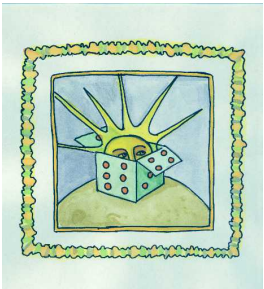


An introduction and case study using extremes

Douglas Nychka, Eric Gilleland, Uli Schnieder
National Center for Atmospheric Research

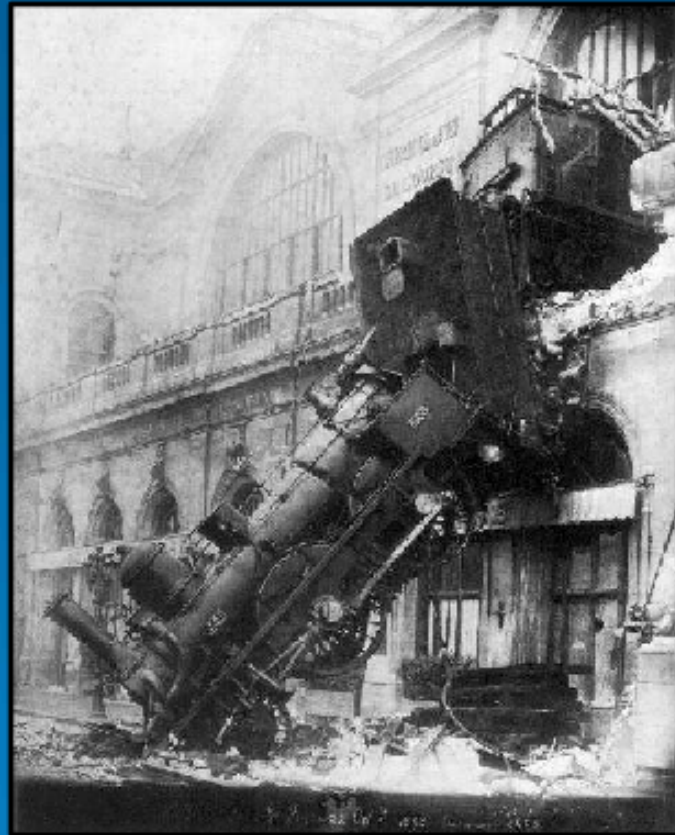
- Some examples
- Extreme value theory and methods (GEV,GPD)
- Space-time model for ozone
- Spatial model for ozone extremes



Extreme Events

“Man can believe
the impossible.
But man can
never believe the
improbable.”

- Oscar Wilde



Surface level ozone

Ozone(O_3) is formed from volatile organic compounds (both pollutants and naturally occurring compounds) emitted into the atmosphere and NO_x in the presence of sunlight.

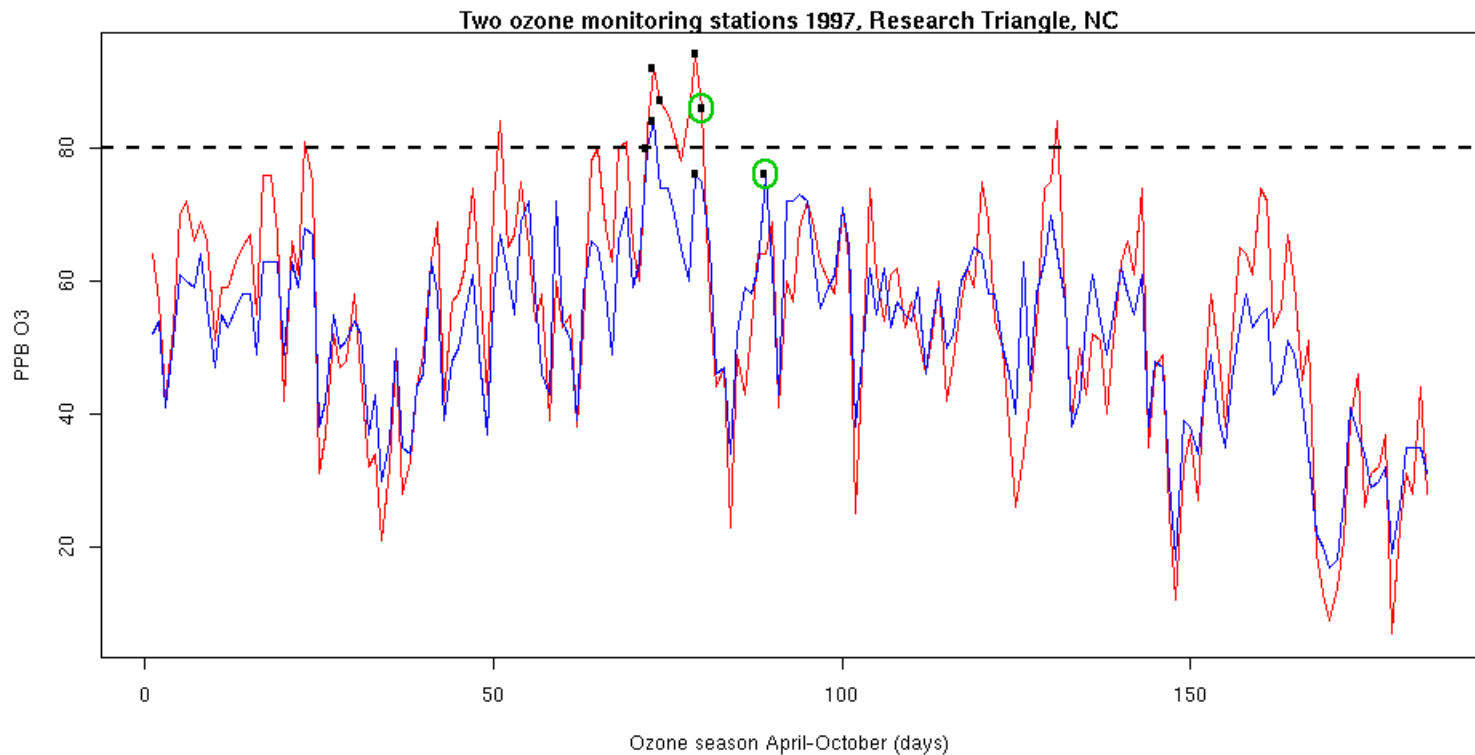
High ozone concentrations cause respiratory problems and sustained lower levels damage vegetation.

US EPA regulations based on the Clean Air Act:

A suggested ozone pollutant standard is based on the fourth *highest* (max) 8-hour daily average (FHDA) recorded during the year. A region is in attainment if the three year average is less than 80 PPB.

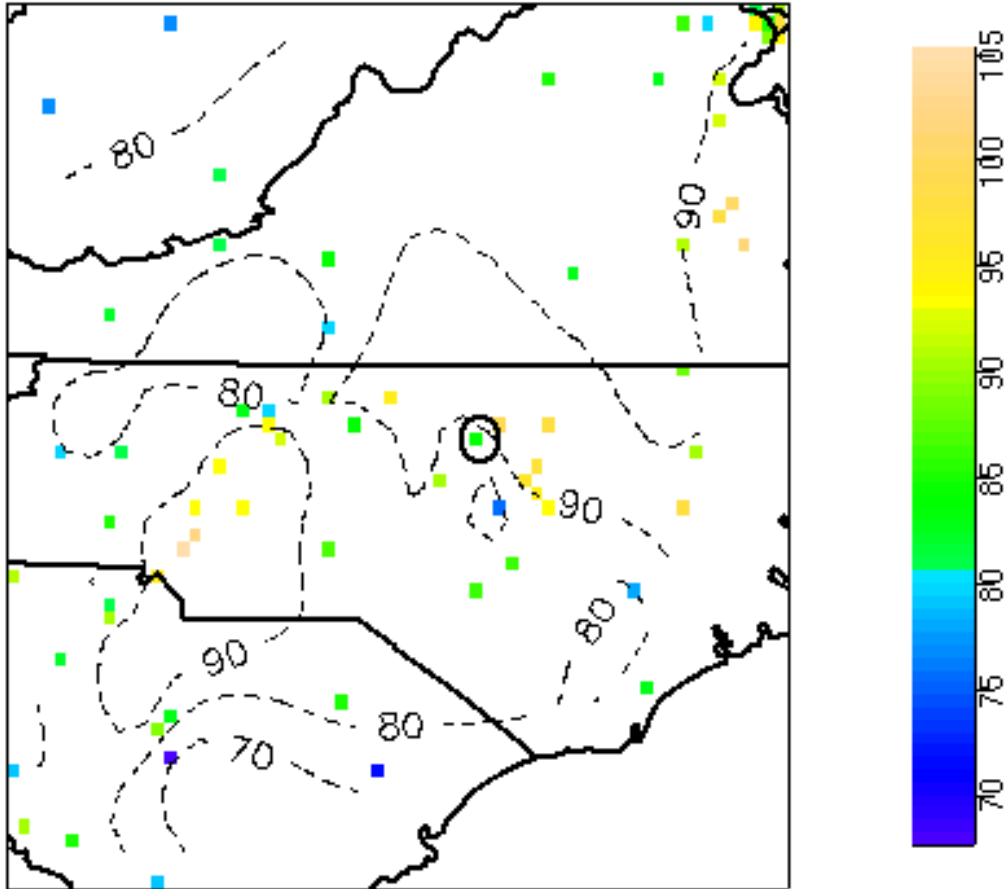
Example of calculating the FHDA statistic

The ozone “season” is 184 days. \approx May-September.



$$FHDA = \left(1 - \frac{4}{184}\right) \text{ quantile of the ozone distribution}$$

RTP study region with FHDA's for 1997



Spatial extremes: our problem today

Based on this example:

Given a spatial process $Z(\mathbf{x})$, what can we say about

$$P(Z(\mathbf{x}) > z_0)$$

when z_0 is large?

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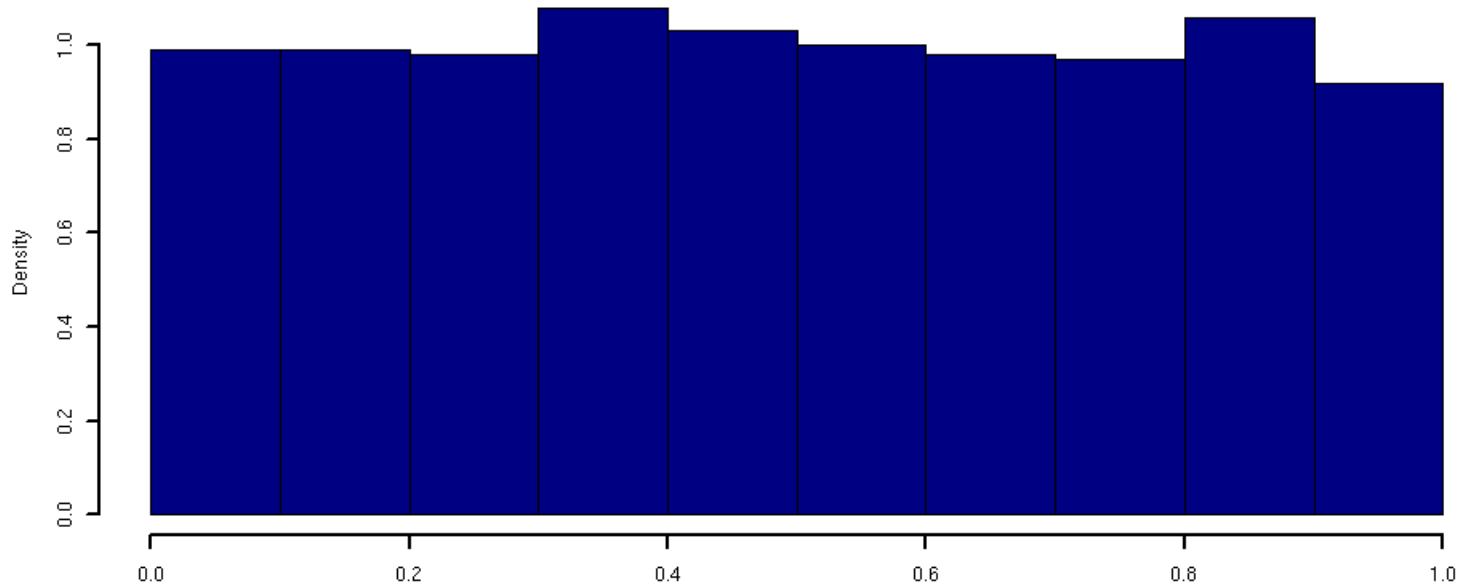
Note:

This is not about dependence between $Z(\mathbf{x})$ and $Z(\mathbf{x}')$ – this is another topic!

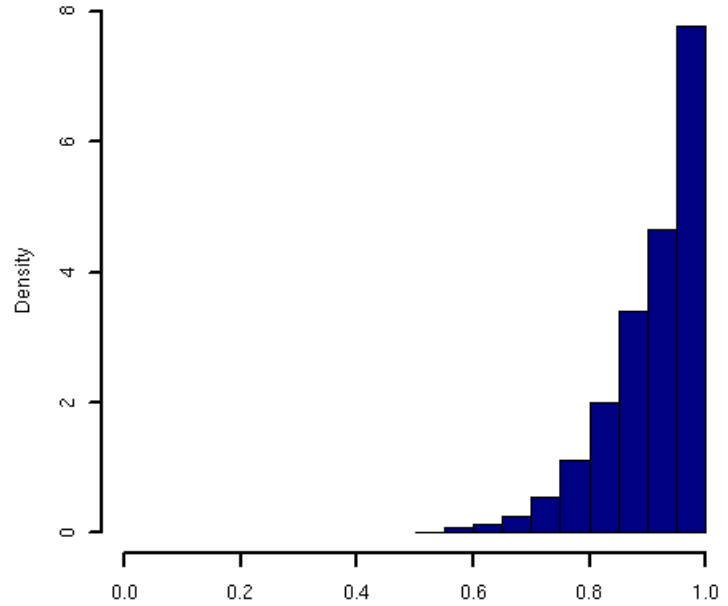
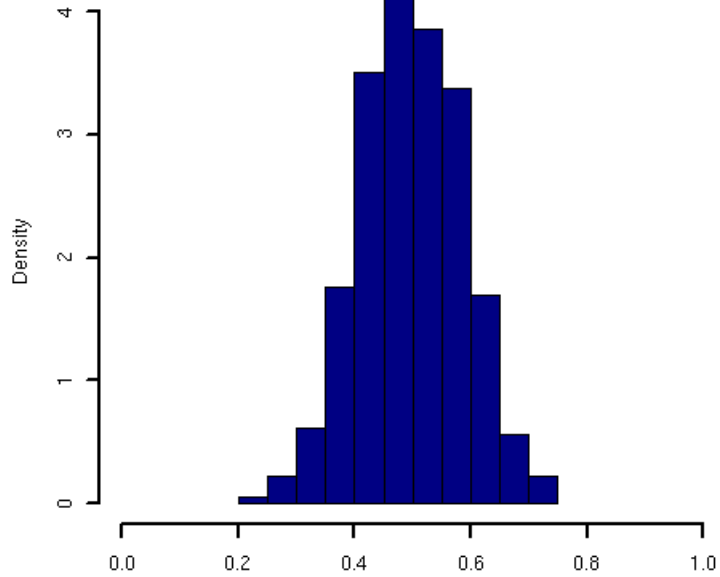
Extreme value distributions

An example

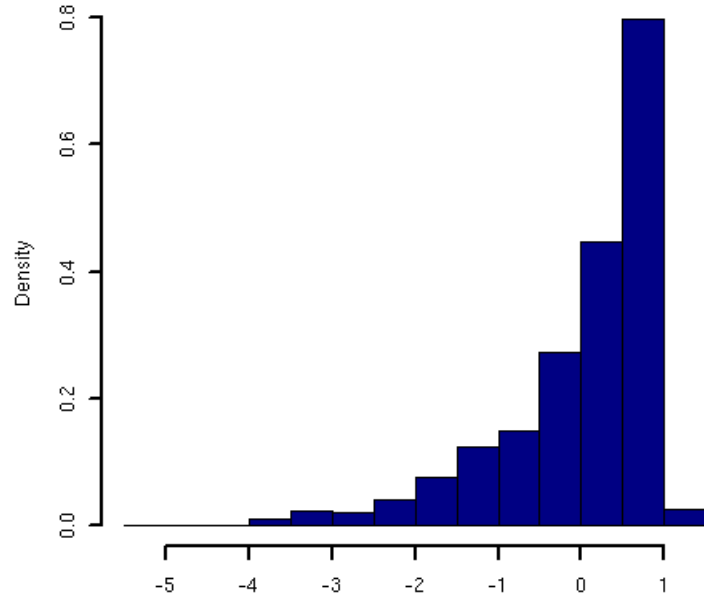
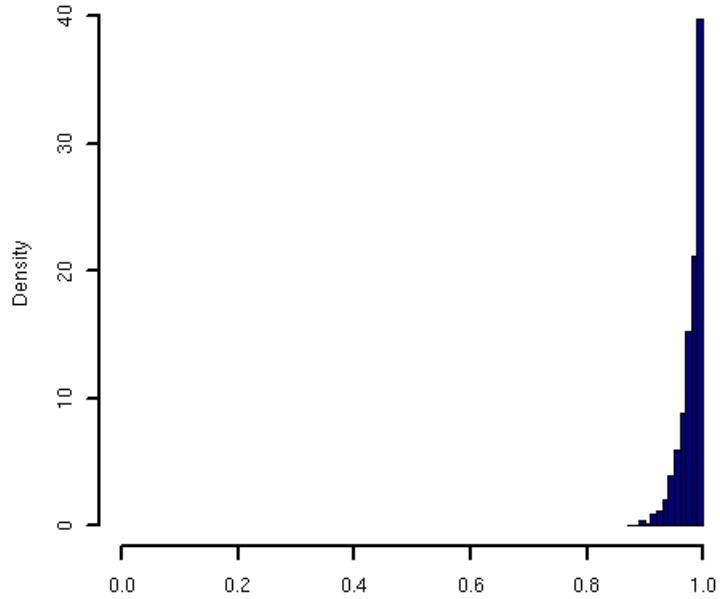
Random sample 1000 Uniforms



Random sample 1000, *mean* of 25 uniforms, *max* of 25



Random sample 1000, max of 100 , standardized



Generalized extreme value distribution (GEV)

GEV cumulative distribution function:

$$F_{GEV}(z) = e^{-(1+\xi(z-\mu)/\sigma)^{-1/\xi}}.$$

Parameters: location (μ), scale (σ) and shape (ξ).

Some points about the GEV

- When the shape is negative, the GEV distribution is zero above $\mu - \sigma/\xi$.
- M_n is the maximum of n random variables,

$$P(M_n < z) \approx F_{GEV}(z),$$

- Special case for the normal, the *Gumbel*

$$F_{\text{Gumbel}}(z) = e^{-e^{-(z-\mu)/\sigma}}.$$

- GEV includes the exponential and Weibul

Generalized Pareto Distribution (GPD)

Exceedence over threshold model

X is random and u is a (large) threshold

Conditional distribution

The probability of X exceeding x given that X is greater than u is

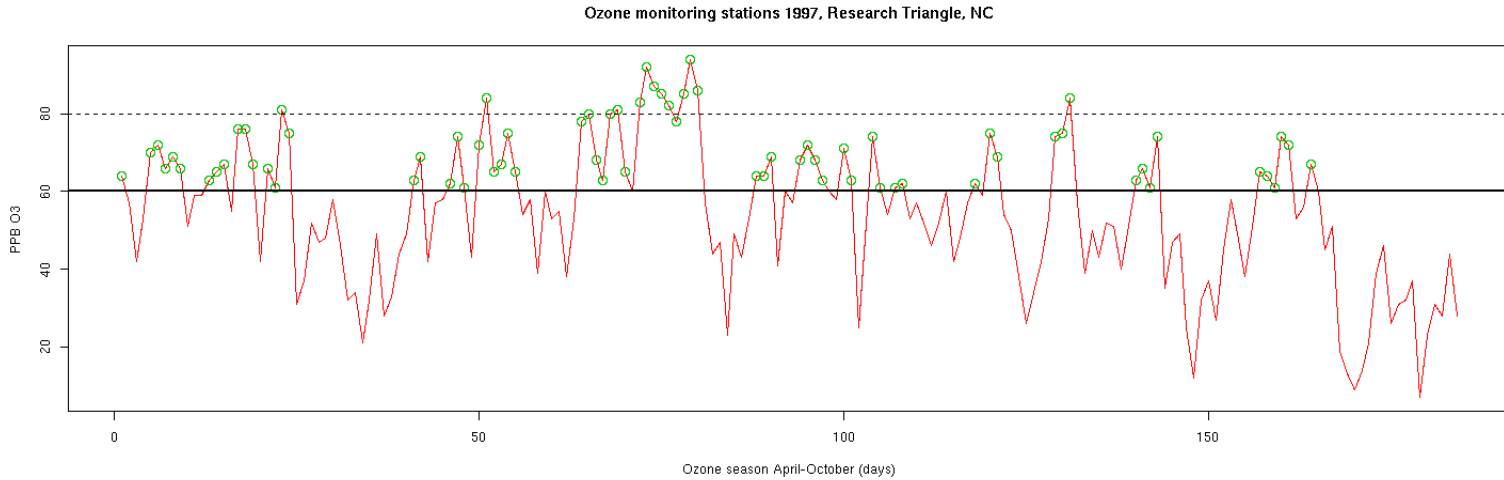
$$P(X > x | X > u) = [X > x | X > u] = \frac{1 - F(x)}{1 - F(u)}$$

The GPD:

$$\frac{1 - F(x)}{1 - F(u)} \approx (1 + \xi(x - u)/(\sigma))^{-1/\xi}$$

for x and u “large”.

Exceedences over Threshold Model



Quantiles and return levels

Given a GEV or GPD model for the tail of a distribution, a useful transformation is the quantile function.

Quantile

For a distribution function, the p -quantile is $x_p = F^{-1}(p)$.

Return levels

- For *annual* maxima the 5 year return level is the $(1 - (1/5)) = .2$ quantile.
- There are 184 days measured in each year for ozone given a GPD fit to *daily* exceedences the 5 year return level is the $1 - 1/(184 * 5)$ quantile.

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Note the GEV and GPD quantiles are nonlinear in their parameters.

Fitting the GPD models to data

Use Maximum likelihood

The likelihood is easy to evaluate and maximize. Using a Bayes method is more difficult

Choosing the threshold for the GPD

Find a range for u where the GPD parameters do not vary much. Or, use a threshold that has some physical basis.

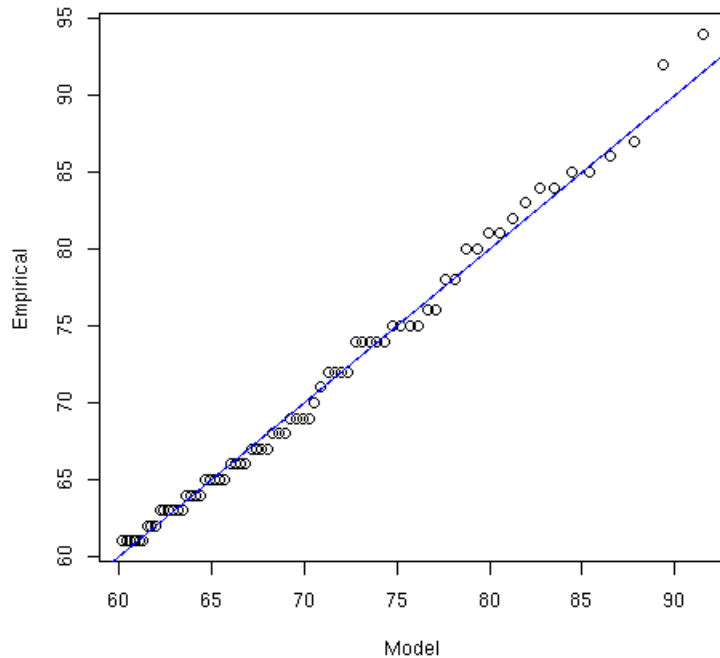
Profile likelihoods are useful for inference on return levels

Approximate confidence intervals and sets are based on the likelihood surface and a χ^2 critical value.

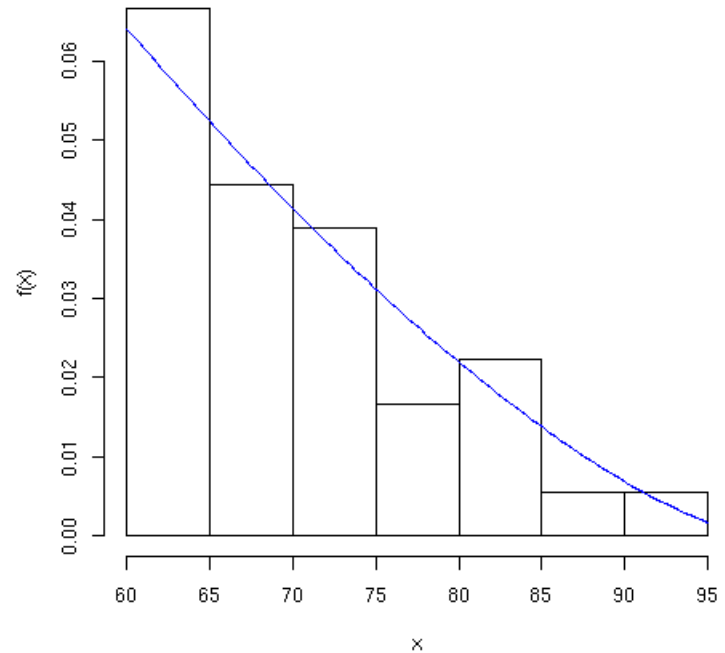
An ozone example

Diagnostic plots fitting the ozone data

Quantile Plot



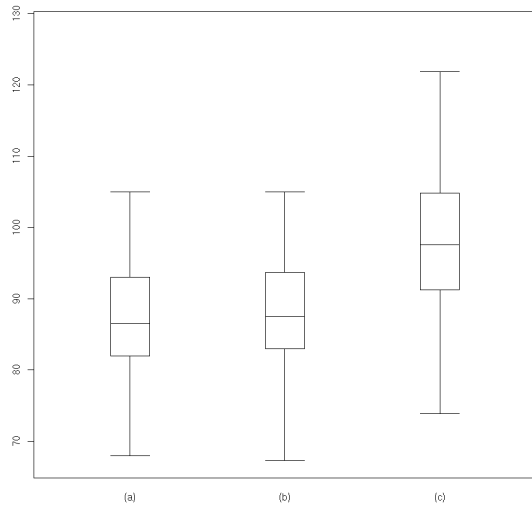
Density Plot



MLEs $\hat{\sigma} = 15.6$ (2.2) and $\hat{\xi} = -0.41$ (.10).

Estimates across station network.

To get an estimate of FHDA substitute $\hat{\sigma}$ and $\hat{\xi}$ into the GPD quantile function (with $p = 1 - 4/184$).



(a) observed FHDA, (b) estimated FHDA and (c) five-year return levels

A modest *space-time* model for ozone

Key idea: Conditional Simulation

For unmonitored locations find the conditional distribution of the FHDA. The distribution of the fields does not have a closed form and so we just generate samples from it.

Space-time model for daily values

In order to simulate from the FHDA field one needs a model for the temporal and spatial dependence of daily ozone. Transformed and scaled daily ozone follows an autoregressive model with spatially correlated shocks.

Model components

Transformation: $y(\mathbf{x}, t)$ = 8-hour ozone at location \mathbf{x} and time t .

$$u(\mathbf{x}, t) = \frac{y(\mathbf{x}, t) - \mu(\mathbf{x}, t)}{\sigma(\mathbf{x})}$$

Autoregression: $u(\mathbf{x}, t) = \rho(\mathbf{x})u(\mathbf{x}, t - 1) + e(\mathbf{x}, t - 1)$

Spatial dependence: $e(\mathbf{x}, t)$ uncorrelated over time and stationary over time.

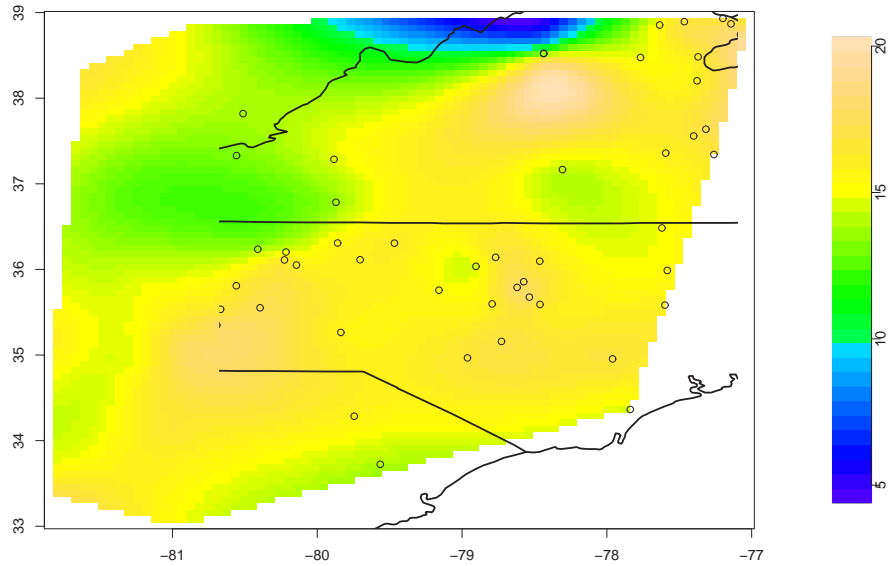
$$COR(e(\mathbf{x}, t), e(\mathbf{x}', t)) = k(\|\mathbf{x} - \mathbf{x}'\|)$$

k is a mixture of exponential covariance functions. Under the assumption of multivariate normality one can generate fields of daily ozone conditional on the observed values.

Transformation

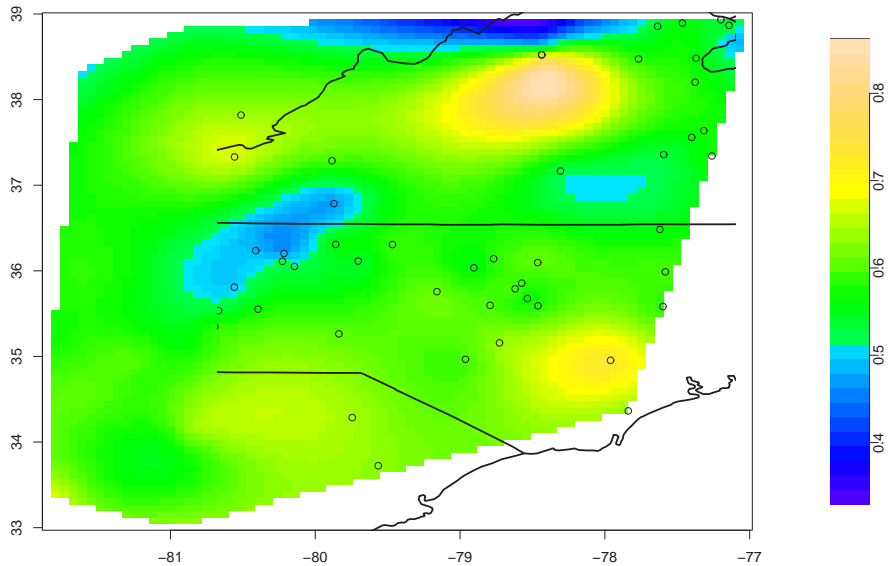
$\mu(\mathbf{x}, t)$ fit for each station location with a sine/cosine expansion and then smoothed over space using PC applied to regression coefficients. Extrapolation to unmonitored locations using interpolating thin plate splines (TPS) .

$\sigma(x)$ also based on TPS interpolation of station estimates.



Autoregressive model

$\rho(\mathbf{x})$ found from autoregression on transformed station data and then extrapolated using TPS

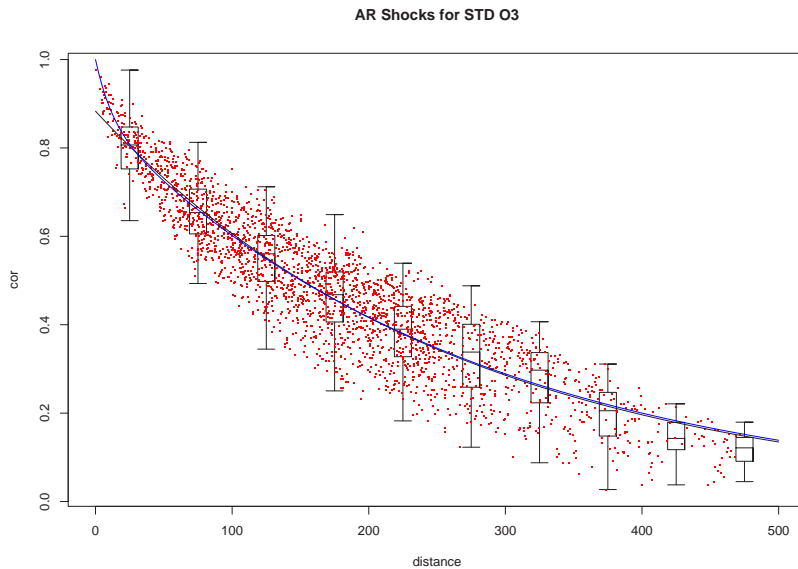


Spatial dependence

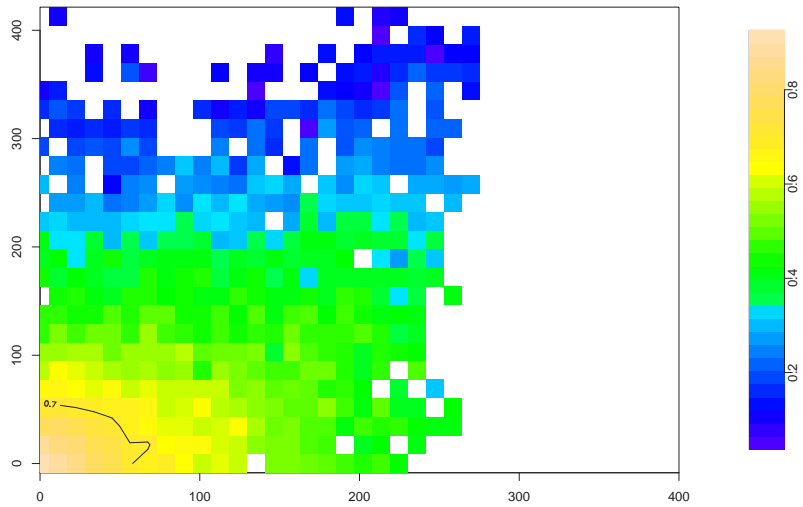
Correlogram of shocks suggests a mixture of exponential covariances

$$k(d) = \alpha e^{-d/\theta_1} + (1 - \alpha) e^{-d/\theta_2}$$

with $\alpha = .09$, $\theta_1 = 18$ (miles) and $\theta_2 = 270$ (miles)



Anisotropy?



Inference for FHDA where we don't measure it.

First discretize this problem

\mathbf{y}_t daily ozone values on a grid and including the stations locations.

$$\mathbf{o} = \begin{pmatrix} \mathbf{y}^s \\ \mathbf{y}^g \end{pmatrix} \quad (1)$$

Generating one year

Starting with an initial field: \mathbf{y}_0

1. *spatial shock* sample from $[e_t^g | e_t^s]$
2. *propagate* $\mathbf{u}_t = \rho \mathbf{u}_{t-1} +$ conditional shocks
3. *back transform* $\mathbf{y}_t = \mathbf{u}_t \boldsymbol{\sigma} + \boldsymbol{\mu}$

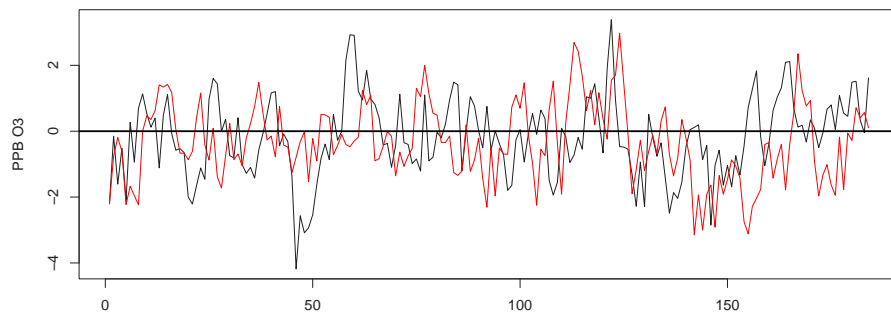
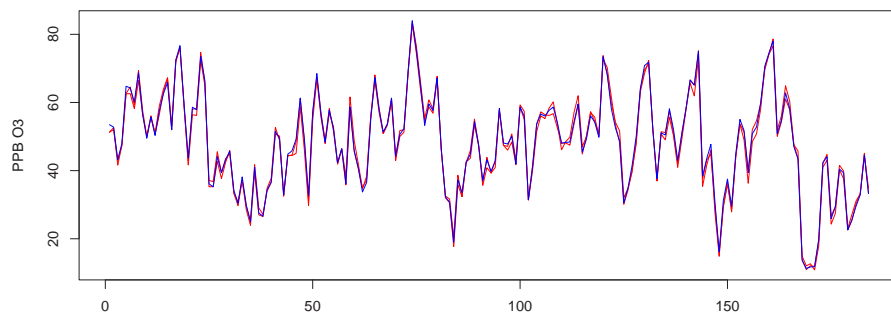
Repeat for entire season.

For each location compute FHDA from the seasons results.

Do this a “1000” times.

Two samples from conditional dist. near RTP, NC

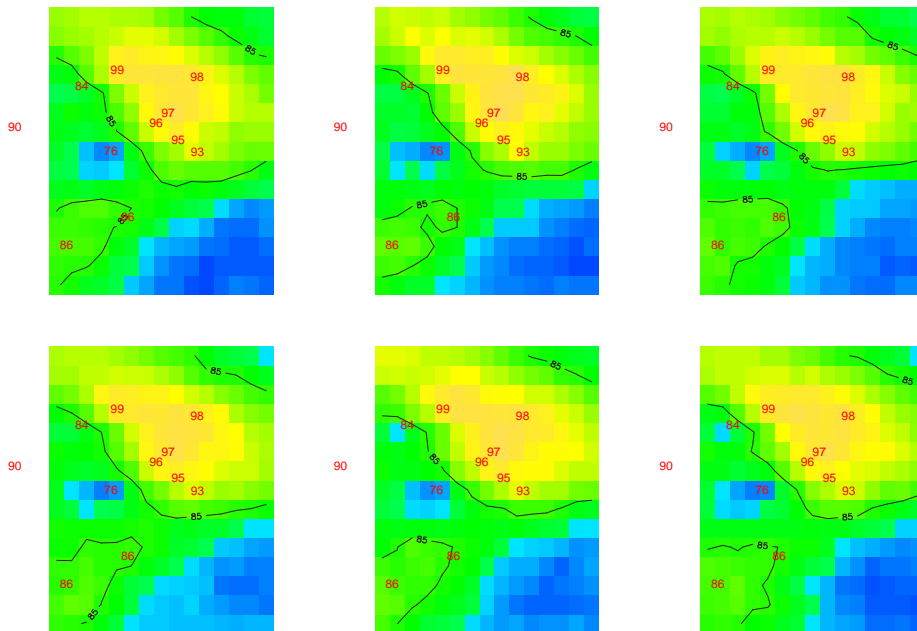
Top: Mean (blue) samples (red)



Below: Differences from mean

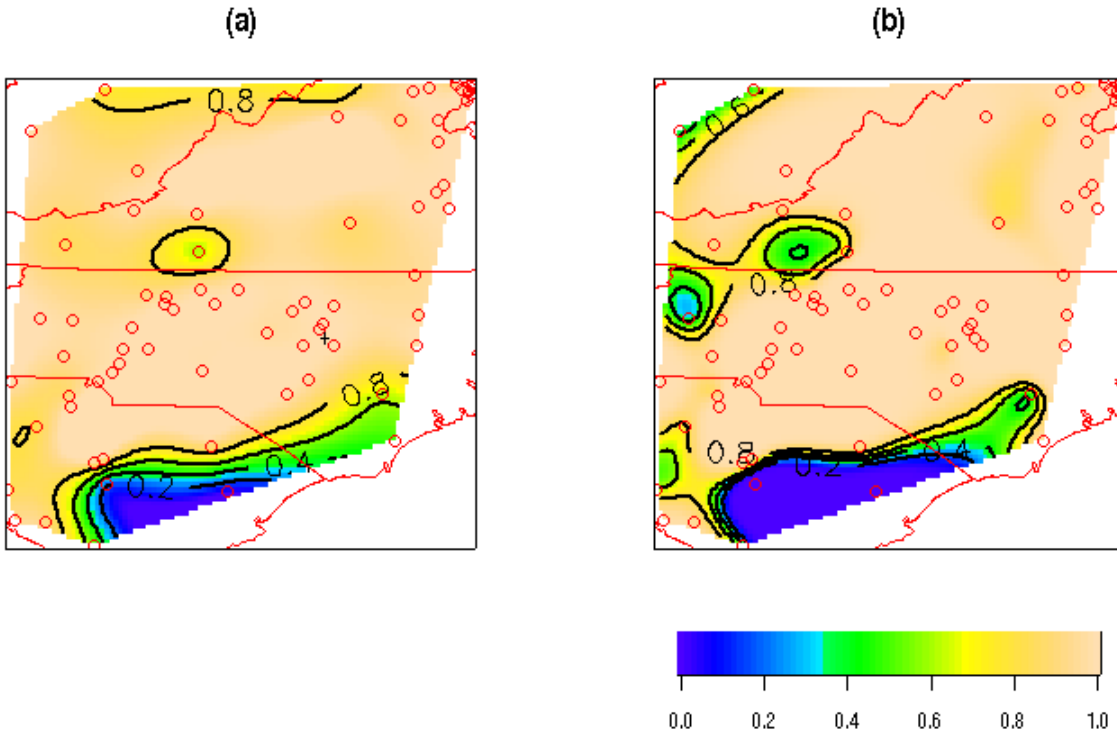
Inference/Posterior

Repeat simulations of a year and accumulate a distribution of FHDA. 6 samples of the field:



Probability of exceeding the ozone standard

(a) Analysis from space-time model (b) Using GPD



A modest *spatial* model for ozone extremes

Predict extremes in ozone at locations where there are not monitoring stations.

Using the GPD model this is can be done by predicting σ and ξ at arbitrary locations.

A hierarchical spatial model

Observation model:

$y(\mathbf{x}, t)$ surface ozone at location \mathbf{x} and time t .

$$[y(\mathbf{x}, t) | \sigma(\mathbf{x}), \xi(\mathbf{x}), u, y > u]$$

A Model for the spatial Process

$$[\sigma(\mathbf{x}), \xi(\mathbf{x}), u | \boldsymbol{\theta}]$$

Prior for hyperparameters

$$[\boldsymbol{\theta}]$$

Joint pdf for data and parameters

Assume that the extreme observations are conditionally independent.

$$\Pi_{i,t}[y(\mathbf{x}_i, t) | \sigma(\mathbf{x}), \xi(\mathbf{x}), u, y > u] \quad [\sigma(\mathbf{x}), \xi(\mathbf{x}), u | \boldsymbol{\theta}] \quad [\boldsymbol{\theta}].$$

t indexes days and i indexes station locations.

A Bayes analysis

For a formal Bayesian analysis, the specification of the joint is a complete recipe for inference on the parameters. Using Bayes Theorem, the posterior for $\sigma(\mathbf{x})$ and $\xi(\mathbf{x})$ given the data $([\sigma(\mathbf{x}), \xi(\mathbf{x}) | y(\mathbf{x}, t), \boldsymbol{\theta}])$ can, in principle, be computed.

Posterior mode

A useful summary of the posterior is to find the parameters that maximize the posterior. This can also be done by maximizing the joint density (because it is proportional).

Some shortcuts and assumptions

ξ , the shape, is constant over space

Justified by univariate fits.

Spatial model for $\sigma(x)$

Assume that $\sigma(x)$ is a Gaussian process with an isotropic Matern covariance function.

Parameters for the Matern

Fix the smoothness of the Matern at $\nu = 2$ and let the range be very large. The only remaining parameter λ is the sill, or variance of the process.

This is a Bayesian description of a thin plate spline model.

More about $\sigma(\mathbf{x})$

λ is the only hyperparameter and we just put an uninformative prior on it.

$$\sigma(\mathbf{x}) = P(\mathbf{x}) + e(\mathbf{x})$$

where P is a linear function of space and e is a smooth process.

As $\lambda \rightarrow \infty$ the surface will tend toward just the linear function.

As $\lambda \rightarrow 0$ the posterior surface will fit the data more closely.

log of the joint distribution

$X\beta$ is a linear function over space.

$$\sum_{i=1}^M l_{GPD}(\mathbf{Y}_i, \sigma(\mathbf{x}_i), \xi) -$$

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$$\lambda(\boldsymbol{\sigma} - \mathbf{X}\boldsymbol{\beta})^T (K^{-1})(\boldsymbol{\sigma} - \mathbf{X}\boldsymbol{\beta})/2 - \log(|K/\lambda|)$$

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$$+C.$$

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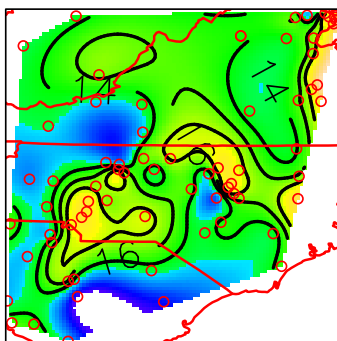
K is the thin-plate spline like covariance for the prior on σ . at the observations.

This is also a penalized likelihood.

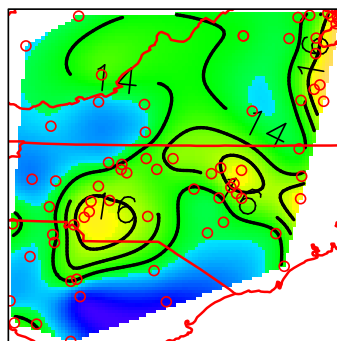
The penalty on σ is due to the covariance and the smoothing parameter, λ .

The profile likelihood surfaces for σ

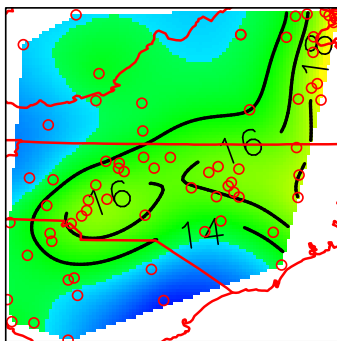
(a) lambda= 0



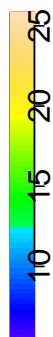
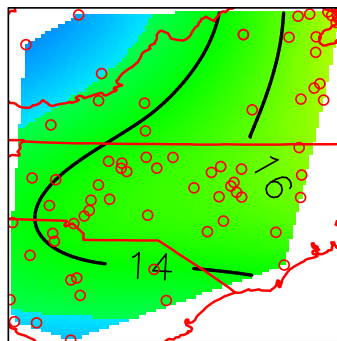
(b) lambda= 1e-6



(c) lambda= 1e-4

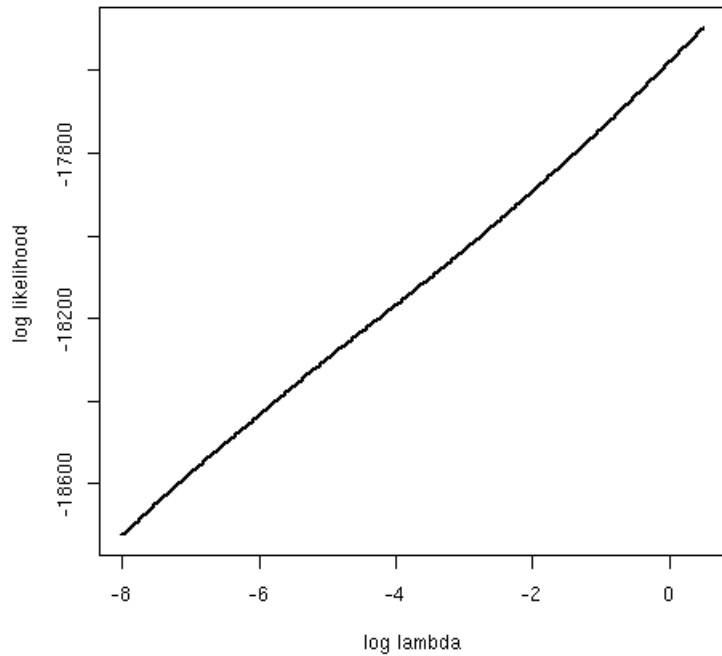


(d) lambda= 1e-2



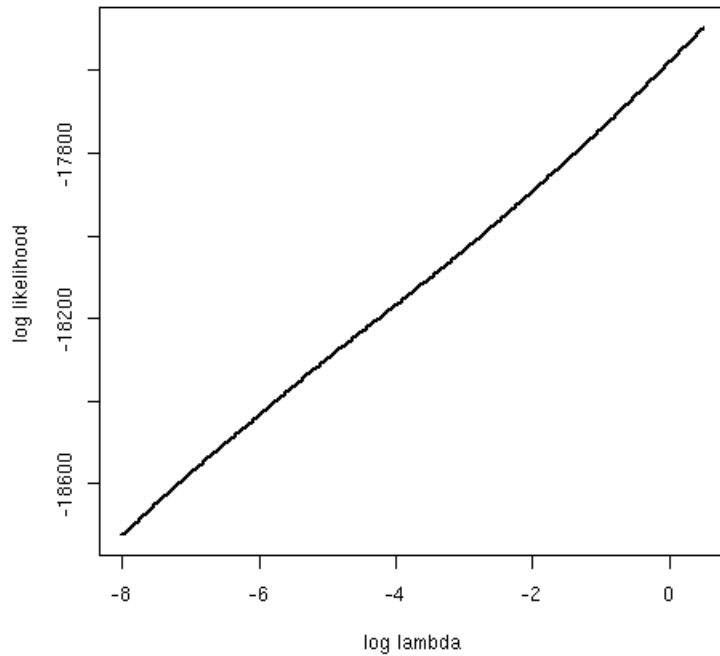
Inference for λ

Profile likelihood for λ



Inference for λ

Profile likelihood for λ



Oops!

Another try

Fit a thin-plate spline to the MLE from the univariate fitting.

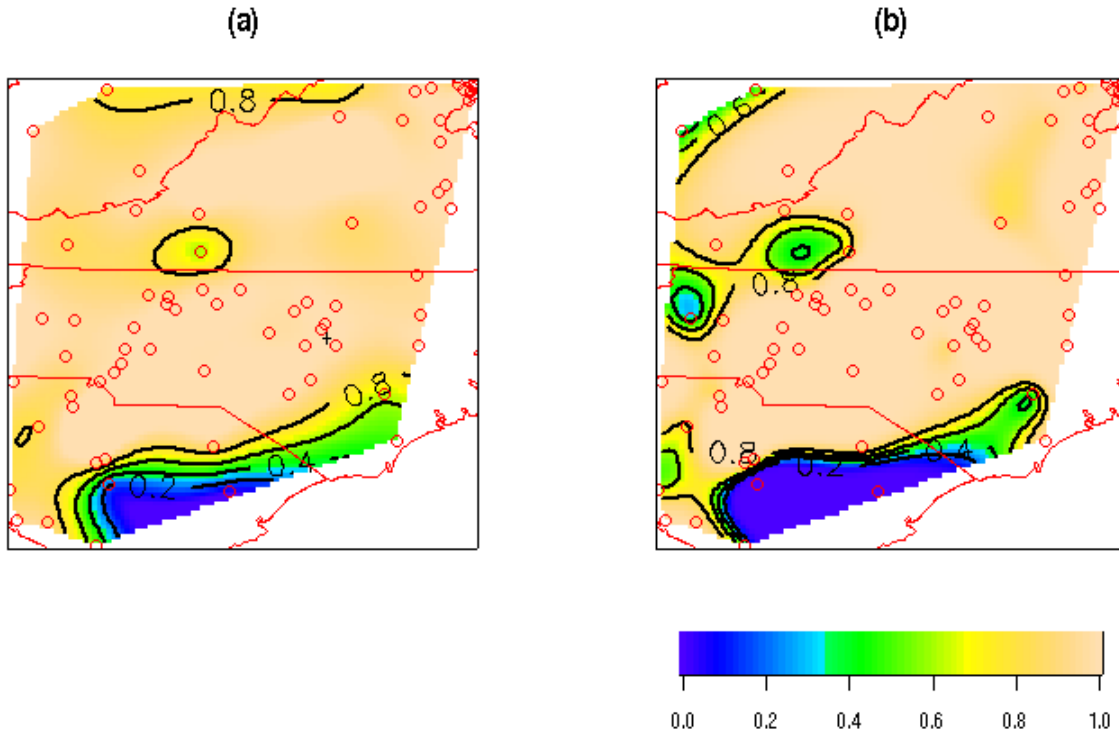
Determine λ by cross-validation:

- For fixed λ omit each location, fit a spline to the remaining points
- predict the value at the omitted location.
- Compare this to the observed value. (difference is called the cross-validated residual)
- Choose the value of λ that minimizes the sum of squares of the CV residuals

When this is done one gets a picture like (c).

Probability of exceeding the ozone standard

(a) Analysis from space-time model (b) Using GPD



Discussion

- Extreme value distributions offer an alternative to modeling tails of a distribution.
- Using two very different approaches the ozone case study ends with a surprisingly similar analysis.
- A more elaborate model would be possible by including more data, both over space and time. Some possible extensions: nonstationary covariances, link function for the GPD parameters and including some temporal dependence.