Quantifying the uncertainty of contour maps

David Bolin
University of Gothenburg

joint work with Finn Lindgren

Banff, July 12, 2017

References and the connection to Peter

Seamocs workshop, Malta 2009

- B. and Lindgren: *Excursion and contour uncertainty regions for latent Gaussian models*, JRRS Series B (2015): 77(1):85-106.
  Acknowledgements: *The authors are grateful to . . . Peter Guttorp for highlighting the need for a thorough treatment of the subject.*

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Contour maps

- B. and Lindgren: *Quantifying the uncertainty of contour maps*, J of Computational and Graphical Statistics (2016).
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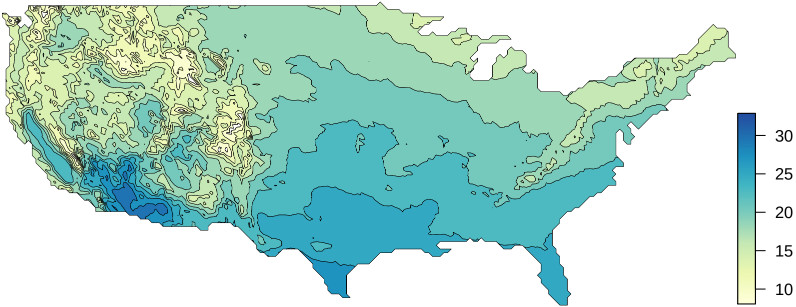
Contour map of US summer mean temperature



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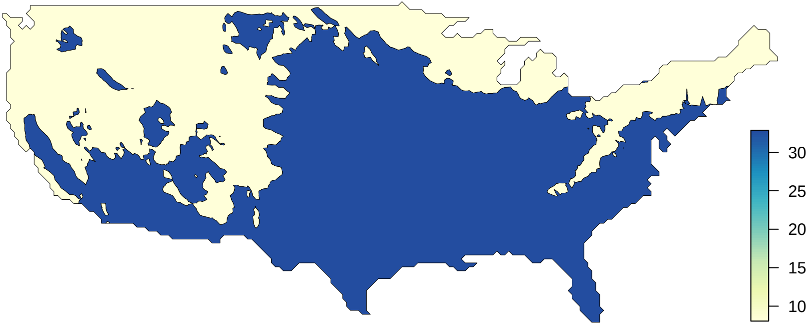

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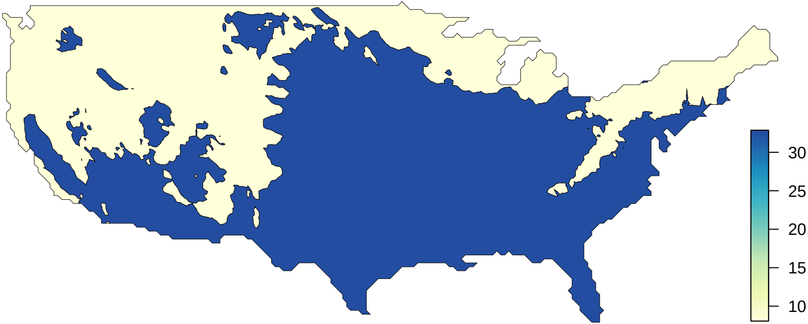

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- Can we put a number on the statistical quality of the contour map?

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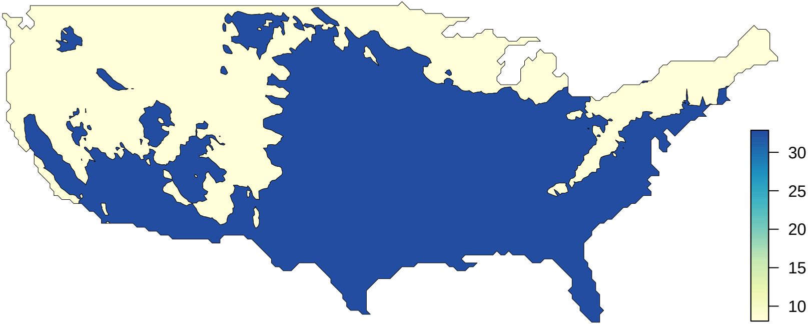
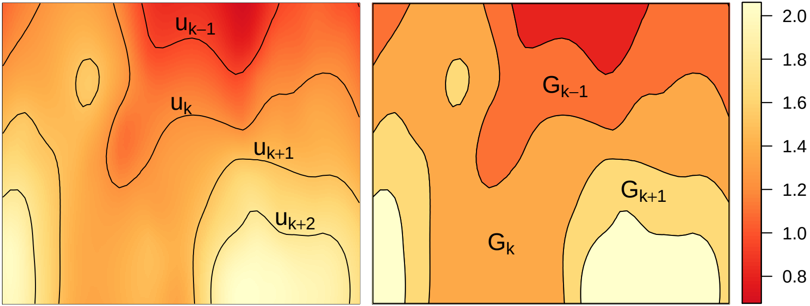


- Can we trust the apparent detail of the level crossings?
- How many contours should we use?
- Can we put a number on the statistical quality of the contour map?
- Fundamental question:
  What *is* the statistical interpretation of a contour map?

Contour maps



For a function f, a contour map $C_f(u_1, \ldots, u_K)$ with K contour levels $u_1 < u_2 < \ldots < u_K$ is the collection of

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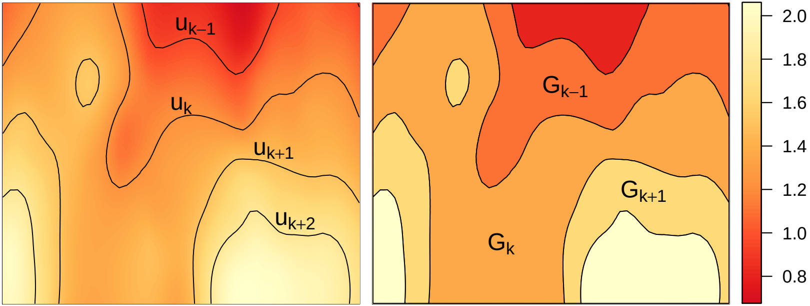

For a function f, a contour map $C_f(u_1, \ldots, u_K)$ with K contour levels $u_1 < u_2 < \ldots < u_K$ is the collection of

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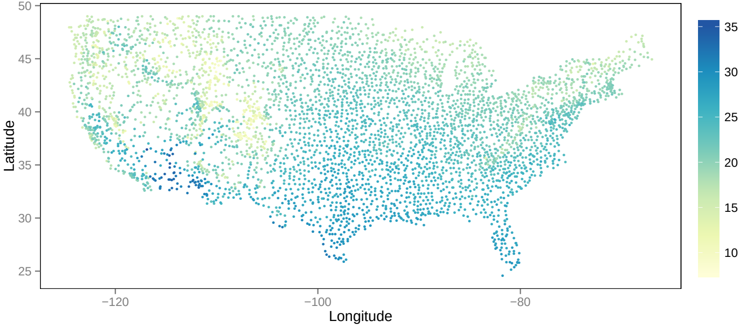
- Level sets $G_k = \{s : u_k < f(s) < u_{k+1}\}$.

Latent Gaussian models



$$\xi(\mathbf{s}) \sim \text{Gaussian random field}$$
$$x(\mathbf{s}) = \mathbf{z}(\mathbf{s})\boldsymbol{\beta} + \xi(\mathbf{s})$$
$$y_i | x(\cdot) \sim \pi(y_i | x(\cdot), \boldsymbol{\theta}), \quad \text{e.g. } \mathsf{N}(x(\mathbf{s}_i), \sigma^2)$$

where $\mathbf{z}(\cdot)$ are explanatory variables and y_i are observations.

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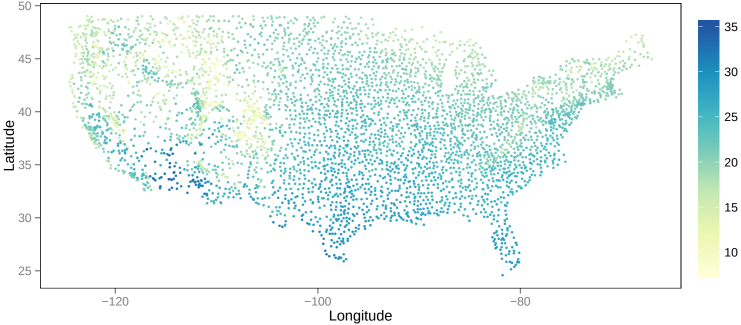

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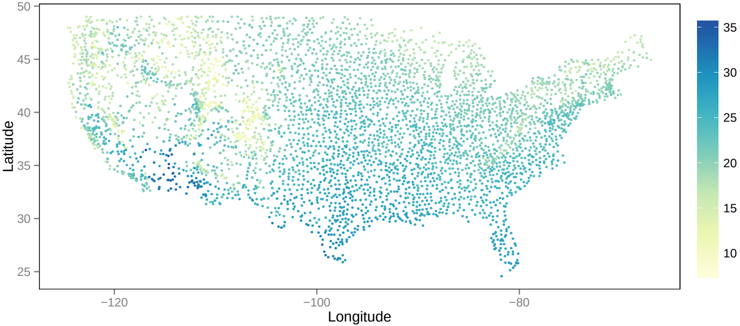

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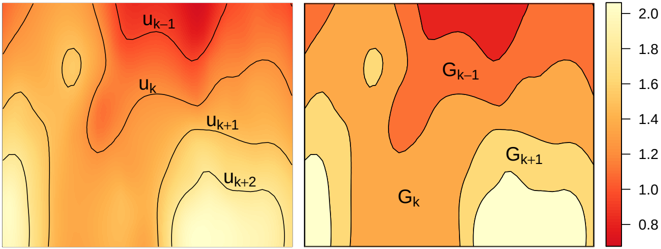
where $\mathbf{z}(\cdot)$ are explanatory variables and y_i are observations.

- A contour map is often reported for $\hat{x}(\mathbf{s}) = \mathsf{E}(x(\mathbf{s})|\mathbf{y})$.
- We interpret the contour map as being informative about x itself.

Interpreting a contour map $C_{\hat{x}}(\mathbf{u})$



- Intuitively, one might interpret a contour map as having

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

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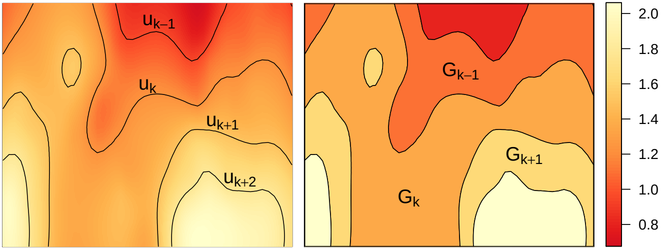

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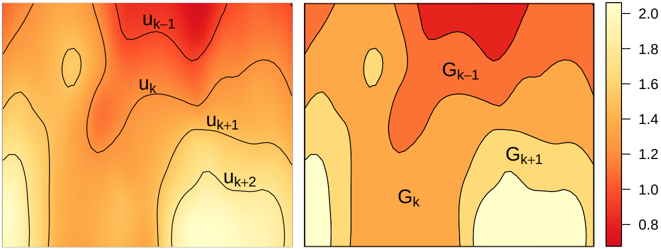

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- This probability will nearly always be close to or equal to zero!
- Polfeldt (1999), *On the quality of contour maps*, Environmetrics, instead considered the marginal probabilities

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

and argued that if $p(\mathbf{s})$ is close to 1 in a large proportion of the region, the contour map is not overconfident.

Contour avoiding sets

We construct an alternative to $p(\mathbf{s})$ that has a joint probability statement.

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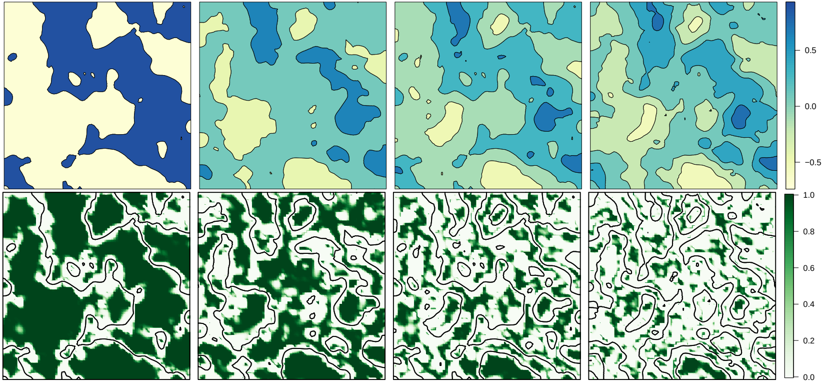
Contour avoiding sets

Let $A_k = \{s : u_k < x(s) < u_{k+1}\}$. The joint $\mathbf{u} = (u_1, \ldots, u_K)$ contour avoiding set is $C_{\mathbf{u},\alpha}(x) = \bigcup_k M_{u_k,\alpha}$, where $M_{\mathbf{u},\alpha} = (M_{u_1,\alpha}, \ldots, M_{u_K,\alpha})$ is given by

$$M_{\mathbf{u},\alpha} = \operatorname*{arg\,max}_{(D_1,\ldots,D_K)} \left\{ \sum_{k=1}^{K} |D_k| : D_k \subseteq G_k, \mathsf{P}\left(\bigcap_k \{D_k \subseteq A_k\} \right) > 1-\alpha \right\},$$

The contour avoiding set is the largest set so that, with probability $1-\alpha$, the intuitive contour map interpretation holds for $\mathbf{s} \in C_{\mathbf{u},\alpha}(X)$.

The contour map function



Given $C_{\bar{u},\alpha}(X)$ we define the *contour map function*

$$F_u(s) = \sup\{1-\alpha; s \in C_{\bar{u},\alpha}\},$$

as a joint probability extension of the Polfeldt idea.

Contour map quality measures

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The P_0 quality measure

Given the contour map function, a simple contour map quality measure, P_0 is given by

$$P_0(x, C_f) = \frac{1}{|\Omega|}\int_\Omega F_{\mathbf{u}}(\mathbf{s})\,\mathrm{d}\mathbf{s}.$$

Loosely speaking, this is the percentage of the total area for which the intuitive interpretation of the contour map holds.

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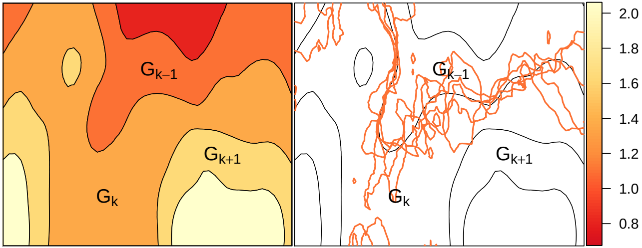
For the contour maps in the example above, we have

$$P_0 = 0.613, \quad P_0 = 0.440, \quad P_0 = 0.394, \quad P_0 = 0.148$$

The "intuitive" interpretation is not the only global interpretation of a contour map!

The P_1 quality measure



Five realisations of u_k contour curves from the posterior for x.

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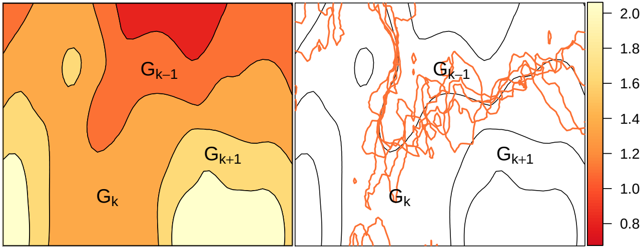
The P_1 quality measure



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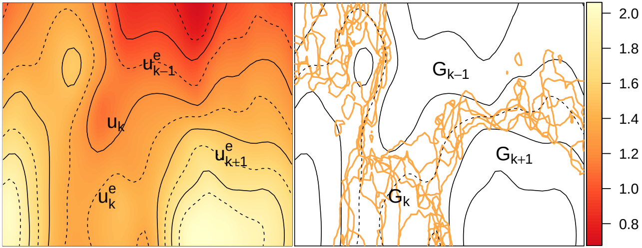
- Another natural interpretation of $C_{\hat{x}}$ is that $G_{k-1} \cup G_k$ should contain all level u_k crossings of the process x.
- Define P_1 as the probability for this occurring:

$$P_1(X, C_f(u_1, \ldots, u_K)) = \mathsf{P}\left(\bigcap_{k=0}^{K} \{u_{k-1} < x(s) < u_{k+2}, s \in G_k\} \right)$$

The P_2 quality measure



Five realisations of u_k^e contour curves from the posterior for x.

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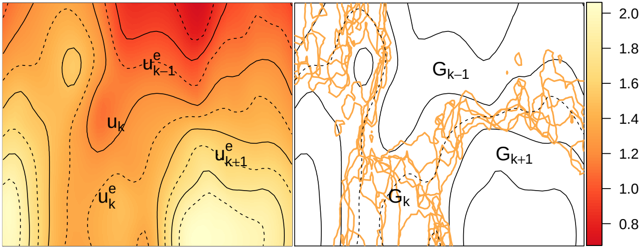

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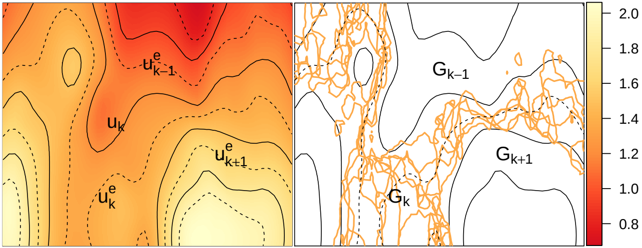

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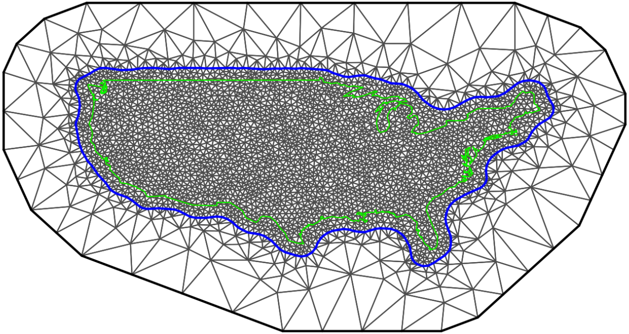
Computational details



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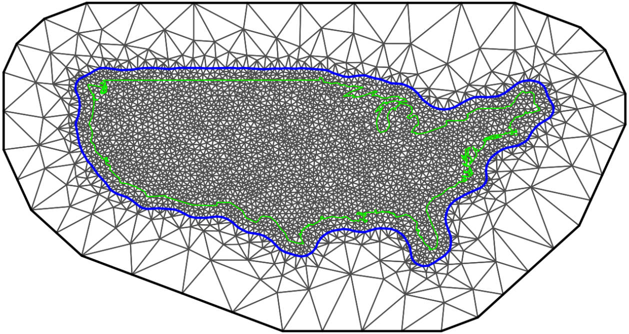

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  - SPDE-based spatial models satisfy this by construction.

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- In a Bayesian setting, one can numerically approximate the posterior probability as

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  where $w_k \propto \pi(\boldsymbol{\theta}_k|\mathbf{y})$ and $\boldsymbol{\theta}_k$ are cleverly chosen parameter configurations (for example as done in INLA).
- Often only a few configurations are needed for accurate results.

Gaussian integrals

Computing the Gaussian probability is done by computing an integral

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

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- For GMRFs, we want to use the sparsity of $\mathbf{Q}$.
- We use a method based on sequential importance sampling.
  - It is based on that a GMRF can be viewed as a non-homogeneous AR-process defined backwards in the indices of $\mathbf{x}$:

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

where $\mathbf{L}$ is the Cholesky factor of $\mathbf{Q}$.

The excursions package

The methods are implemented in the R package `excursions`

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Important functions in the package:

- `excursions`: Compute uncertainty regions for individual contour curves, excursion sets, and excursion functions.
- `contourmap`: Compute contour maps, quality measures, and contour map functions.
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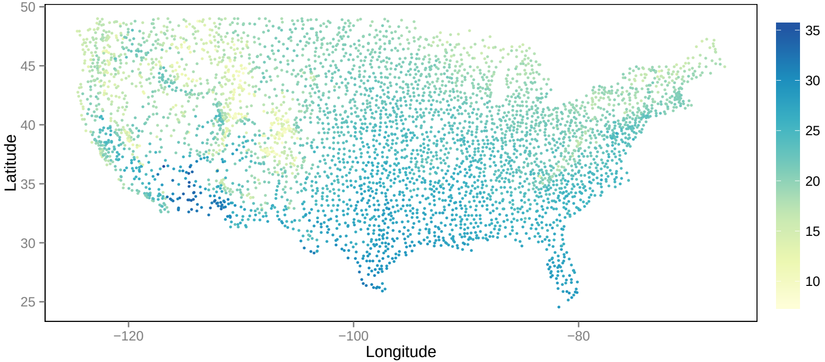
Specialized versions of the functions:

- Interface to R-INLA: e.g. `excursions.inla`
- Functions to analyze MCMC output: e.g. `excursions.mc`

Back to the US temperatures

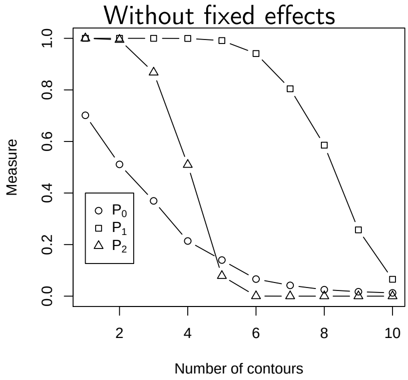


Measurements at approximately 8000 locations.

Estimate the true temperature surface using the model:

- Likelihood: $Y_i \sim \mathsf{N}(X(s_i), \sigma^2)$.
- Latent temperature model: $x(s)$ is a Gaussian Matérn field.

Contour map quality measures



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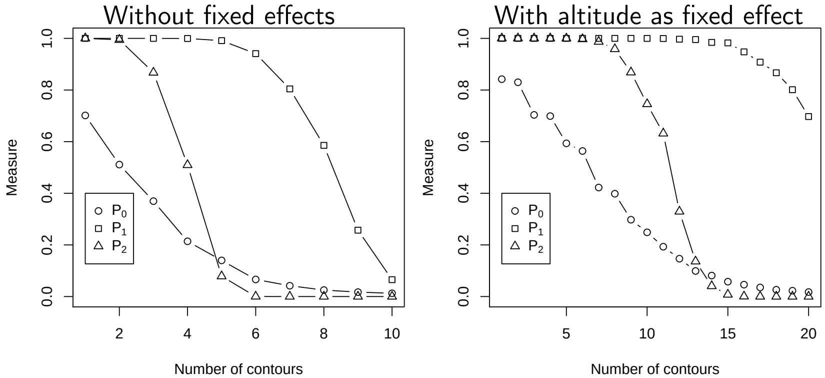
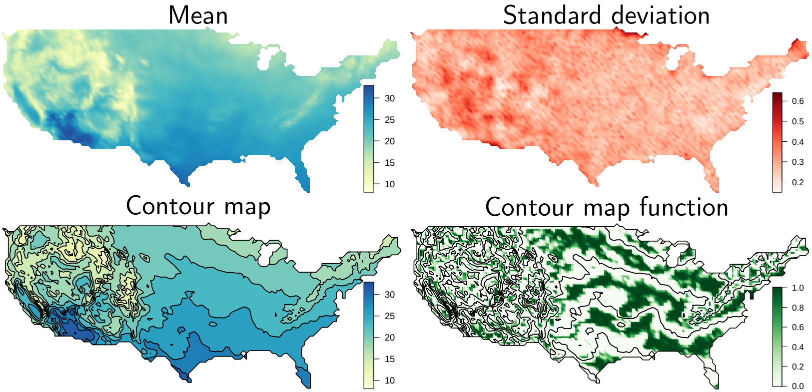


The spatial predictions are more uncertain in a model without spatial explanatory variables (left) than in a model using elevation (right).

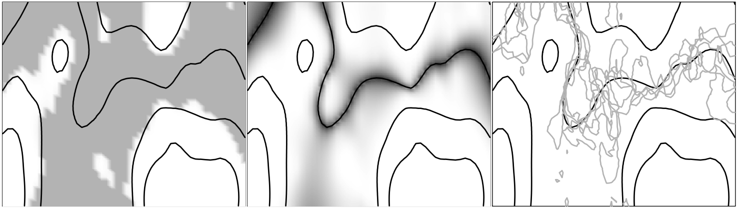
Without explanatory variables, use 3 contours. With elevation, use 10.

Results



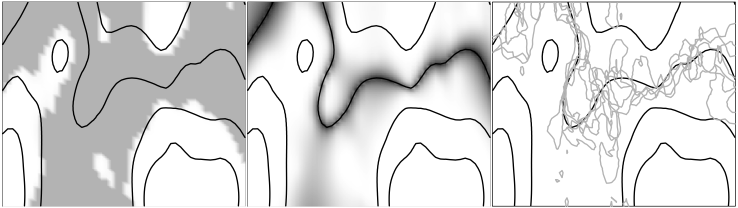
With 10 contour levels the contour map above has $P_2 \approx 0.95$.

Alternative methods for uncertainty visualization



Is a contour map the best way of visualizing the uncertainty?

Alternative methods for uncertainty visualization



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Methods for drawing contours with uncertainty:

- Add credible band to the contours.

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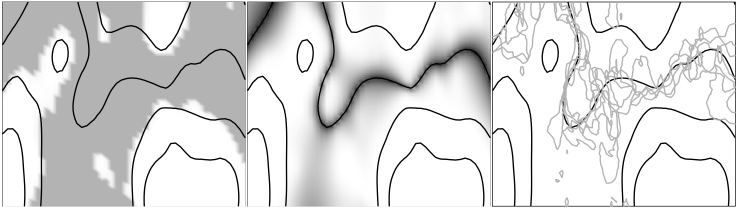

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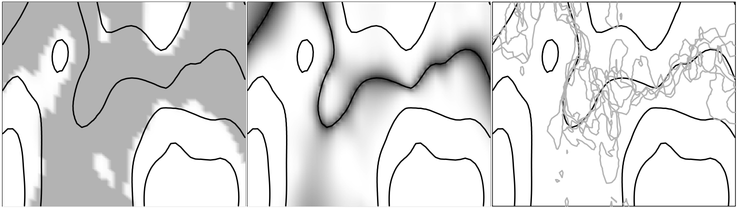

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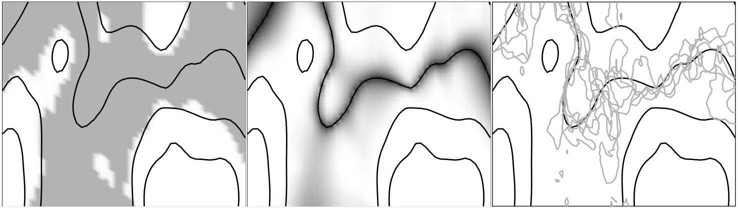

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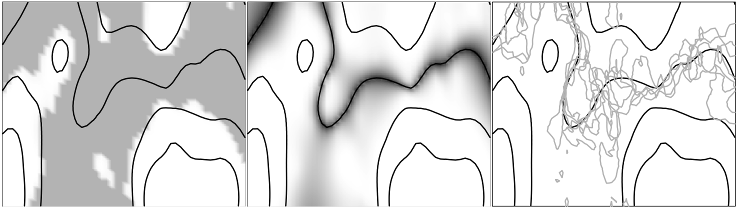

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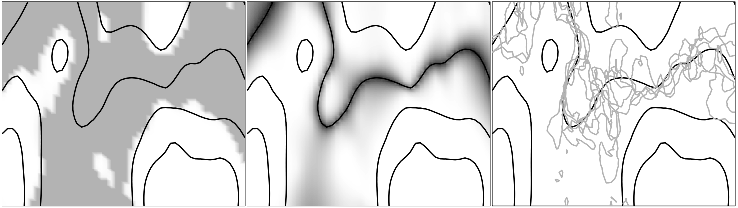

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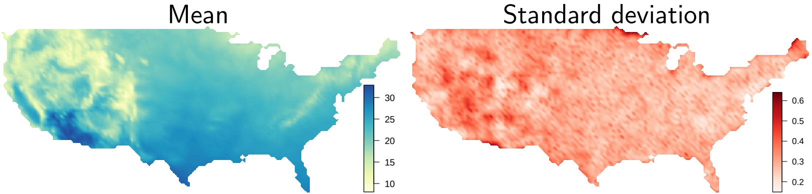

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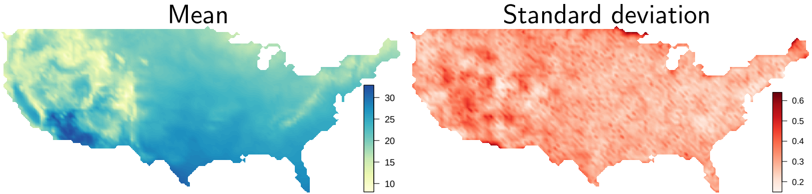

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There are many other ways to visualize the uncertainty:

- Two maps: One of a point estimate and one of posterior standard deviations.
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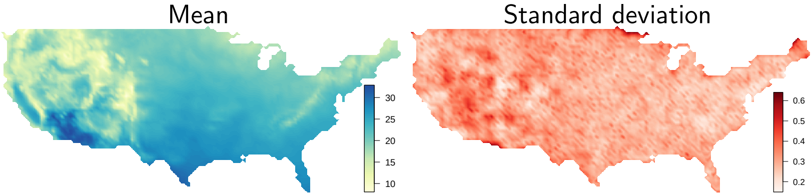

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Is there a best alternative?

Questions for the breakout session

Join the discussion in Breakout session G tomorrow!

1. What is the best way of visualizing estimates of spatial fields and their uncertainties?
2. How should one do visualization for more complicated scenarios:
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Thanks for your attention!