Quantifying the uncertainty of contour maps

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Scotland

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Contour map for US summer mean temperature

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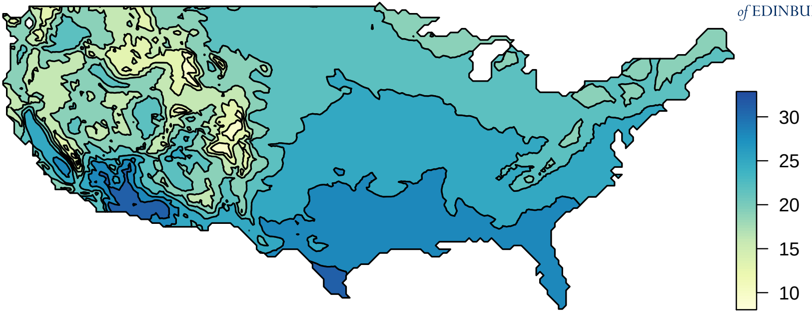

- Can we trust the apparent details af the level crossings?
- How many levels should we sensibly use?
- Can we put a number on the statistical quality of the contour map?
- Fundamental question:
  What *is* the statistical interpretation of a contour map?
- To answer these questions we need methods for efficient calculations for random fields.

GMRFs: Gaussian Markov random fields

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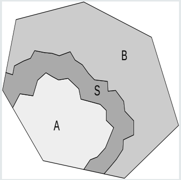
Continuous domain GMRFs ((Rozanov, 1977)

If $x(\boldsymbol{s})$ is a (stationary) Gaussian random field on Ω with covariance function $R_x(\boldsymbol{s}, \boldsymbol{s}')$, it fulfills the *global Markov property*

$$\{x(\mathcal{A}) \perp x(\mathcal{B}) | x(\mathcal{S}), \text{ for all } \mathcal{AB}\text{-separating sets } \mathcal{S} \subset \Omega\}$$

if the power spectrum can be written as $1/S_x(\boldsymbol{\omega}) =$ polynomial in $\boldsymbol{\omega}$, for some polynomial order p.
Generally: Markov if the precision operator is local.



Discrete domain GMRFs

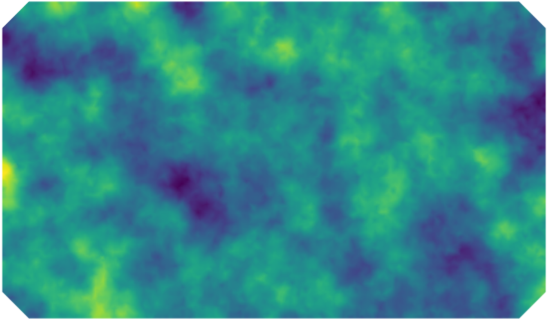
$\boldsymbol{x} = (x_1, \ldots, x_n) \sim \mathsf{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$ is Markov with respect to a neighbourhood structure $\{\mathcal{N}_i, i = 1, \ldots, n\}$ if $Q_{ij} = 0$ whenever $j \neq \mathcal{N}_i \cup i$.

- Continuous domain basis representation with Markov weights: $x(\boldsymbol{s}) = \sum_{k=1}^{n} \Psi_k(\boldsymbol{s}) x_k$
- Many stochastic PDE solutions are Markov in continuous space, and can be approximated by *Markov weights on local basis functions*.

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

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

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



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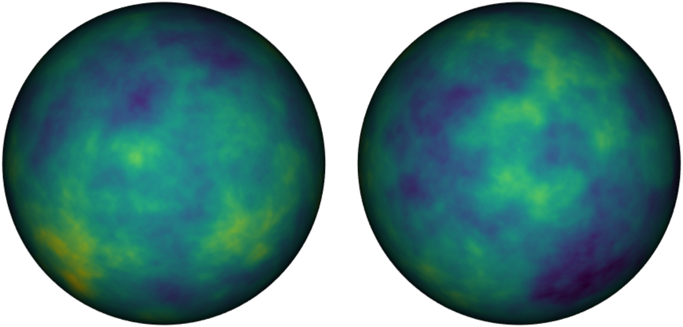

GMRFs based on SPDEs (Lindgren et al., 2011)

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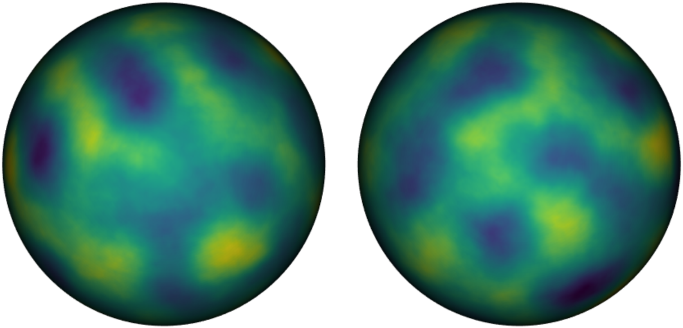
GMRF representations of SPDEs can be constructed for oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$(\kappa^2 e^{i\pi\theta} - \Delta)(\tau\, x(\boldsymbol{s})) = \mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{s} \in \Omega$$



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

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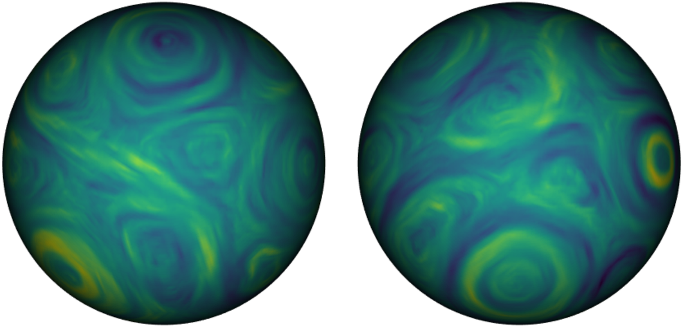
GMRF representations of SPDEs can be constructed for oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

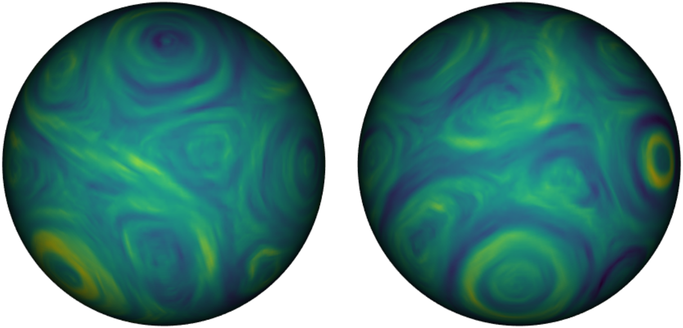
$$(\kappa_{\boldsymbol{s}}^2 + \nabla \cdot \boldsymbol{m}_{\boldsymbol{s}} - \nabla \cdot \boldsymbol{M}_{\boldsymbol{s}} \nabla)(\tau_{\boldsymbol{s}} x(\boldsymbol{s})) = \mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{s} \in \Omega$$



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

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

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



Spatial latent Gaussian models

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Consider a simple hierarchical spatial generalised linear model

$$\begin{aligned} \boldsymbol{\beta} &\sim \mathsf{N}(\mathbf{0}, \boldsymbol{I}\sigma_\beta^2), \\ \xi(\boldsymbol{s}) &\sim \text{Gaussian (Markov) random field}, \\ x(\boldsymbol{s}) &= \boldsymbol{z}(\boldsymbol{s})\boldsymbol{\beta} + \xi(\boldsymbol{s}), \\ (y_i|x) &\sim \pi(y_i|x(\cdot), \boldsymbol{\theta}), \quad \text{e.g. } \mathsf{N}(x(\boldsymbol{s}_i), \sigma_e^2), \end{aligned}$$

where $\boldsymbol{z}(\cdot)$ are spatially indexed explanatory variables, and y_i are conditionally independent observations.

- A contour curve for a level u crossing is typically calculated as the level u crossing of $\widehat{x} = \mathsf{E}[x(\boldsymbol{s})|\boldsymbol{y}]$.
- In practice, we want to interpret it as being informative about the potential level crossings of the random field $x(\boldsymbol{s})$ itself.
- We need access to high dimensional joint probabilities in the posterior density $\pi(\boldsymbol{x}|\boldsymbol{y})$.

Posterior probabilities

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

Numerical integration

Numerically approximate the excursion probability by approximating the posterior integral as

$$\mathsf{P}(\boldsymbol{a} < \boldsymbol{x} < \boldsymbol{b}|\boldsymbol{y}) = \mathsf{E}[\mathsf{P}(\boldsymbol{a} < \boldsymbol{x} < \boldsymbol{b}|\boldsymbol{y},\boldsymbol{\theta})] \approx \sum_k w_k \mathsf{P}(\boldsymbol{a} < \boldsymbol{x} < \boldsymbol{b}|\boldsymbol{y},\boldsymbol{\theta}_k),$$

where each parameter configuration $\boldsymbol{\theta}_k$ is provided by R-INLA and the weights w_k are chosen proportional to $\pi(\boldsymbol{\theta}_k|\boldsymbol{y})$.

- Often only a few configurations $\boldsymbol{\theta}_k$ are needed.
- Quantile corrections and other techniques from INLA can be added

A sequential Monte-Carlo algorithm

- A GMRF can be viewed as a non-homogeneous AR-process defined backwards in the indices of $\boldsymbol{x} \sim \mathsf{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$.
- Let $\boldsymbol{L}$ be the Cholesky factor in $\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^{\top}$. 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 $n-i$ components as I_i,

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

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

Contours and excursions

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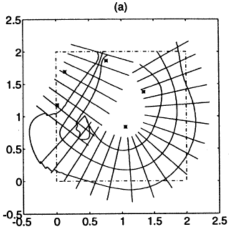
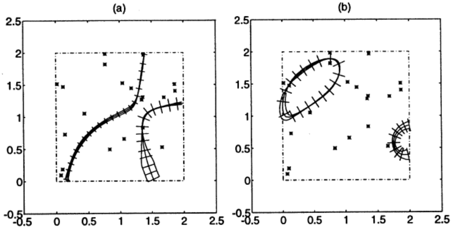
- Lindgren, Rychlik (1995): *How reliable are contour curves? Confidence sets for level contours*, Bernoulli
  Regions with a single expected crossing
- Polfeldt (1999) *On the quality of contour maps*, Environmetrics
  How many contour curves should one use?
- Neither paper considered joint probabilities
- 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.





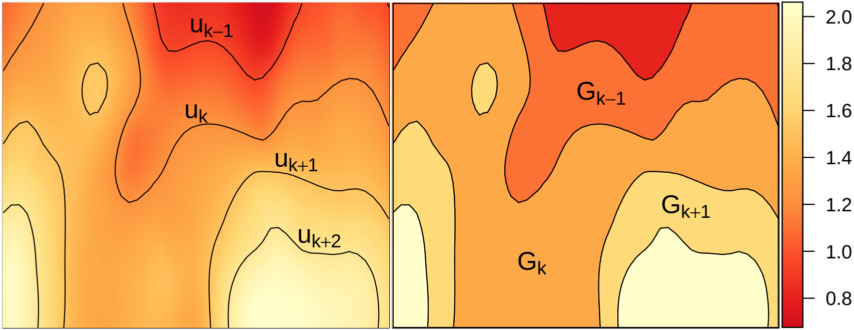
Level sets

Level sets

Given a function $f(\boldsymbol{s})$, $\boldsymbol{s} \in \Omega$ and levels

$$-\infty = u_0 < u_1 < u_2 < \cdots < u_K < u_{K+1} = +\infty,$$

the *level sets* are $G_k(f) = \{\boldsymbol{s};\ u_k < f(\boldsymbol{s}) < u_{k+1}\}$, $k = 0, \ldots, K$.



Joint and marginal probabilities

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Now, consider a contour map based on a point estimate $\widehat{x}(\cdot)$.

Intuitively, we might consider the joint probability

$$\mathsf{P}(u_k < x(\boldsymbol{s}) < u_{k+1}, \text{ for all } \boldsymbol{s} \in G_k(\widehat{x}) \text{ and all } k)$$

Unfortunately, this will nearly always be close to or equal to zero!

Polfeldt (1999) instead considered the marginal probability field

$$p(\boldsymbol{s}) = \mathsf{P}(u_k < x(\boldsymbol{s}) < u_{k+1} \text{ for } k \text{ such that } \boldsymbol{s} \in G_k(\widehat{x}))$$

The argument is then that if $p(\boldsymbol{s})$ is close to 1 in a large proportion of space, the contour map is not overconfident.

We extend this notion to alternative joint probability statements.

Contour avoiding sets and the contour map function

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Contour avoiding sets

The *contour avoiding sets* $M_{\boldsymbol{u},\alpha} = (M^0_{\boldsymbol{u},\alpha}, \ldots, M^K_{\boldsymbol{u},\alpha})$ are given by

$$M_{\boldsymbol{u},\alpha} = \underset{(D_0,\ldots,D_K)}{\operatorname{argmax}} \left\{ \sum_{k=0}^{K} |D_k| : \mathsf{P}\left(\bigcap_{k=0}^{K} \{D_k \subseteq G_k(x)\} \right) \geq 1-\alpha \right\}$$

where D_k are disjoint and open sets. The joint contour avoiding set is then $C_{\boldsymbol{u},\alpha}(x) = \bigcup_{k=0}^{K} M^k_{\boldsymbol{u},\alpha}$.

Note: $C_{\boldsymbol{u},\alpha}(x)$ is the largest set so that with probability at least $1-\alpha$, the intuitive contour map interpretation is fulfilled for $\boldsymbol{s} \in C_{\boldsymbol{u},\alpha}(x)$.

The *contour map function* $F_{\boldsymbol{u}}(\boldsymbol{s}) = \sup\{1-\alpha;\ \boldsymbol{s} \in C_{\boldsymbol{u},\alpha}\}$ is a joint probability extension of the Polfeldt idea.

Quality measures

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Let $C_{\boldsymbol{u}}(\widehat{x})$ denote a contour map based on a point estimate of x.

Three quality measures

P_0: The proportion of space where the intuitive contour map interpretation holds jointly: $P_0(x, C_{\boldsymbol{u}}(\widehat{x})) = \frac{1}{|\Omega|}\int_\Omega F_{\boldsymbol{u}}(\boldsymbol{s})\,\mathrm{d}\boldsymbol{s}$

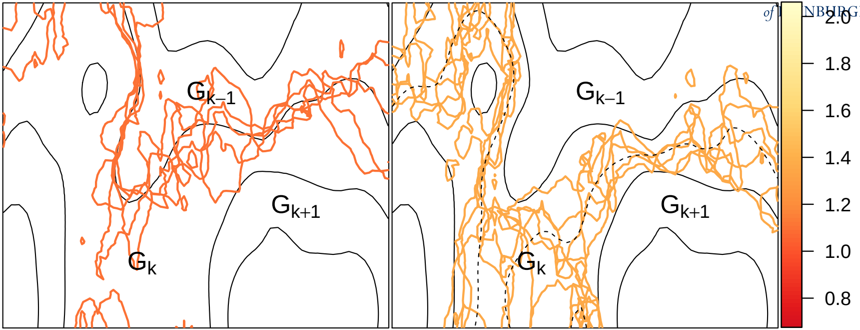
P_1: Joint credible regions for u_k crossings:

$$P_1(x, C_{\boldsymbol{u}}(\widehat{x})) = \mathsf{P}\left(\cap_k \{x(\boldsymbol{s}) < u_k \text{ where } \widehat{x}(\boldsymbol{s}) < u_{k-1}\} \cap \{x(\boldsymbol{s}) > u_k \text{ where } \widehat{x}(\boldsymbol{s}) > u_{k+1}\}\right)$$

P_2: Joint credible regions for $u_k^e = \frac{u_k + u_{k+1}}{2}$ crossings:

$$P_2(x, C_{\boldsymbol{u}}(\widehat{x})) = \mathsf{P}\left(\cap_k \{x(\boldsymbol{s}) < u_k^e \text{ where } \widehat{x}(\boldsymbol{s}) < u_k\} \cap \{x(\boldsymbol{s}) > u_k^e \text{ where } \widehat{x}(\boldsymbol{s}) > u_{k+1}\}\right)$$

Interpretation of P_1 and P_2

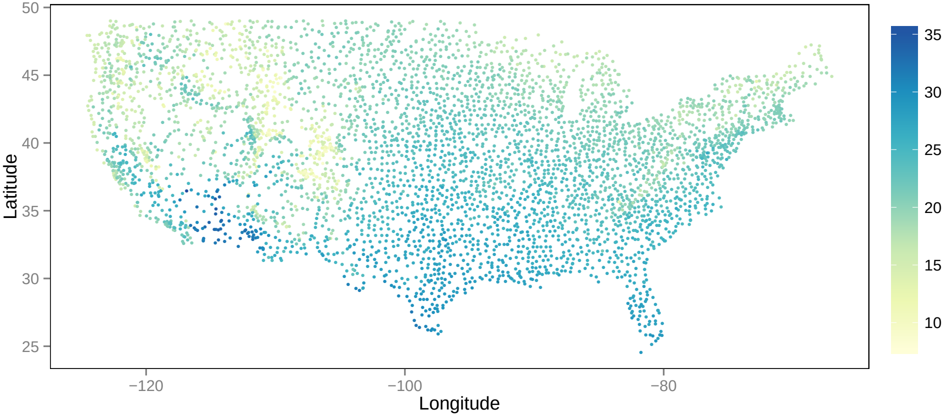


Five realisations of contour curves from the posterior distribution for x are shown.

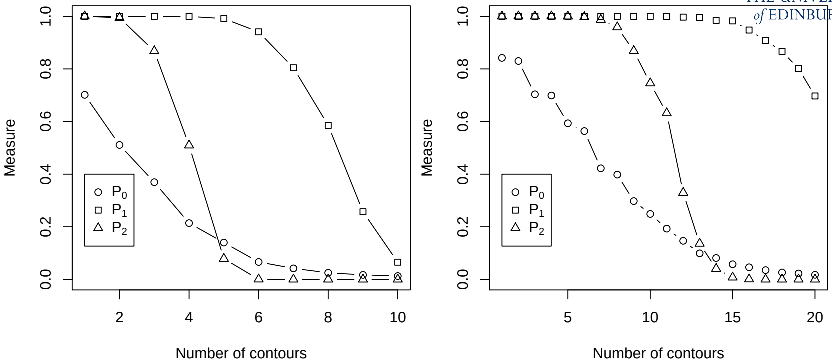
Note the fundamental difference in smoothness between the contours of $\widehat{x}$ and x!

Additional note for theorists:
The process x is not a member of its own RKHS, but $\hat{x}$ usually is.
This is a feature, not a bug.

Mean summer temperature measurements for 1997



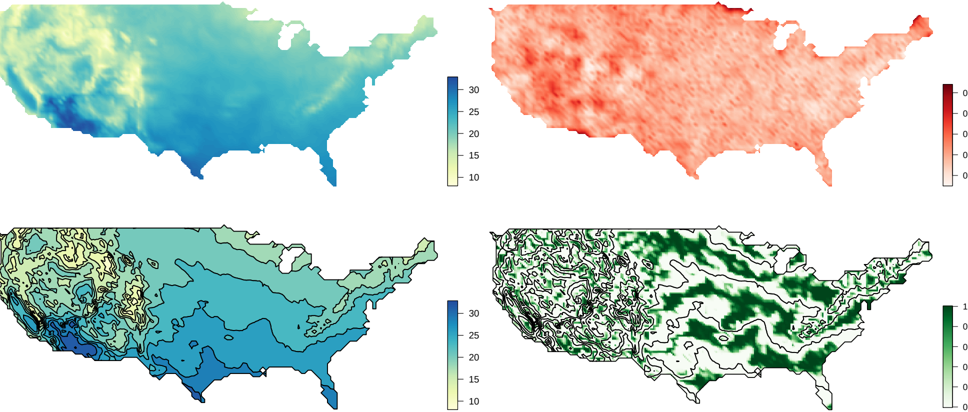
Contour map quality for different K and different models



The spatial predictions are more uncertain in a model without spatial explanatory variables (left) than in a model using elevation (right).

P_1 consistently admits about double the number of contour levels in comparison with P_2, as expected from the probabilistic interpretations.

Posterior mean, s.d., contour map, and F_u, for $K = 8$



Contour map quality measure: $P_2 = 0.958$

Summary

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- Drawn contours are usually non-linear functions of point estimates
- Point estimate contour shapes do not match actual structure
- Recast the uncertainty problem as probabilistic excursion sets
- Excursion formulation allows discontinuities, avoiding the hypothesis testing *equal to the level* trap
- Recursive Monte Carlo integration for high dimensional probabilities
- General concept not tied to a specific computational method
- Instead of drawing too many contours, should often consider either
  - using a continuous colour scale, showing the entire point estimate, or
  - using only a specific contour of interest, e.g. "regulation air quality limit"

References

- David Bolin and Finn Lindgren (2015): Excursion and contour uncertainty regions for latent Gaussian models, *JRRS Series B*, 77(1):85–106
- David Bolin and Finn Lindgren (2016): Quantifying the uncertainty of contour maps, *J of Computational and Graphical Statistics*.
- David Bolin and Finn Lindgren (2018, to appear): Calculating Probabilistic Excursion Sets and Related Quantities Using `excursions`, *J of Statistical Software*. `https://arxiv.org/abs/1612.04101`
- David Bolin and Finn Lindgren: R CRAN package `excursions` (dev on `https://bitbucket.com/davidbolin/excursions`)

```
contourmap(mu = expectation, Q = precision)
contourmap.inla(result.inla) # INLA or inlabru output
continuous(..., geometry) # Interpret on continuous domain
```

- Lindgren, F., Rue, H. and Lindström, J. (2011): An explicit link between Gaussian fields and Gaussian Markov eandom fields: the stochastic partial differential equation approach (with discussion); *JRSS Series B*, 73(4):423–498