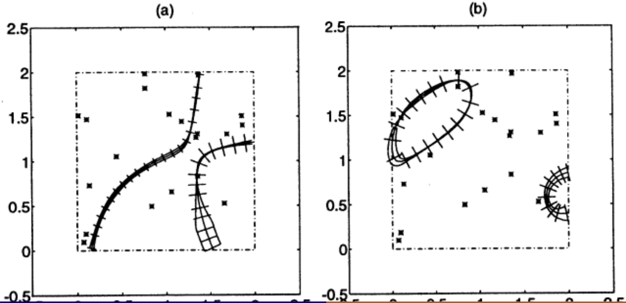


Figure 9. 50% confidence bands in Example 1 for level (a) $u = 0$, (b) $u = 2$; $n = 5$.



Definitions for functions

Excursion sets for functions

Given a function $f(s)$, $s \in \Omega$, the positive and negative excursion sets for a level u are

$$A_u^+(f) = \{s \in \Omega; f(s) > u\} \quad \text{and} \quad A_u^-(f) = \{s \in \Omega; f(s) < u\}.$$

Contour sets for functions

Given a function $f(s)$, $s \in \Omega$, the contour set A_u^c for a level u is

$$A_u^c(f) = \left(A_u^+(f)^o \cup A_u^-(f)^o\right)^c$$

where A^o is the interior and A^c the complement of the set A.

Excursion sets for random fields

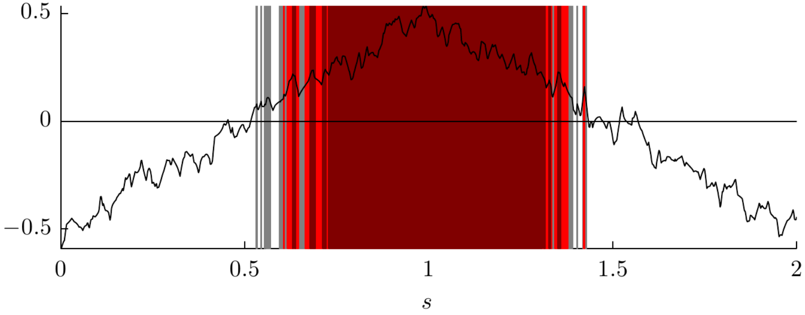
Excursion sets

Let $x(s)$, $s \in \Omega$ be a random process. The positive and negative level u excursion sets with probability $1-\alpha$ are

$$E^+_{u,\alpha}(x) = \arg\max_D \{|D| : \mathsf{P}(D \subseteq A^+_u(x)) \geq 1-\alpha\}.$$
$$E^-_{u,\alpha}(x) = \arg\max_D \{|D| : \mathsf{P}(D \subseteq A^-_u(x)) \geq 1-\alpha\}.$$

- $E^+_{u,\alpha}(x)$ is the largest set so that the level u is exceeded *at all locations* in the set with probability $1-\alpha$.
- Another possible definition of an excursion set would be a set that contains *all excursions* with probability $1-\alpha$. This set is given by $E^-_{u,\alpha}(x)^c$.

Example 1: Gaussian process with exponential covariance



- Gaussian process with exponential covariance function.
- $E^{+}_{0,0.05}(x)$ is shown in red.
- The grey area contains $\{s : \mathsf{P}(x(s) > 0) > 0.95\}$.
- The dark red set is the Bonferroni lower bound.
- The black curve is the kriging estimate of $x(s)$.

Contour sets

Level avoiding sets

Let $x(s)$, $s \in \Omega$ be a random process. The pair of level u avoiding sets with probability $1-\alpha$, $(M^+_{u,\alpha}(x), M^-_{u,\alpha}(x))$, is equal to

$$\underset{(D^+,D^-)}{\arg\max}\{|D^- \cup D^+| : \mathsf{P}(D^- \subseteq A^-_u(x),\ D^+ \subseteq A^+_u(x)) \geq 1-\alpha\}.$$

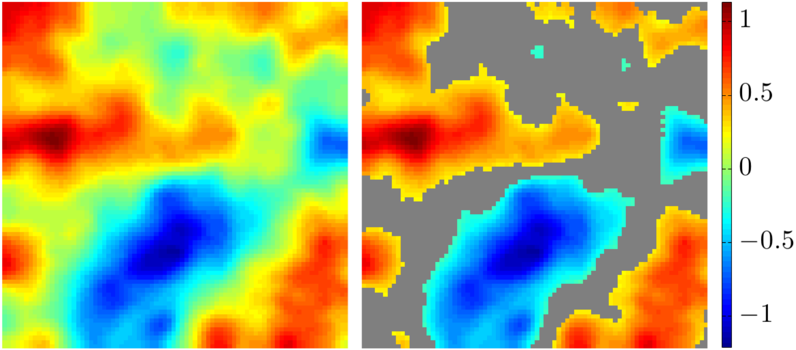
Uncertainty region for contour sets

Let $(M^+_{u,\alpha}(x), M^-_{u,\alpha}(x))$ be the pair of level avoiding sets. The uncertainty region for the contour set of level u is then

$$E^c_{u,\alpha}(x) = \left(M^+_{u,\alpha}(x)^o \cup M^-_{u,\alpha}(x)^o\right)^c.$$

- $E^c_{u,\alpha}$ is the smallest set such that with probability $1-\alpha$ *all* level u crossings of x are in the set.

Example 2: Gaussian Matérn field



- Gaussian Matérn field measured under Gaussian noise.
- Left panel shows the kriging estimate, in the right panel $E^c_{0,0.05}(x)$ is superimposed in grey.
- The complement of $E^c_{u,\alpha}$ is the union of the pair of level avoiding sets.

Excursion functions

- The set $E^{+}_{u,\alpha}(x)$ does not provide any information about the locations not contained in the set.
- It would instead be good to have is something similar to p-values, but which can be interpreted simultaneously.

Excursion functions

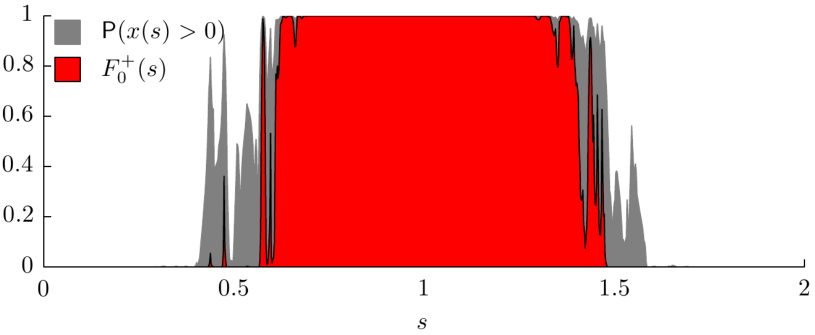
The positive and negative u excursion functions are given by

$$F_u^{+}(s) = \sup\{1-\alpha; s \in E^{+}_{u,\alpha}\},$$
$$F_u^{-}(s) = \sup\{1-\alpha; s \in E^{-}_{u,\alpha}\}.$$

Similarly, the level avoidance and contour functions are given by

$$F_u(s) = \sup\{1-\alpha; s \in (E^{c}_{u,\alpha})^{c}\},$$
$$F_u^{c}(s) = 1 - F_u(s).$$

Example 1 (cont): Excursion functions



- $E_{u,\alpha}^+$ is retrieved as the $1 - \alpha$ excursion set of $F_u^+(s)$.
- If the function takes a value close to one, the process likely exceeds the level at that location.
- If the value of the function is close to zero, it is more unlikely that the process exceeds the level at that location.

Outline of the method

- There are, in principle, two main problems that have to be solved in order to find the excursion sets.
  1. Probability calculation: e.g. calculate the probability $\mathsf{P}(D \subseteq A_u^+(x))$ for a given set D.
  2. Shape optimization: find the largest region D satisfying the required probability constraint.
- In practice it may not be computationally feasible to solve the problems separately.
- Instead we propose a slightly different strategy that will minimize the number of calls to the integration method.
- The method is based on using an increasing parametric family for the excursion sets in combination with a sequential integration routine.

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Outline of the method

Calculating excursion sets using a one-parameter family

Assume that $\pi(\mathbf{x})$ is Gaussian and that $D(\rho)$ is a parametric family, such that $D(\rho_1) \subseteq D(\rho_2)$ if $\rho_1 < \rho_2$. The following strategy is then used to calculate $E^+_{u,\alpha}$.

- Choose a suitable (sequential) integration method.
- Reorder the nodes to the order they will be added to the excursion set when the parameter ρ is increased.
- sequentially add nodes to the set D and in each step update the probability $\mathsf{P}(D \subseteq A^+_u(x))$. Stop as soon as this probability falls below $1 - \alpha$.
- $E^+_{u,\alpha}$ is given by the last set D for which $\mathsf{P}(D \subseteq A^+_u(x)) \geq 1 - \alpha$.

Gaussian integrals

- For a Gaussian vector $\mathbf{x}$, the probabilities $\mathsf{P}(D \subseteq A_u^+(x))$, $\mathsf{P}(D \subseteq A_u^-(x))$, and $\mathsf{P}(D^+ \subseteq A_u^+(x), D^- \subseteq A_u^-(x))$ can all be written on the form

$$I(\mathbf{a}, \mathbf{b}, \Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \int_{\mathbf{a}\leq\mathbf{x}\leq\mathbf{b}} \exp(-\frac{1}{2}\mathbf{x}^\top\Sigma^{-1}\mathbf{x})\,\mathrm{d}\mathbf{x},$$

- $\mathbf{a}$ and $\mathbf{b}$ are vectors depending on the mean value of $\mathbf{x}$, the domain D, and on u.
- There have been considerable research efforts devoted to approximating integrals of this form in recent years[1].
- For GMRFs, we want to use the sparsity of $\mathbf{Q}$.
- We use a method based on sequential importance sampling.

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Parametric families for excursion sets

- The parametric families are based on the marginal quantiles of $x(s)$, $\mathsf{P}(x(s) \leq q_\rho(s)) = \rho$, which are easy to calculate.

One-parameter family

Let $q_\rho(s)$ be the marginal quantiles for $x(s)$, then a one-parameter family for the positive and negative u excursion sets is given by

$$D_1^+(\rho) = \{s; \mathsf{P}(x(s) > u) \geq 1 - \rho\} = A_u^+(q_\rho),$$
$$D_1^-(\rho) = \{s; \mathsf{P}(x(s) < u) \geq 1 - \rho\} = A_u^-(q_{1-\rho}).$$

- Using this parametric family is equivalent to finding a threshold value for the marginal excursion probabilities to get the correct simultaneous significance level.
- This simple one-parameter family can be extended in a number of ways, e.g. by smoothing the marginal quantiles.

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Extension to a latent Gaussian setting

- In practice, we cannot use the previous computations unless we are in a purely Gaussian setting with known parameters.
- A more general model is a latent Gaussian setting, where the posterior distribution can be written as

$$\pi(\mathbf{x}|\mathbf{y}) = \int \pi(\mathbf{x}|\mathbf{y}, \boldsymbol{\theta})\pi(\boldsymbol{\theta}|\mathbf{y})\,\mathrm{d}\boldsymbol{\theta},$$

  where $\mathbf{y}$ is data and $\boldsymbol{\theta}$ a parameter vector.
- Integrated Nested Laplace Approximations (INLA) are used to estimate the posterior distributions.
- The method is extended by numerically approximating the posterior integral as a weighted sum of Gaussian probabilities,

$$\mathrm{P}(\mathbf{a} < \mathbf{x} < \mathbf{b}|\mathbf{y}) \approx \sum_{i=1}^{k} \pi(\boldsymbol{\theta}_i|\mathbf{y})\mathrm{P}(\mathbf{a} < \mathbf{x} < \mathbf{b}|\mathbf{y}, \boldsymbol{\theta}_i).$$

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Air pollution (PM_{10}) data

- The limit value fixed by the European directive 2008/50/EC for PM_{10} is $50\mu g/m^3$. The daily mean concentration cannot exceed this value more than 35 days in a year.
- A region where this value is periodically exceeded is the Piemonte region in northern Italy.
- Cameletti et al (2012/13)[2] investigated an SPDE/GMRF model for PM_{10} concentration in the region.
- The goal is to analyse exceedance probabilities of the limit value.
- Daily PM_{10} data measured at 24 monitoring stations during 182 days in the period October 2005 - March 2006.

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Model

- The following measurement equation is assumed,

$$y(\mathbf{s}_i, t) = x(\mathbf{s}_i, t) + \mathcal{E}(\mathbf{s}_i, t),$$

where $\mathcal{E}(\mathbf{s}_i, t) \sim \mathsf{N}(0, \sigma_{\mathcal{E}}^2)$ is Gaussian measurement noise, both spatially and temporally uncorrelated.

- $x(\mathbf{s}_i, t)$ is the latent field assumed to be on the form

$$x(\mathbf{s}_i, t) = \sum_{k=1}^{p} z_k(\mathbf{s}_i, t)\beta_k + \xi(\mathbf{s}_i, t),$$

where the $p = 9$ covariates z_k are used.

- ξ is assumed to follow first order AR-dynamics in time

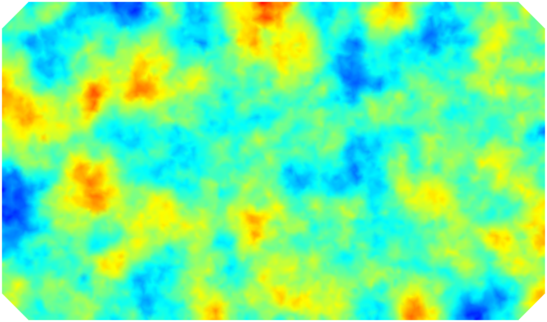
$$\xi(\mathbf{s}_i, t) = a\xi(\mathbf{s}_i, t-1) + \omega(\mathbf{s}_i, t),$$

where $|a| < 1$ and $\omega(\mathbf{s}_i, t)$ is a zero-mean temporally independent Gaussian process with spatial Matérn covariances.

GMRFs based on SPDEs (Lindgren et al., 2011)

GMRF representations of SPDEs can be constructed for to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$(\kappa^2 - \Delta)(\tau\, x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



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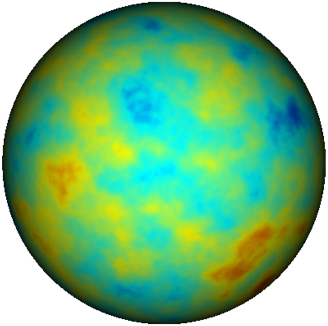

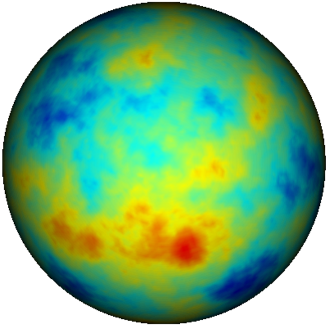

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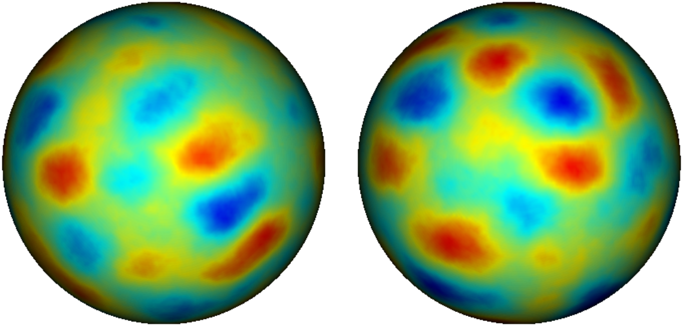

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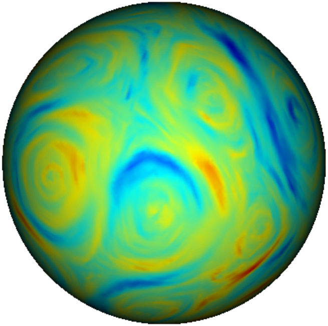
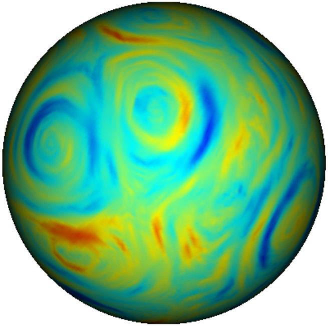
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)(\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega \text{s}$$





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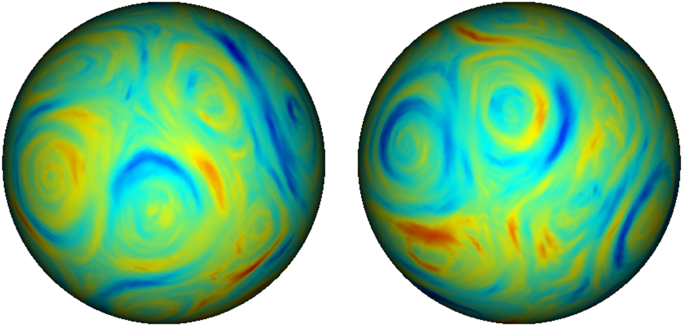
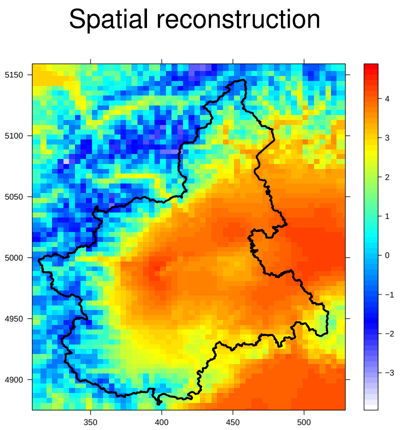
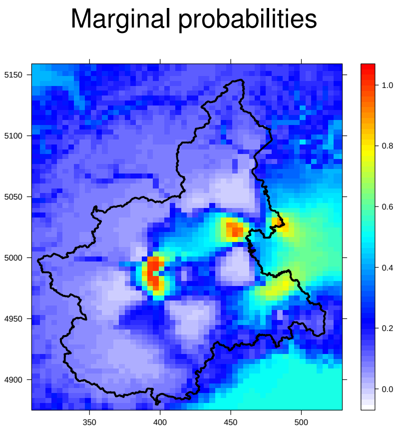
$$\left(\frac{\partial}{\partial t} + \kappa^2_{\mathbf{u},t} + \nabla \cdot \mathbf{m}_{\mathbf{u},t} - \nabla \cdot \mathbf{M}_{\mathbf{u},t} \nabla\right) (\tau_{\mathbf{u},t} x(\mathbf{u}, t)) = \mathcal{E}(\mathbf{u}, t), \quad (\mathbf{u}, t) \in \Omega \times \mathbb{R}$$



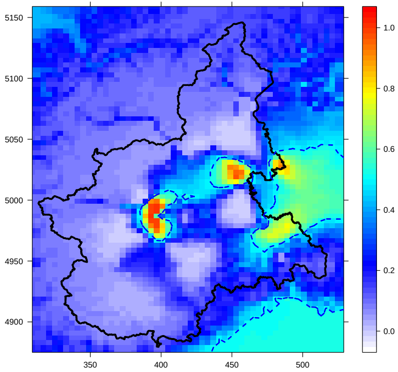
Results for January 30, 2006



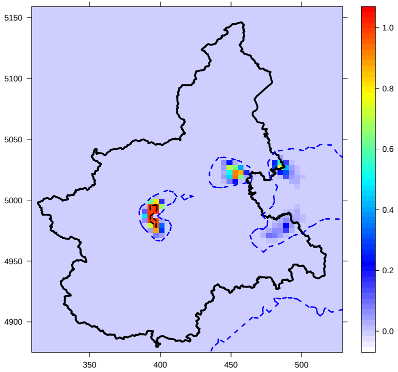


Results for January 30, 2006

Marginal probabilities



$F^{+}_{50}(s)$



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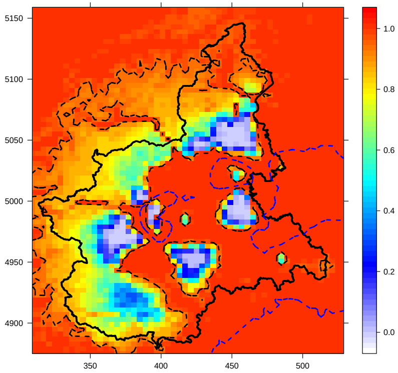
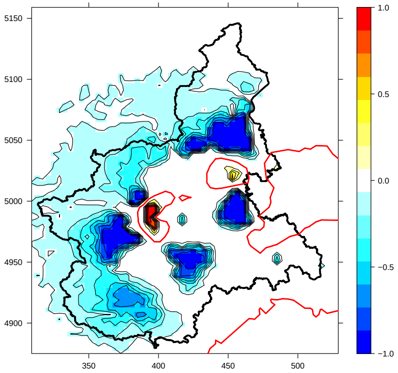
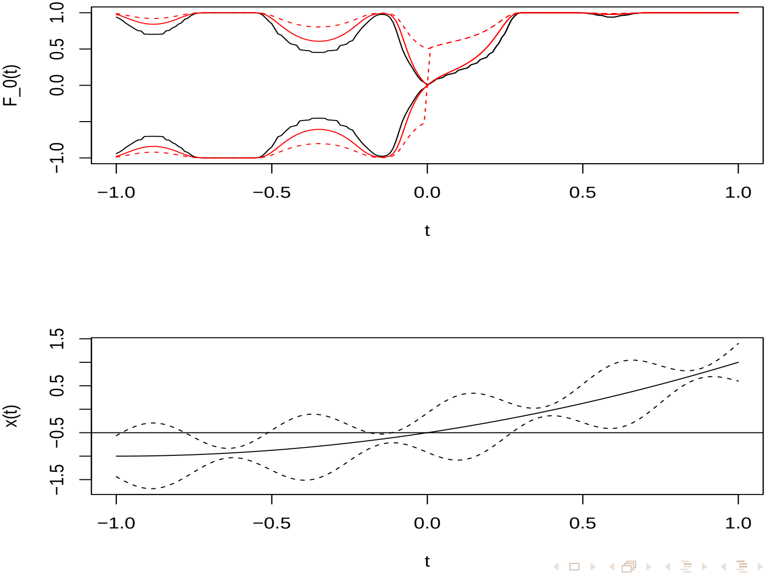
Contour function $F^c_{50}(s)$



Signed avoidance $\pm F_{50}(s)$



The signed avoidance function



Future and current

- Investigate if/when the more complicated parametric families are needed.
- For excursion sets, compare results with other thresholding methods and a sample based method by French and Sain.
- For contour uncertainty sets, compare with the methods by Lindgren and Rychlik (1995).
- Combine method with the work by Polfeldt (1999) to make quantitative statements about joint contour map reliability.
- R package `excursions`, on CRAN:

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excursions(alpha=0.05, u=0, type=">",
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```

References

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A sequential Monte-Carlo algorithm

- a GMRF can be viewed as a non-homogeneous AR-process defined backwards in the indices of $\mathbf{x}$.
- Let L be the Cholesky factor of $\mathbf{Q}$, then

$$x_i|x_{i+1},\ldots,x_n \sim \mathsf{N}\left(\mu_i - \frac{1}{L_{ii}}\sum_{j=i+1}^{n} L_{ji}(x_j-\mu_j), L_{ii}^{-2}\right),$$

- Denote the integral of the last $d-i$ components as I_i,

$$I_i = \int_{a_i}^{b_i} \pi(x_i|x_{i+1:d}) \cdots \int_{a_{d-1}}^{b_{d-1}} \pi(x_{d-1}|x_d) \int_{a_d}^{b_d} \pi(x_d)\,\mathrm{d}x,$$

- $x_i|x_{i+1:d}$ only depends on the elements in $x_{\mathcal{N}_i\cap\{i+1:d\}}$.
- Estimate the integrals using sequential importance sampling.
- in each step x_j is sampled from the truncated Gaussian distribution $1(a_j < x_j < b_j)\pi(x_j|x_{j+1:d})$.
- The importance weights can be updated recursively.

Parametric families for excursion sets

Parametric family for level avoiding sets

Let $D_1^+(\rho_1)$ and $D_1^-(\rho_2)$ be given by the one-parameter family.

- A two-parameter family for the pair of level avoiding sets is obtained as $(D_1^+(\rho_1), D_1^-(\rho_2))$.
- A one-parameter family is obtained by requiring that $\rho_1 = \rho_2 = \rho$.

- The one-parameter family can be used in the method without modifications to estimate level avoiding sets and contour uncertainty regions.
- The two-parameter family requires a modified method where one of the parameters is optimized using e.g. golden section search.

Extension to a latent Gaussian setting

- Assuming that $\pi(\mathbf{x}|\mathbf{y},\boldsymbol{\theta})$ is,or can be approximated as, Gaussian, there are several ways to calculate the excursion probabilities. One of which is

Numerical integration

Numerically approximate the excursion probability by approximating the posterior integral as

$$\mathsf{P}(\mathbf{a}<\mathbf{x}<\mathbf{b}) = \mathsf{E}(\mathsf{P}(\mathbf{a}<\mathbf{x}<\mathbf{b}|\boldsymbol{\theta})) \approx \sum_{i=1}^{k} w_i \mathsf{P}(\mathbf{a}<\mathbf{x}<\mathbf{b}|\boldsymbol{\theta}_i),$$

where the configuration $\{\boldsymbol{\theta}_i\}$ is taken from INLA and the weights w_i are chosen proportional to $\pi(\boldsymbol{\theta}_i|\mathbf{y})$.

- Often only a few configurations $\{\boldsymbol{\theta}_i\}$ are needed.