# Bayesian inference & process convolution models

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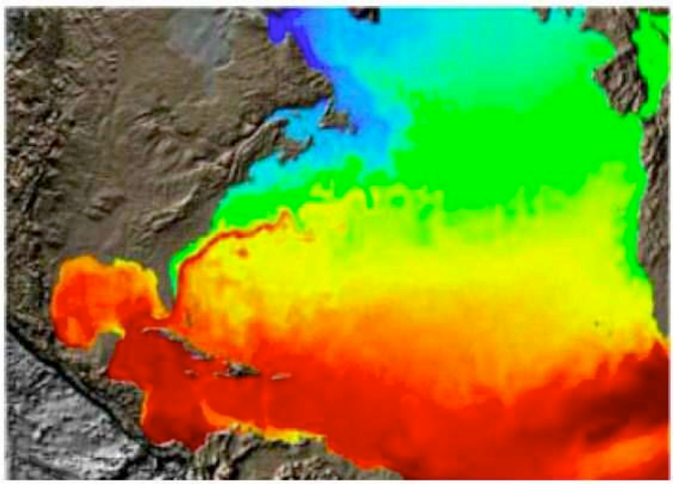
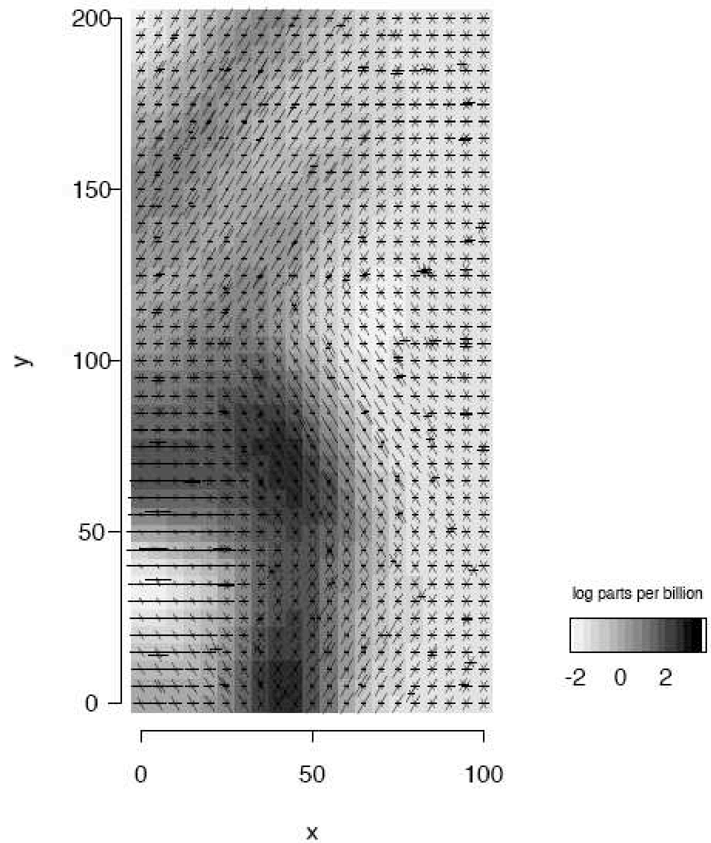


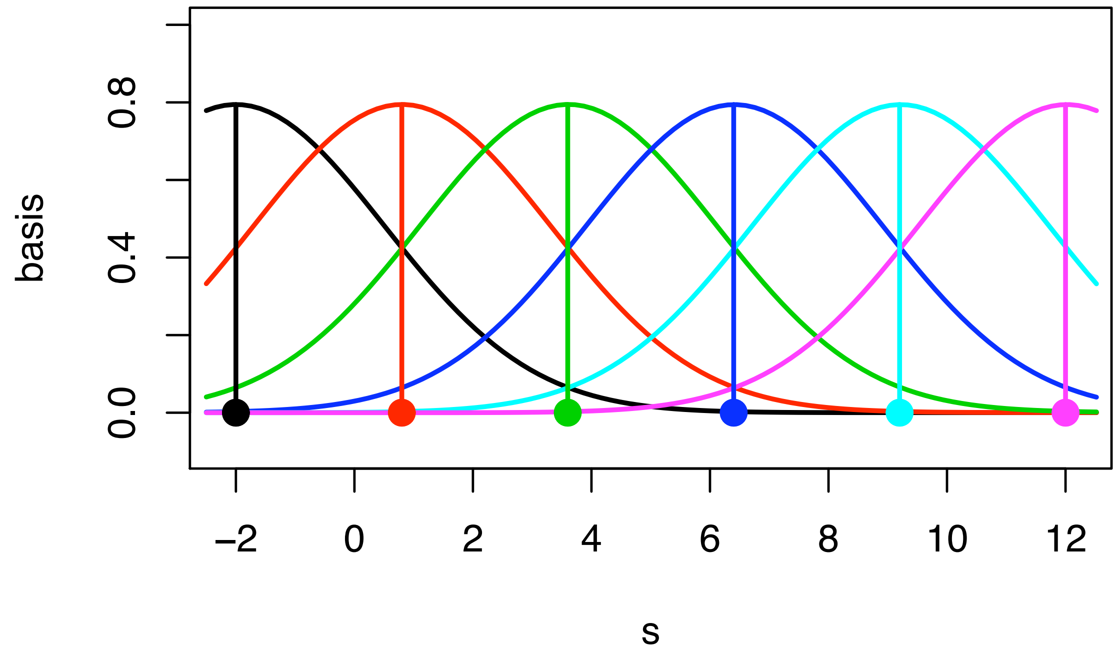
North Atlantic temperatures



# MOVING AVERAGE SPATIAL MODELS

# Kernel basis representation for spatial processes $z(s)$

Define $m$ basis functions $k_1(s), \ldots, k_m(s)$.




Here $k_j(s)$ is normal density cetered at spatial location $\omega_j$:

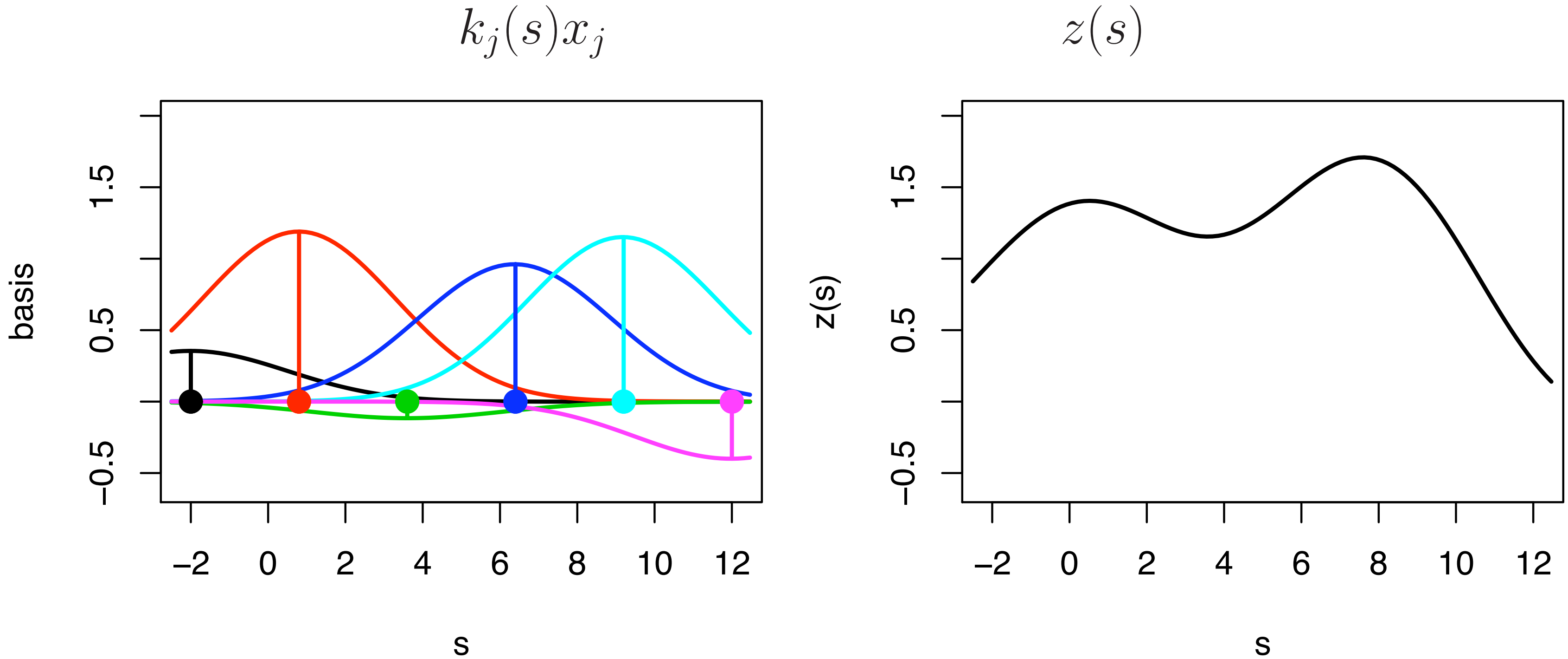
$$k_j(s) = \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2}(s - \omega_j)^2\}$$

set $z(s) = \sum_{j=1}^{m} k_j(s) x_j$ where $x \sim N(0, I_m)$.

Can represent $z = (z(s_1), \ldots, z(s_n))^T$ as $z = Kx$ where

$$K_{ij} = k_j(s_i)$$

# $x$ and $k(s)$ determine spatial processes $z(s)$

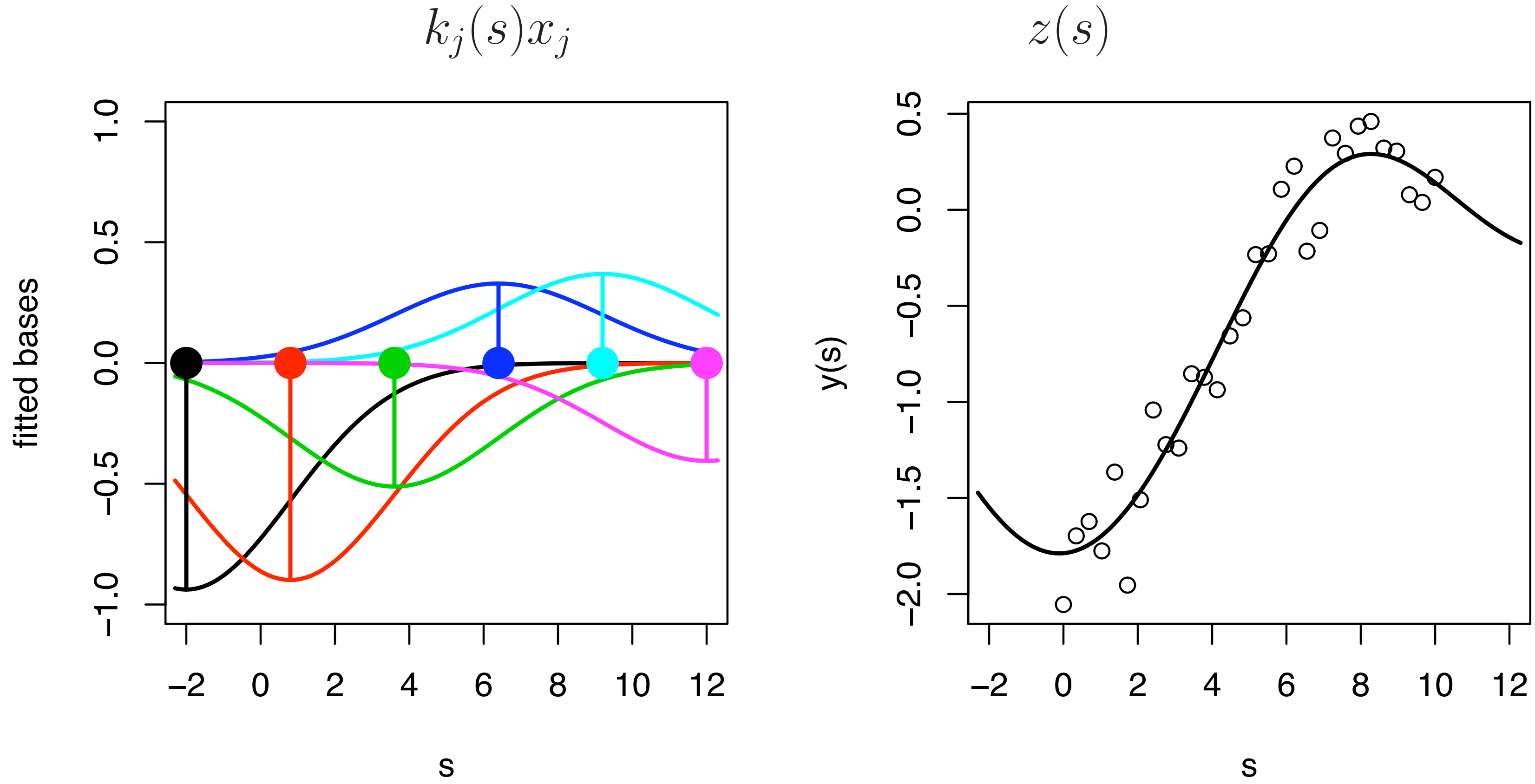



Continuous representation:

$$z(s) = \sum_{j=1}^{m} k_j(s)x_j \text{ where } x \sim N(0, I_m).$$

Discrete representation: For $z = (z(s_1), \ldots, z(s_n))^T$, $z = Kx$ where $K_{ij} = k_j(s_i)$

# Estimate $z(s)$ by specifying $k_j(s)$ and estimating $x$




Discrete representation: For $z = (z(s_1), \ldots, z(s_n))^T$, $z = Kx$ where $K_{ij} = k_j(s_i)$

$\Rightarrow$ standard regression model: $y = Kx + \epsilon$

# Formulation for the 1-d example

Data $y = (y(s_1), \ldots, y(s_n))^T$ observed at locations $s_1, \ldots, s_n$. Once knot locations $\omega_j,\ j = 1, \ldots, m$ and kernel choice $k(s)$ are specified, the remaining model formulation is trivial:

Likelihood:

$$L(y|x, \lambda_y) \propto \lambda_y^{\frac{n}{2}} \exp\left\{-\frac{1}{2}\lambda_y (y - Kx)^T (y - Kx)\right\}$$

where $K_{ij} = k(\omega_j - s_i)$.

Priors:

$$\begin{aligned}
\pi(x|\lambda_x) &\propto \lambda_x^{\frac{m}{2}} \exp\left\{-\frac{1}{2}\lambda_x x^T x\right\} \\
\pi(\lambda_x) &\propto \lambda_x^{a_x - 1} \exp\{-b_x \lambda_x\} \\
\pi(\lambda_y) &\propto \lambda_y^{a_y - 1} \exp\{-b_y \lambda_y\}
\end{aligned}$$

Posterior:

$$\begin{aligned}
\pi(x, \lambda_x, \lambda_y|y) \propto\ & \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\} \times \\
& \lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5x^T x]\right\}
\end{aligned}$$

# Posterior and full conditionals

Posterior:

$$\begin{aligned}\pi(x, \lambda_x, \lambda_y | y) \;\propto\; & \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\} \times \\ & \lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5x^T x]\right\}\end{aligned}$$

Full conditionals:

$$\begin{aligned}\pi(x | \cdots) \;&\propto\; \exp\{-\frac{1}{2}[\lambda_y x^T K^T K x - 2\lambda_y x^T K^T y + \lambda_x x^T x]\} \\ \pi(\lambda_x | \cdots) \;&\propto\; \lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5x^T x]\right\} \\ \pi(\lambda_y | \cdots) \;&\propto\; \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\}\end{aligned}$$



Gibbs sampler implementation

$$\begin{aligned}x | \cdots \;&\sim\; N((\lambda_y K^T K + \lambda_x I_m)^{-1} \lambda_y K^T y, (\lambda_y K^T K + \lambda_x I_m)^{-1}) \\ \lambda_x | \cdots \;&\sim\; \Gamma(a_x + \frac{m}{2}, b_x + .5x^T x) \\ \lambda_y | \cdots \;&\sim\; \Gamma(a_y + \frac{n}{2}, b_y + .5(y - Kx)^T (y - Kx))\end{aligned}$$

# Gibbs sampler: intuition

## Gibbs sampler for a bivariate normal density

$$\pi(z) = \pi(z_1, z_2) \propto \begin{vmatrix} 1 & \rho \\ \rho & 1 \end{vmatrix}^{-\frac{1}{2}} \exp\left\{-\frac{1}{2} \begin{pmatrix} z_1 & z_2 \end{pmatrix} \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}^{-1} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}\right\}$$

Full conditionals of $\pi(z)$:

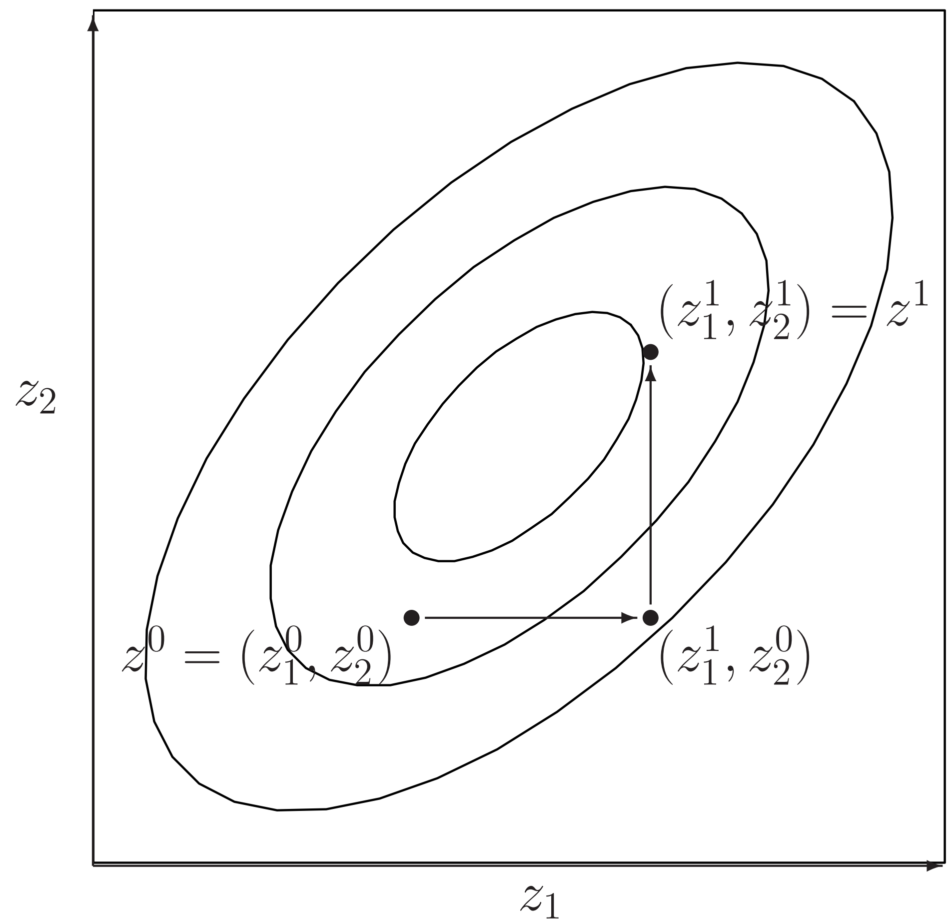
$$\begin{aligned} z_1|z_2 &\sim N(\rho z_2, 1-\rho^2) \\ z_2|z_1 &\sim N(\rho z_1, 1-\rho^2) \end{aligned}$$

- initialize chain with

$$z^0 \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

- draw $z_1^1 \sim N(\rho z_2^0, 1-\rho^2)$

now $(z_1^1, z_2^0)^T \sim \pi(z)$

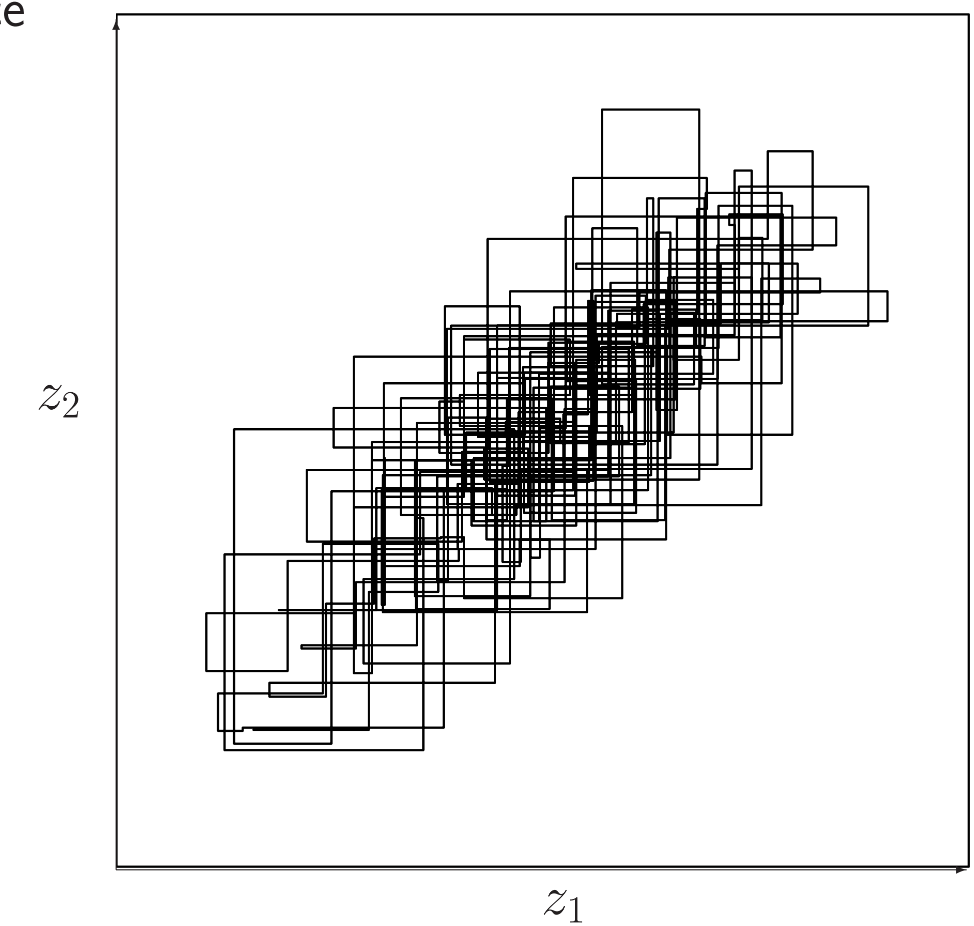


# Gibbs sampler: intuition

Gibbs sampler gives $z^0, z^2, \ldots, z^T$ which can be treated as dependent draws from $\pi(z)$.

If $z^0$ is not a draw from $\pi(z)$, then the initial realizations will not have the correct distribution. In practice, the first 100?, 1000? realizations are discarded.

The draws can be used to make inference about $\pi(z)$:




- Posterior mean of $z$ is estimated by:

$$\begin{pmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \end{pmatrix} = \frac{1}{T} \sum_{k=1}^{T} \begin{pmatrix} z_1^k \\ z_2^k \end{pmatrix}$$

- Posterior probabilities:

$$\widehat{P}(z_1 > 1) = \frac{1}{T} \sum_{k=1}^{T} I[z_1^k > 1]$$

$$\widehat{P}(z_1 > z_2) = \frac{1}{T} \sum_{k=1}^{T} I[z_1^k > z_2^k]$$

- 90% interval: $(z_1^{[5\%]}, z_1^{[95\%]})$.

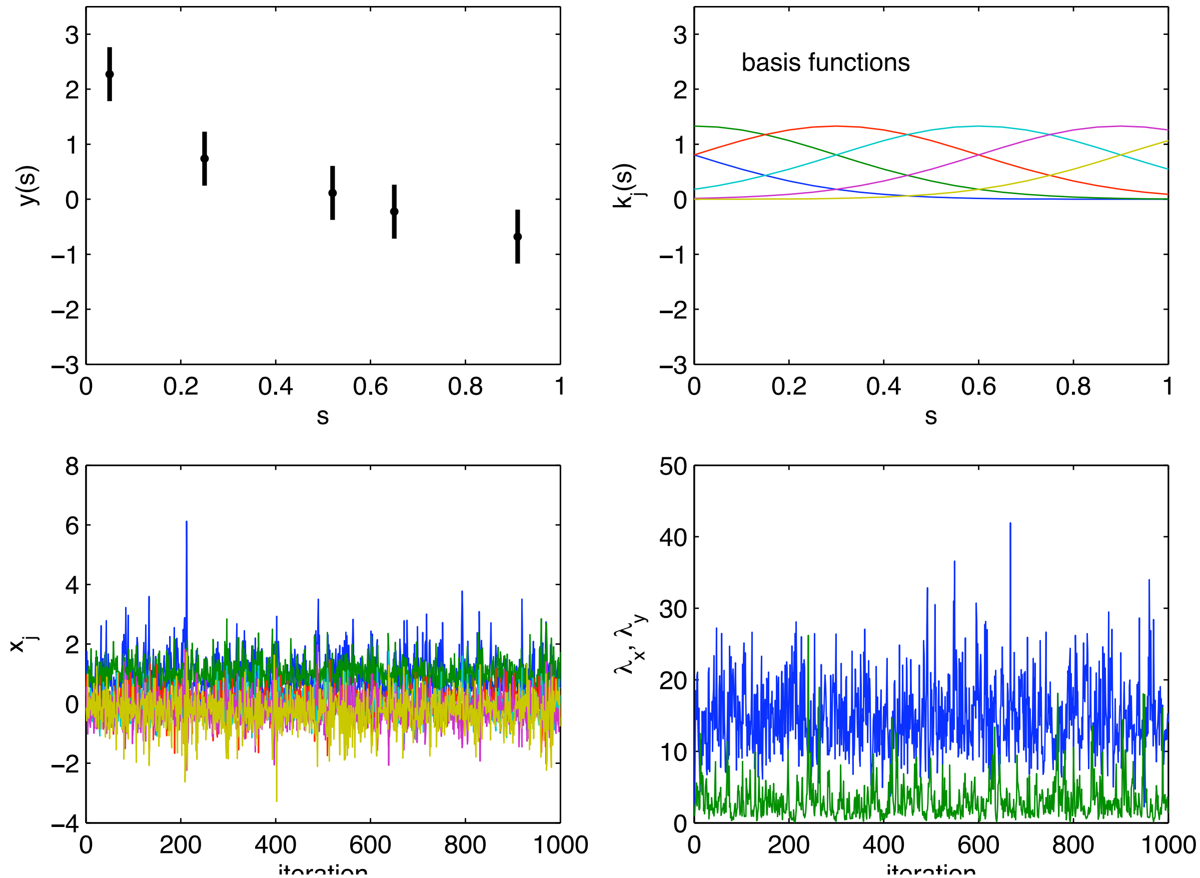
# 1-d example

$m = 6$ knots evenly spaced between $-.3$ and $1.2$.

$n = 5$ data points at $s = .05, .25, .52, .65, .91$.

$k(s)$ is $N(0, \text{sd} = .3)$

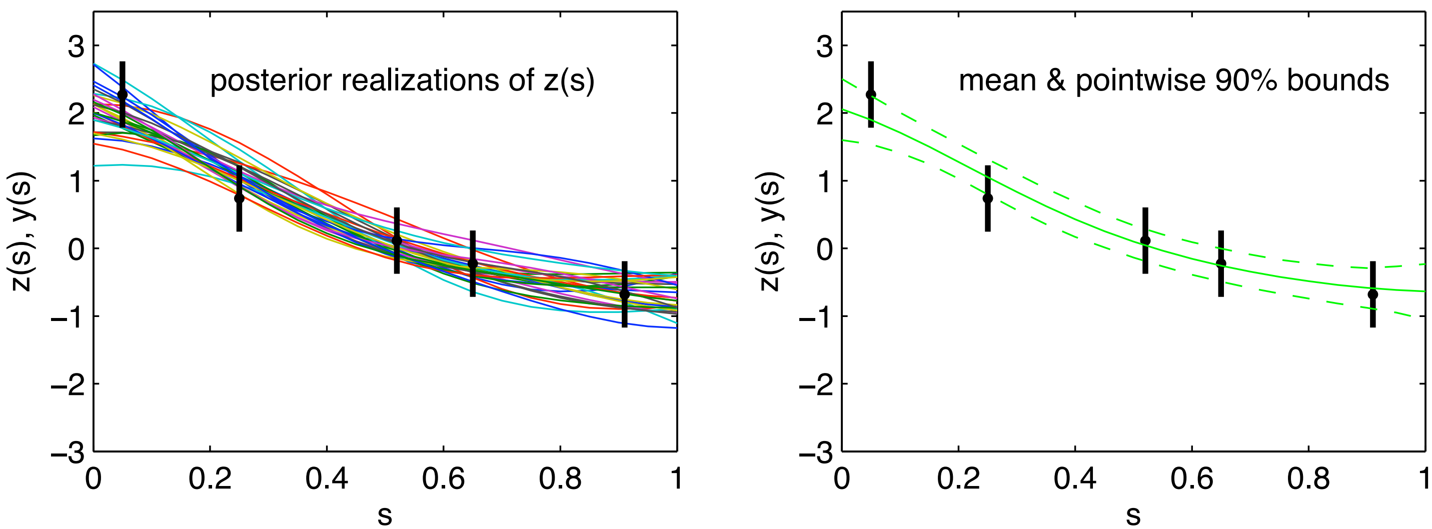
$a_y = 10$, $b_y = 10 \cdot (.25^2) \Rightarrow$ strong prior at $\lambda_y = 1/.25^2$; $a_x = 1$, $b_x = .001$



# 1-d example

From posterior realizations of knot weights $x$, one can construct posterior realizations of the smooth fitted function $z(s) = \Sigma_{j=1}^{m} k_j(s) x_j$.

Note strong prior on $\lambda_y$ required since $n$ is small.

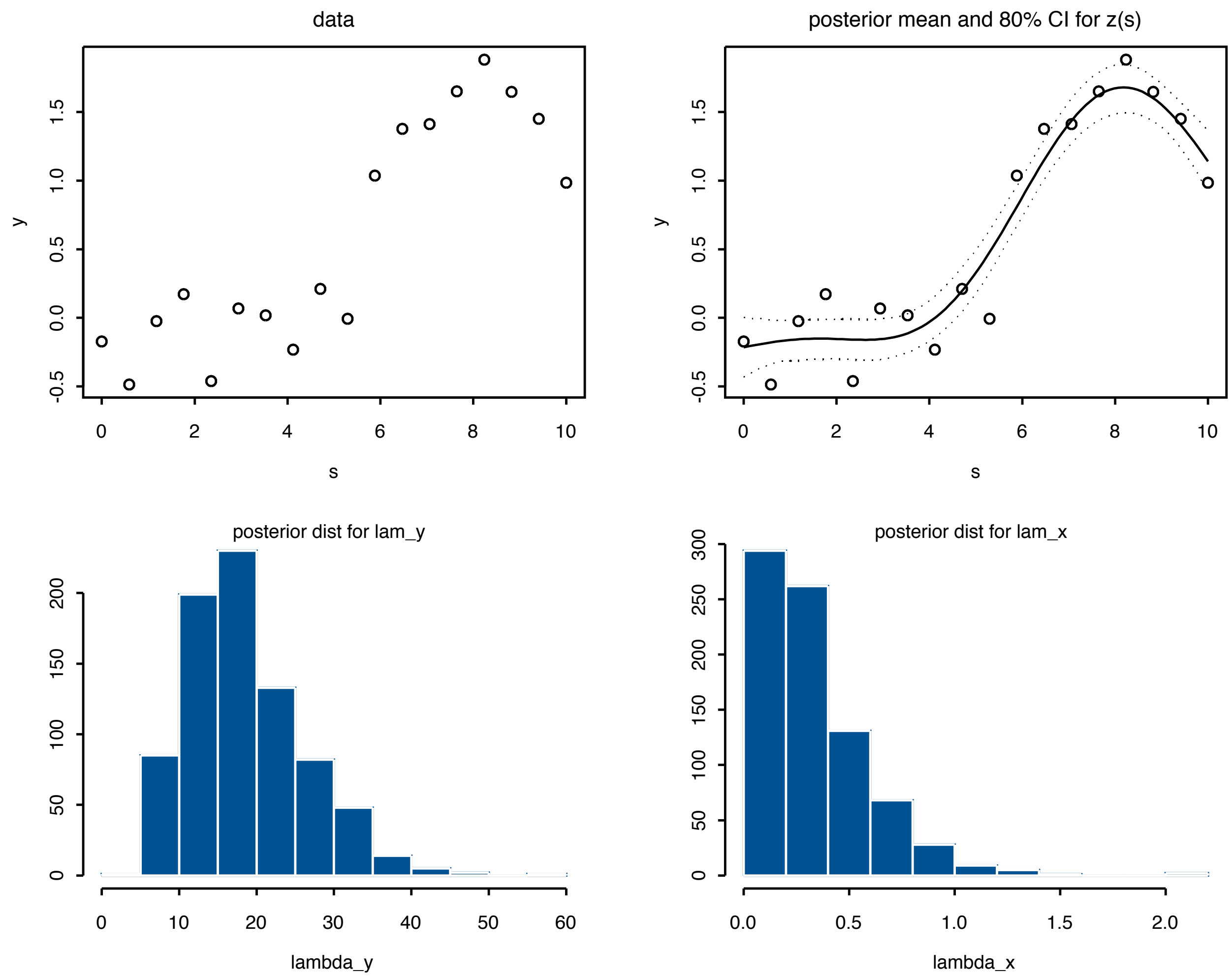


# 1-d example

$m = 20$ knots evenly spaced between $-2$ and $12$.

$n = 18$ data points evenly spaced between 0 and 10.

$k(s)$ is $N(0, \text{sd} = 2)$

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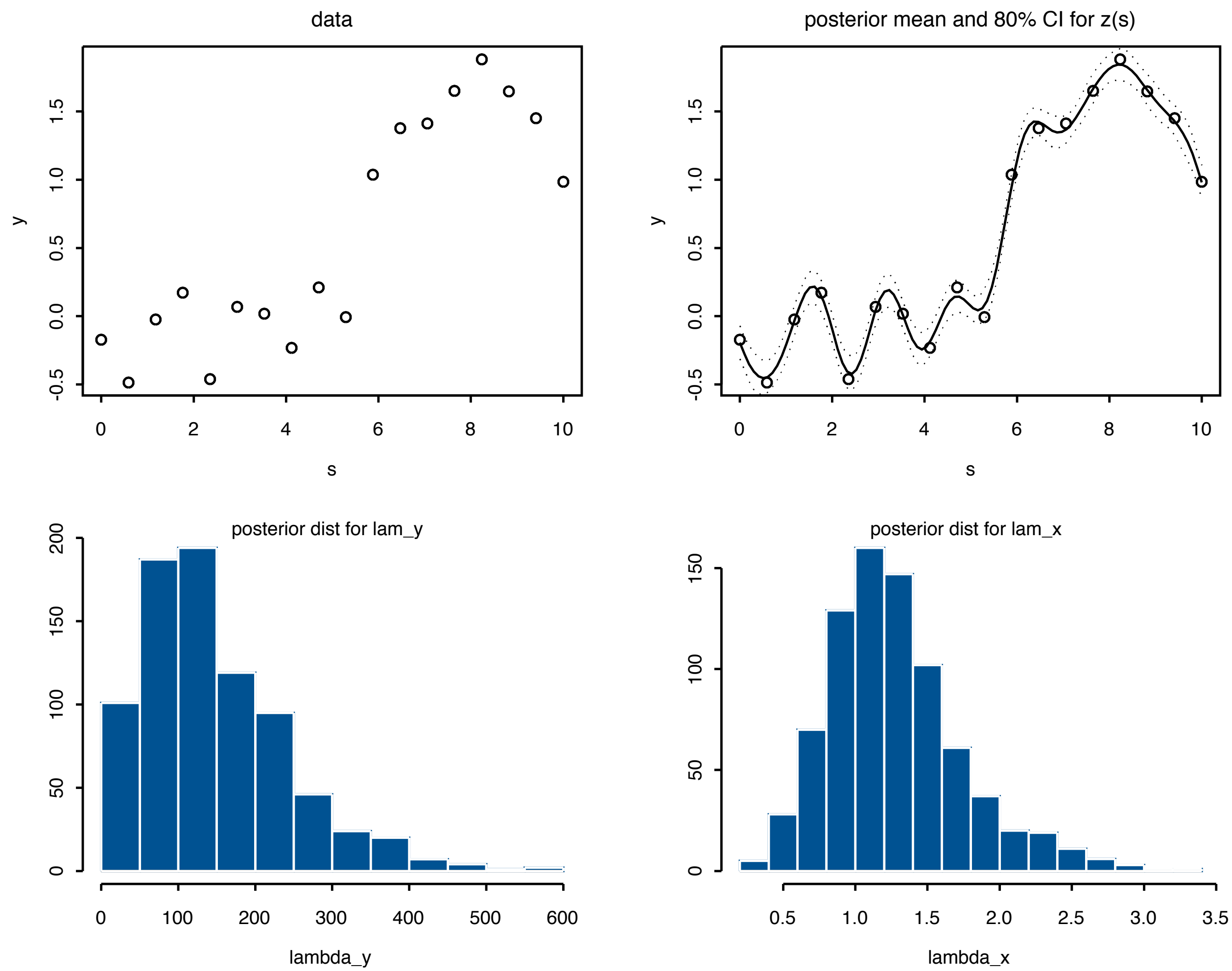
# 1-d example

$m = 20$ knots evenly spaced between $-2$ and $12$.

$n = 18$ data points evenly spaced between 0 and 10.

$k(s)$ is $N(0, \text{sd} = 1)$



# Basis representations for spatial processes $z(s)$

Represent $z(s)$ at spatial locations $s_1, \dots, s_n$.

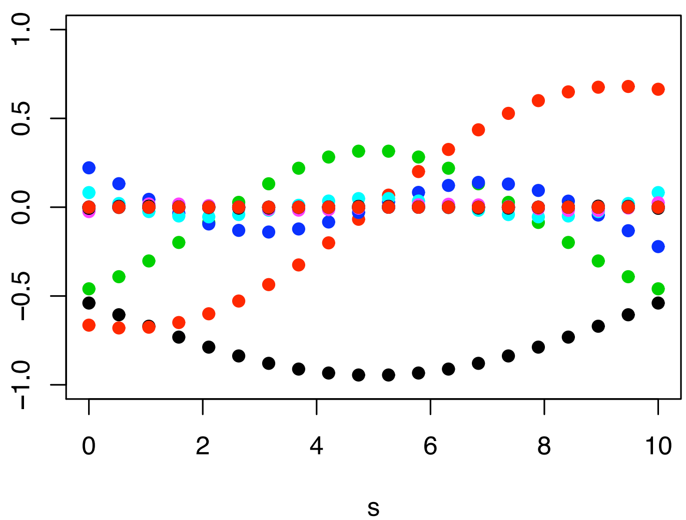
$z = (z(s_1), \dots, z(s_n))^T \sim N(0, \Sigma_z)$.

Recall

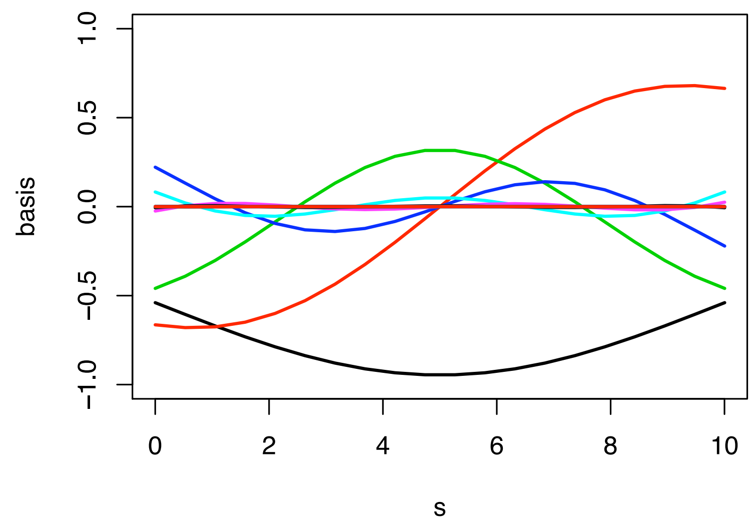
$$z = Kx, \text{ where } KK^T = \Sigma_z \text{ and } x \sim N(0, I_n).$$

Gives a discrete representation of $z(s)$ at locations $s_1, \dots, s_n$.

discrete representation




continuous representation




$$z(s_i) = \sum_{j=1}^{n} K_{ij} x_j \qquad z(s) = \sum_{j=1}^{n} k_j(s) x_j$$

Columns of $K$ give basis functions.

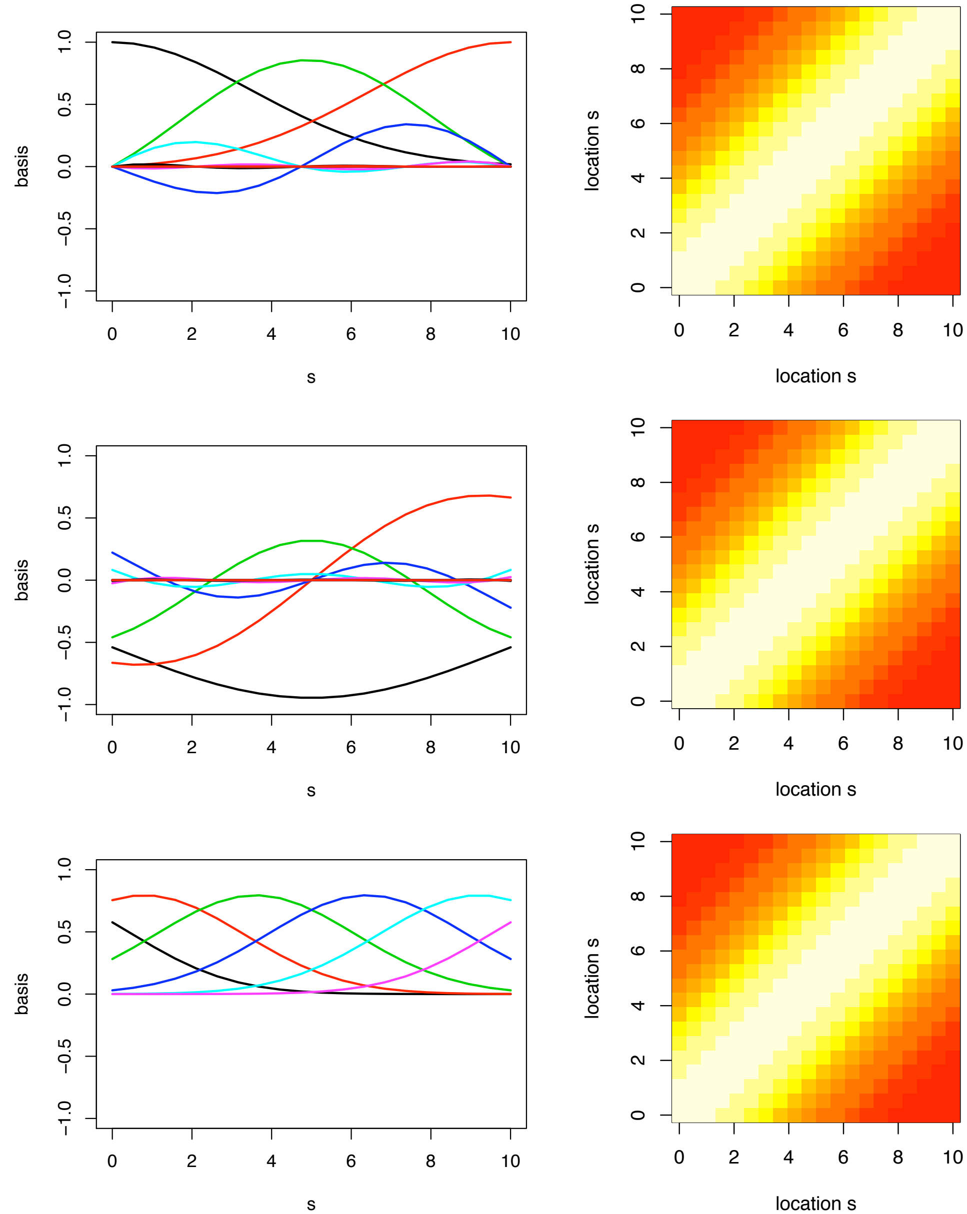
Can use a subset of these basis functions to reduce dimensionality.

| decomposition | basis | covariance |
| --- | --- | --- |

Cholesky (w/piv)

SVD

kernels



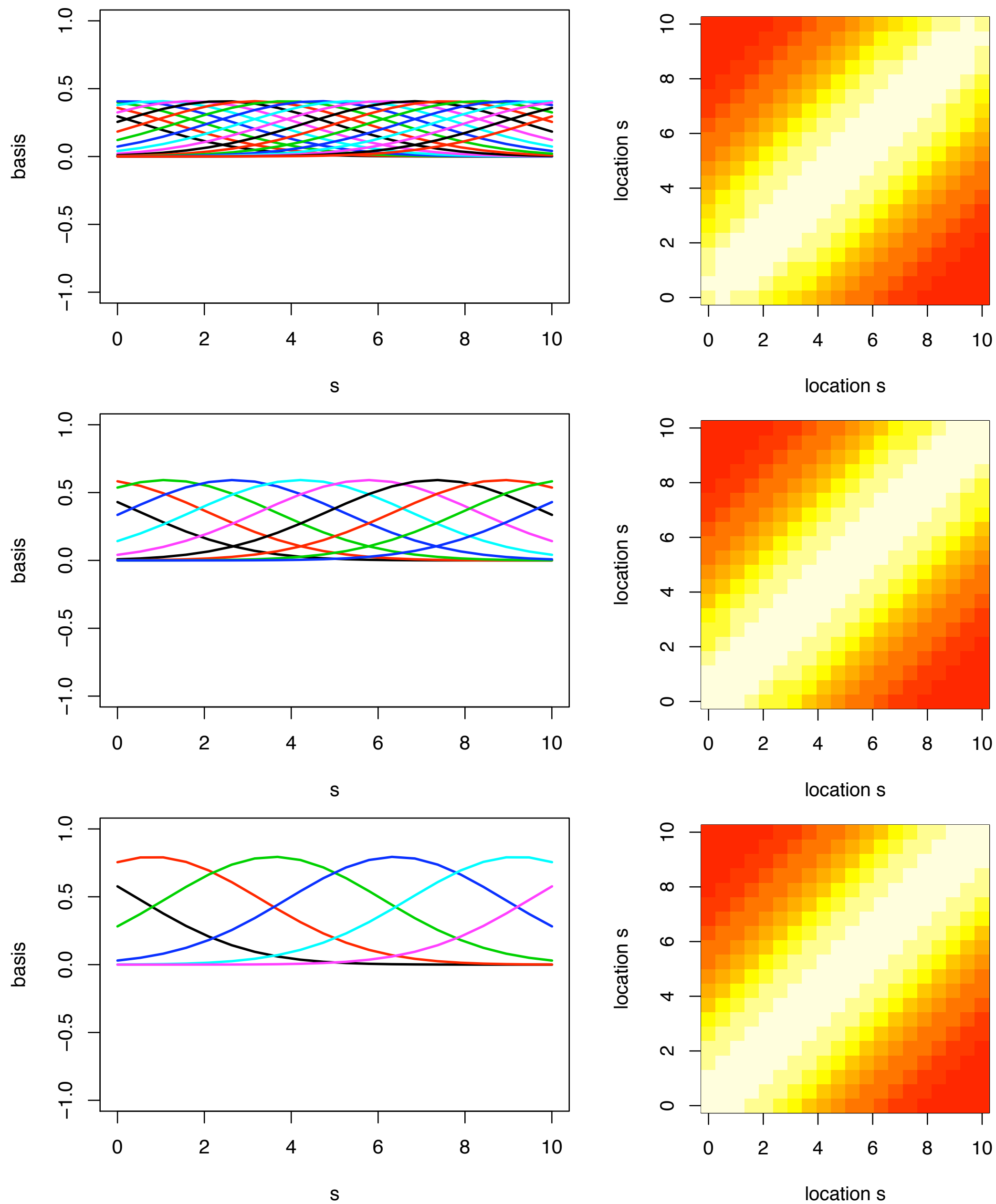
# How many basis kernels?

Define $m$ basis functions $k_1(s), \ldots, k_m(s)$.

$m = 20$?

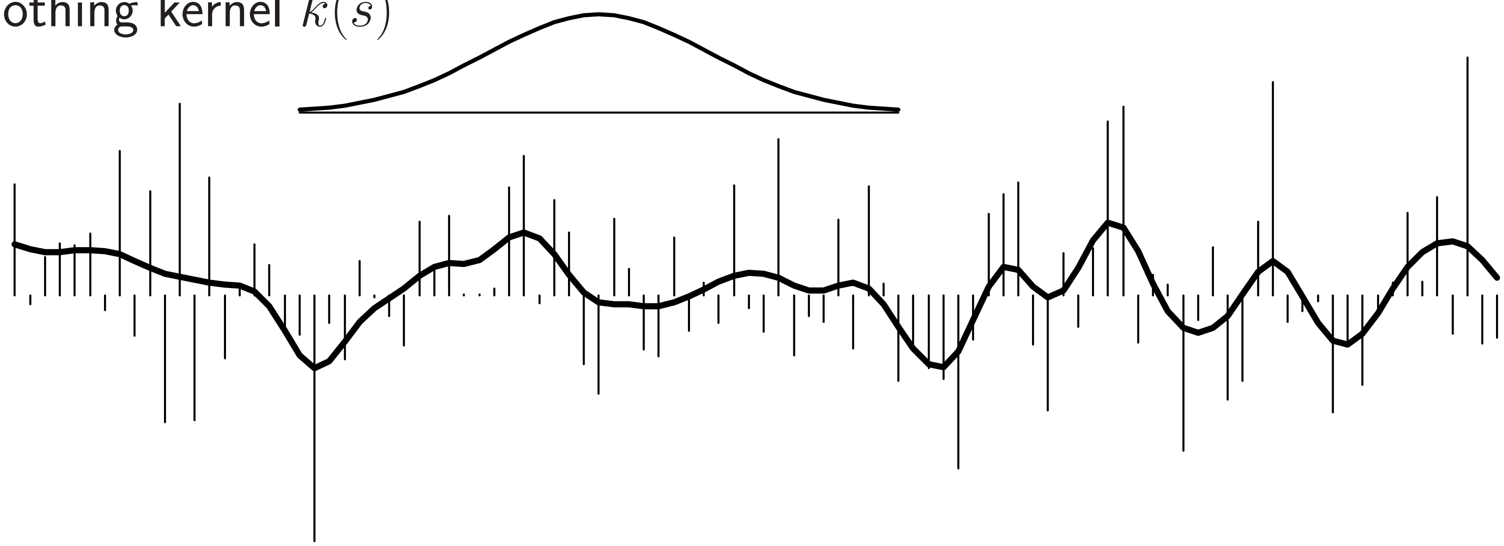
$m = 10$?

$m = 6$?



# Moving average specifications for spatial models $z(s)$

smoothing kernel $k(s)$



white noise process $x = (x_1, \ldots, x_m)$ at spatial locations $\omega_1, \ldots, \omega_m$.

$$x \sim N(0, \frac{1}{\lambda_x} I_m)$$

spatial process $z(s)$ constructed by convolving $x$ with smoothing kernel $k(s)$

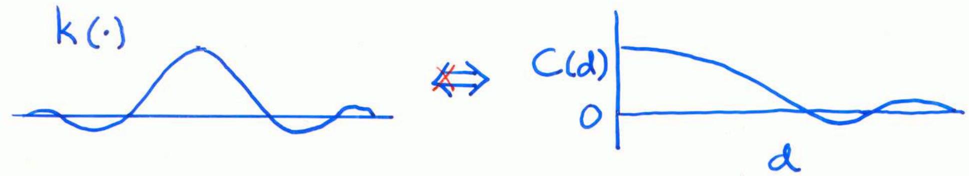
$$z(s) = \sum_{j=1}^{m} x_j k(\omega_j - s)$$

$\Rightarrow z(s)$ is a Gaussian process with mean 0 and covariance given by

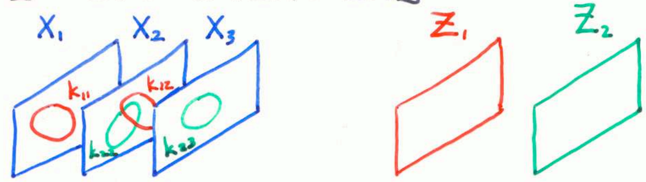
$$\text{Cov}(z(s), z(s')) = \frac{1}{\lambda_x} \sum_{j=1}^{m} k(\omega_j - s) k(\omega_j - s')$$

# USES

## "NON-PARAMETRIC" COVARIANCE FUNCTION



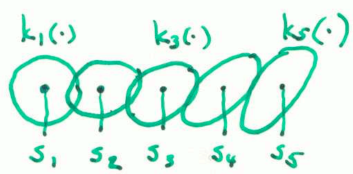

## MULTIVARIATE SPECIFICATIONS

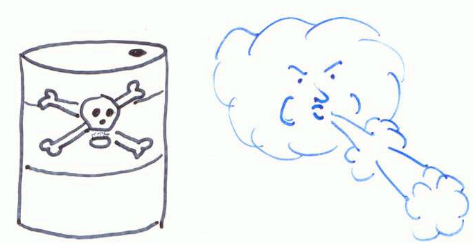



$Z_1 = k_{11} * X_1 + k_{12} * X_2$ $\quad$ $Z_2 = k_{22} * X_2 + k_{23} * X_3$

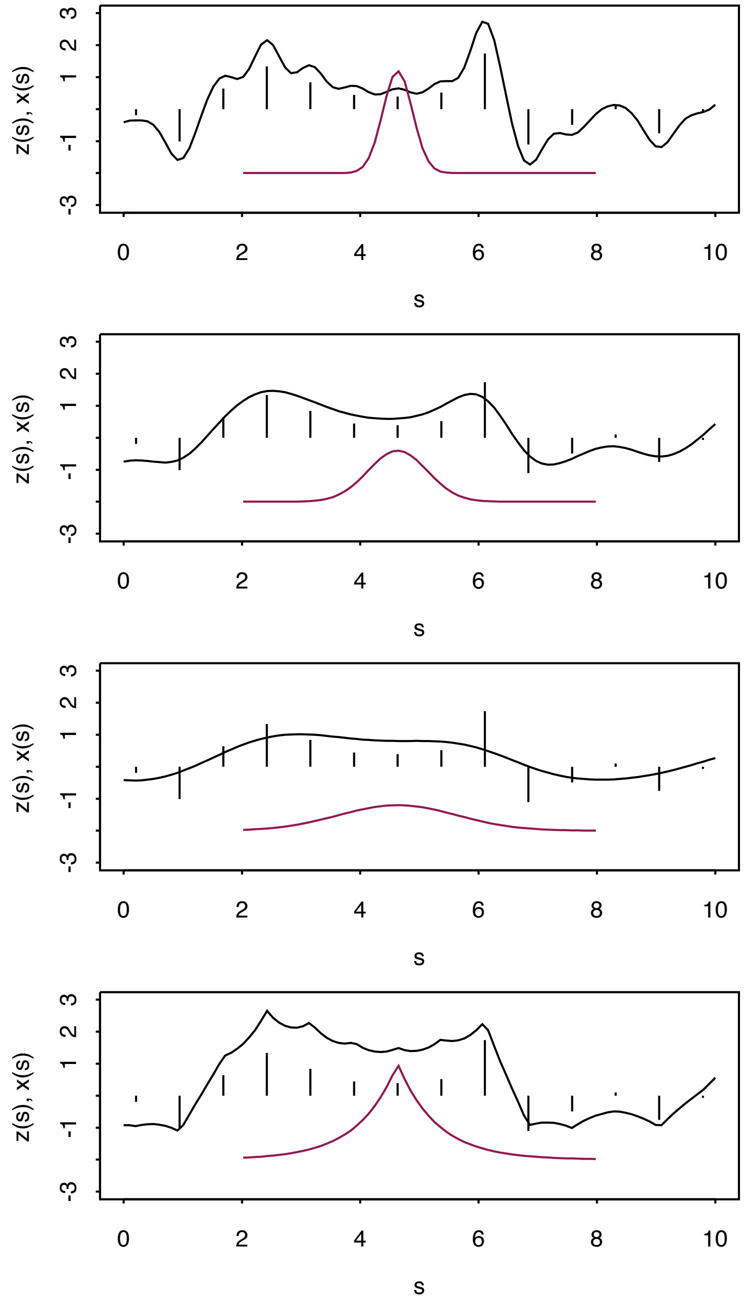
## EDGES


## NON STATIONARITY



# Example: constructing 1-d models for $z(s)$




$m = 20$ knot locations

$\omega_1, \ldots, \omega_m$ equally spaced between $-2$ and 12.

$x = (x_1, \ldots, x_m)^T \sim N(0, I_m)$

$z(s) = \Sigma_{k=1}^{m} k(\omega_k - s)x_k$

$k(s)$ is a normal density with sd $= \frac{1}{4}, \frac{1}{2},$ and 1
4th frame uses $k(s) = 1.4\exp\{-1.4|s|\}$.

General points:

- smooth kernels required
- spacing depends on kernel width

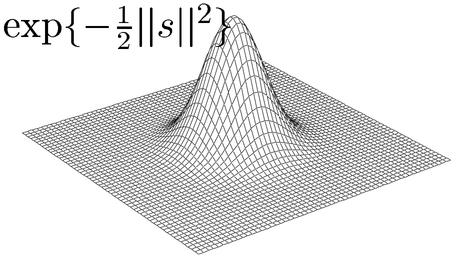
– knot spacing $\leq 1$ sd for normal $k(s)$

- kernel width is equivalent to scale parameter i GP models

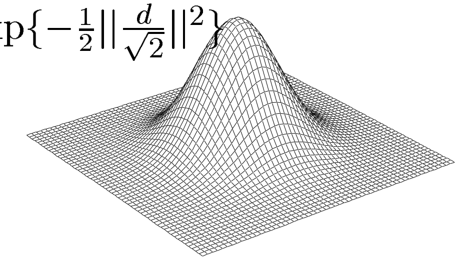
# kernels and induced covariance functions

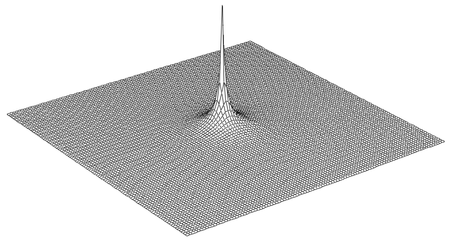
| **kernel** | **covariance function** |
|---|---|

$k(s) \propto \exp\{-\frac{1}{2}||s||^2\}$

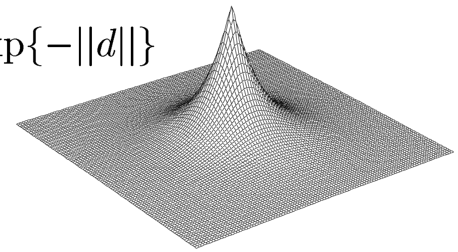


$c(d) \propto \exp\{-\frac{1}{2}||\frac{d}{\sqrt{2}}||^2\}$

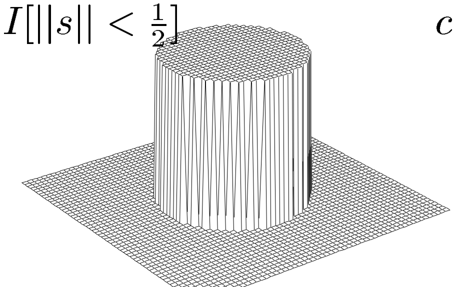




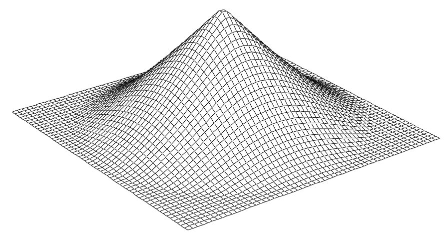
$c(d) \propto \exp\{-||d||\}$



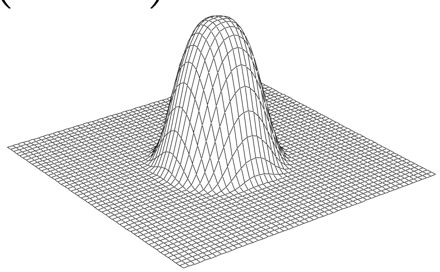
$k(s) \propto I[||s|| < \frac{1}{2}]$

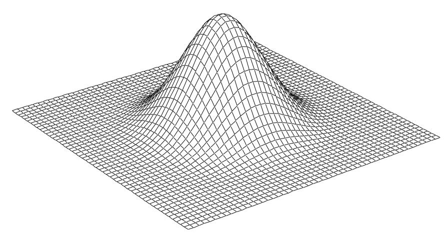


$c(d) \propto (1 - \frac{3}{2}||d|| + \frac{1}{2}||d||^3)I[d < 1]$



$k(s) \propto \left(1 - \frac{||s||^3}{r^3}\right)^3 I[s \leq r]$





# MRF formulation for the 1-d example

Data $y = (y(s_1), \ldots, y(s_n))^T$ observed at locations $s_1, \ldots, s_n$. Once knot locations $\omega_j,\ j = 1, \ldots, m$ and kernel choice $k(s)$ are specified, the remaining model formulation is trivial:

Likelihood:

$$L(y|x, \lambda_y) \propto \lambda_y^{\frac{n}{2}} \exp\left\{-\frac{1}{2}\lambda_y (y - Kx)^T (y - Kx)\right\}$$

where $K_{ij} = k(\omega_j - s_i)x_j$.

Priors:

$$\begin{aligned}
\pi(x|\lambda_x) &\propto \lambda_x^{\frac{m}{2}} \exp\left\{-\frac{1}{2}\lambda_x x^T W x\right\} \\
\pi(\lambda_x) &\propto \lambda_x^{a_x - 1} \exp\{-b_x \lambda_x\} \\
\pi(\lambda_y) &\propto \lambda_y^{a_y - 1} \exp\{-b_y \lambda_y\}
\end{aligned}$$

Posterior:

$$\begin{aligned}
\pi(x, \lambda_x, \lambda_y|y) \propto\ & \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\} \times \\
& \lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5x^T W x]\right\}
\end{aligned}$$

# Posterior and full conditionals (MRF formulation)

Posterior:

$$\pi(x, \lambda_x, \lambda_y | y) \propto \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\} \times$$
$$\lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5 x^T W x]\right\}$$

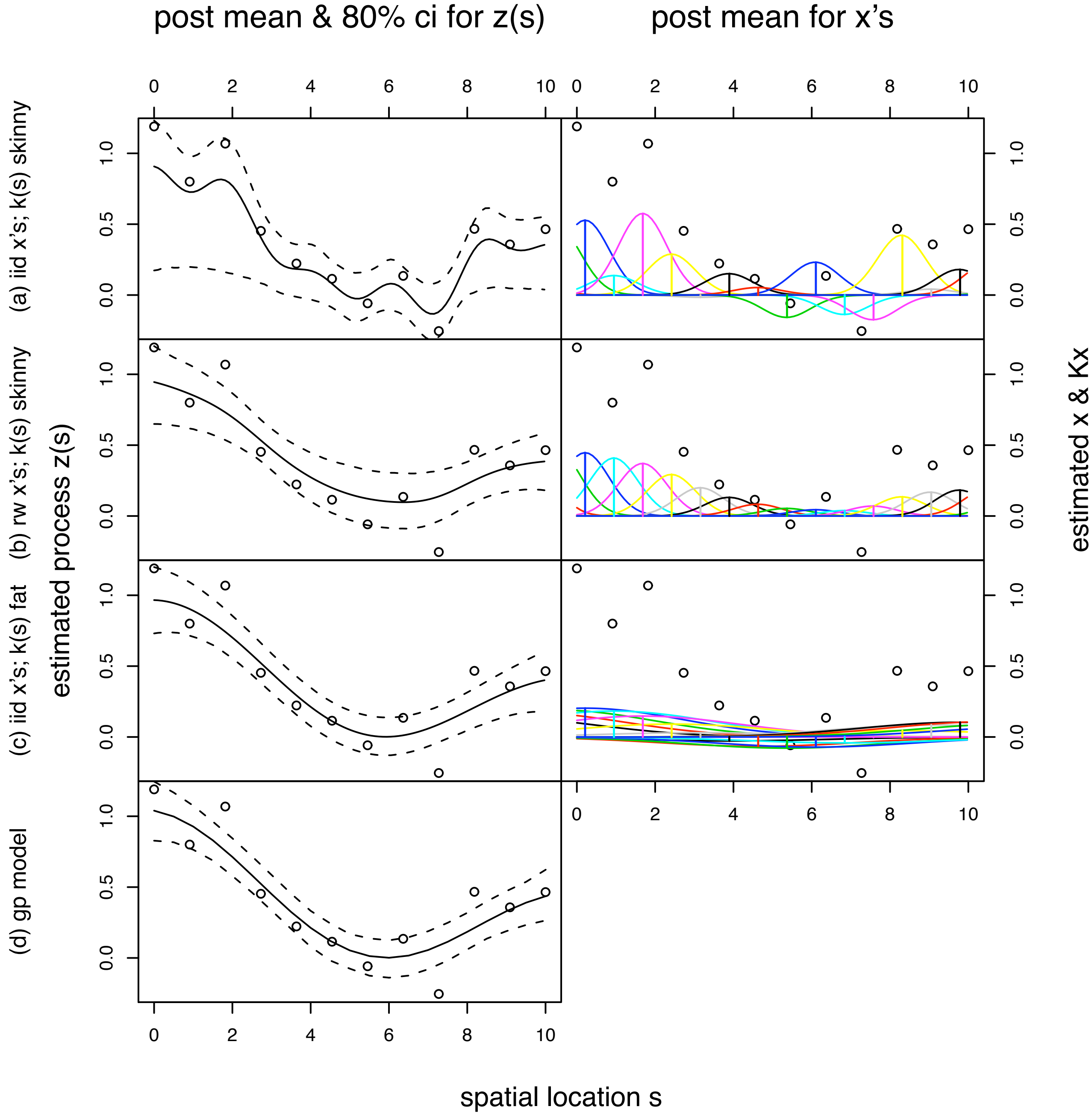
Full conditionals:

$$\pi(x | \cdots) \propto \exp\{-\frac{1}{2}[\lambda_y x^T K^T K x - 2\lambda_y x^T K^T y + \lambda_x x^T W x]\}$$
$$\pi(\lambda_x | \cdots) \propto \lambda_x^{a_x + \frac{m}{2} - 1} \exp\left\{-\lambda_x [b_x + .5 x^T W x]\right\}$$
$$\pi(\lambda_y | \cdots) \propto \lambda_y^{a_y + \frac{n}{2} - 1} \exp\left\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\right\}$$

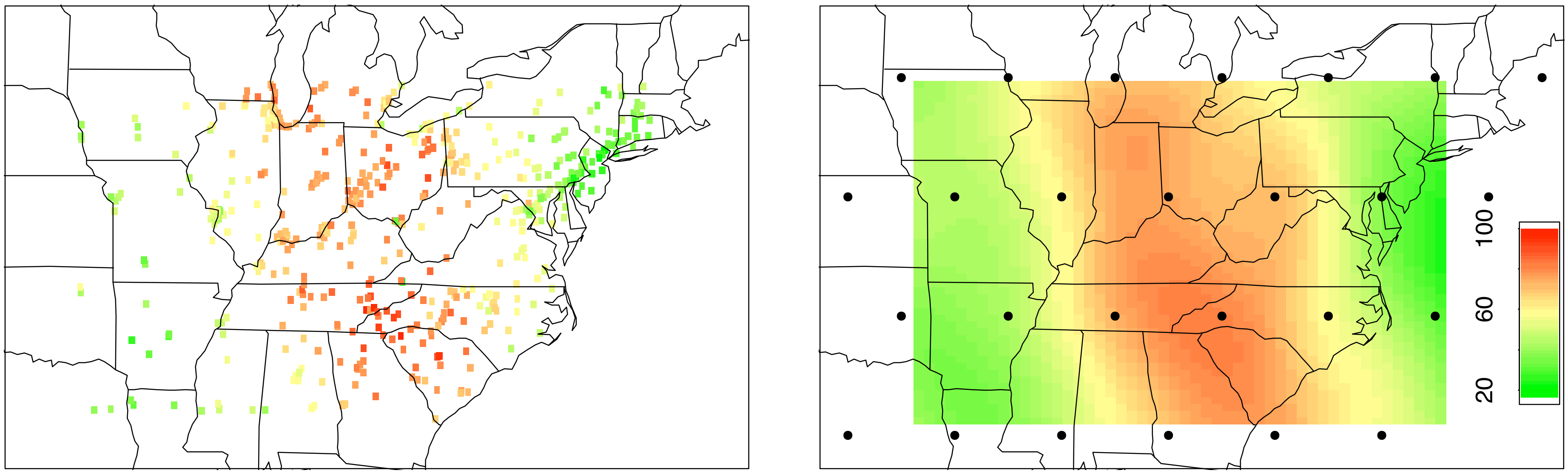
Gibbs sampler implementation

$$x | \cdots \sim N((\lambda_y K^T K + \lambda_x W)^{-1} \lambda_y K^T y, (\lambda_y K^T K + \lambda_x W)^{-1})$$
$$\lambda_x | \cdots \sim \Gamma(a_x + \frac{m}{2}, b_x + .5 x^T x)$$
$$\lambda_y | \cdots \sim \Gamma(a_y + \frac{n}{2}, b_y + .5(y - Kx)^T (y - Kx))$$

# 1-d example - using MRF prior for $x$



# 8 hour max for ozone on a summer day in the Eastern US






$n = 510$ ozone measurements

$\omega_k$'s laid out on a hexagonal lattice as shown.

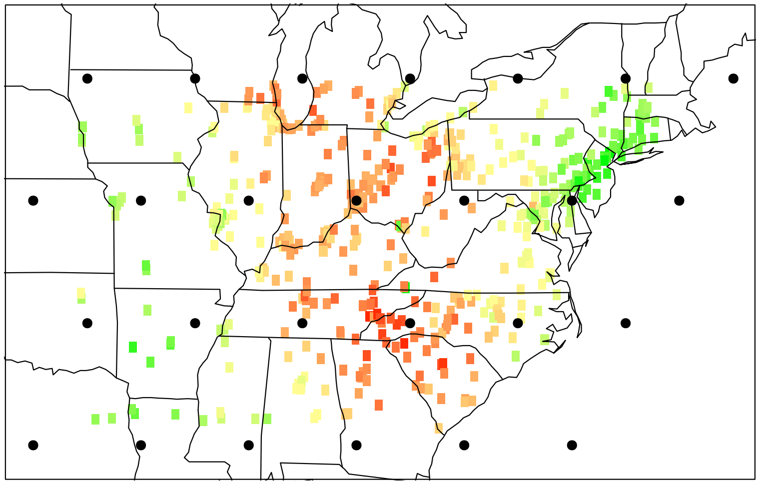
$k(s)$ is circular normal, with sd $=$ lattice spacing.

Choice of width for $k(s)$:

- could look at empirical variogram
- could estimate using ML or cross-validation
- could treat as additional parameter in posterior

# A multiresolution spatial model formulation

$$z(s) = z_{\text{coarse}}(s) + z_{\text{fine}}(s)$$

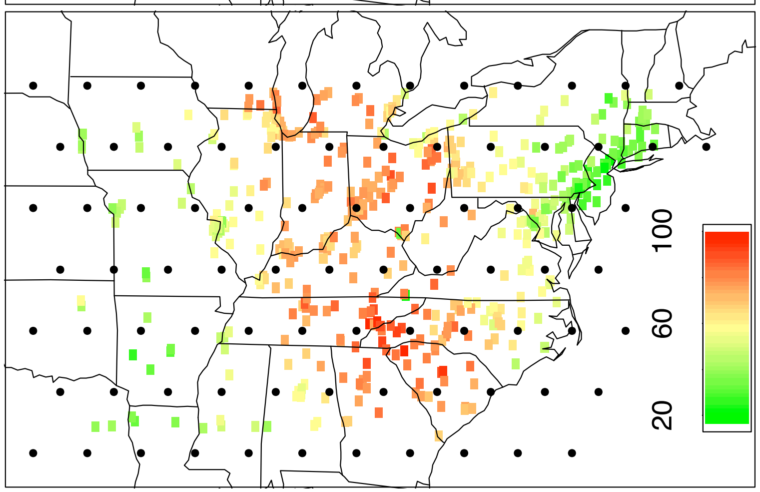


Coarse process:

$m_c = 27$ locations $\omega_1^c, \ldots, \omega_{m_c}^c$ on a hexagonal grid.

$x_c = (x_{c1}, \ldots, x_{cm_c})^T \sim N(0, \frac{1}{\lambda_c} I_{m_c})$

coarse smoothing kernel $k_c(s)$ is normal with sd = coarse grid spacing.




Fine process:

$m_f = 87$ locations $\omega_1^f, \ldots, \omega_{m_f}^f$ on a hexagonal grid.

$x_f = (x_{f1}, \ldots, x_{fm_f})^T \sim N(0, \frac{1}{\lambda_f} I_{m_f})$

fine smoothing kernel $k_f(s)$ is normal with sd = fine grid spacing.

note: coarse kernel width is twice the fine kernel width.

# Multiresolution formulation and full conditionals

Model:

$$
\begin{aligned}
y &= K_c x_c + K_f x_f + \epsilon \\
y &= Kx + \epsilon
\end{aligned}
$$

where

$$
K = \begin{pmatrix} K_c & K_f \end{pmatrix} \text{ and } x = \begin{pmatrix} x_c \\ x_f \end{pmatrix}
$$

Define

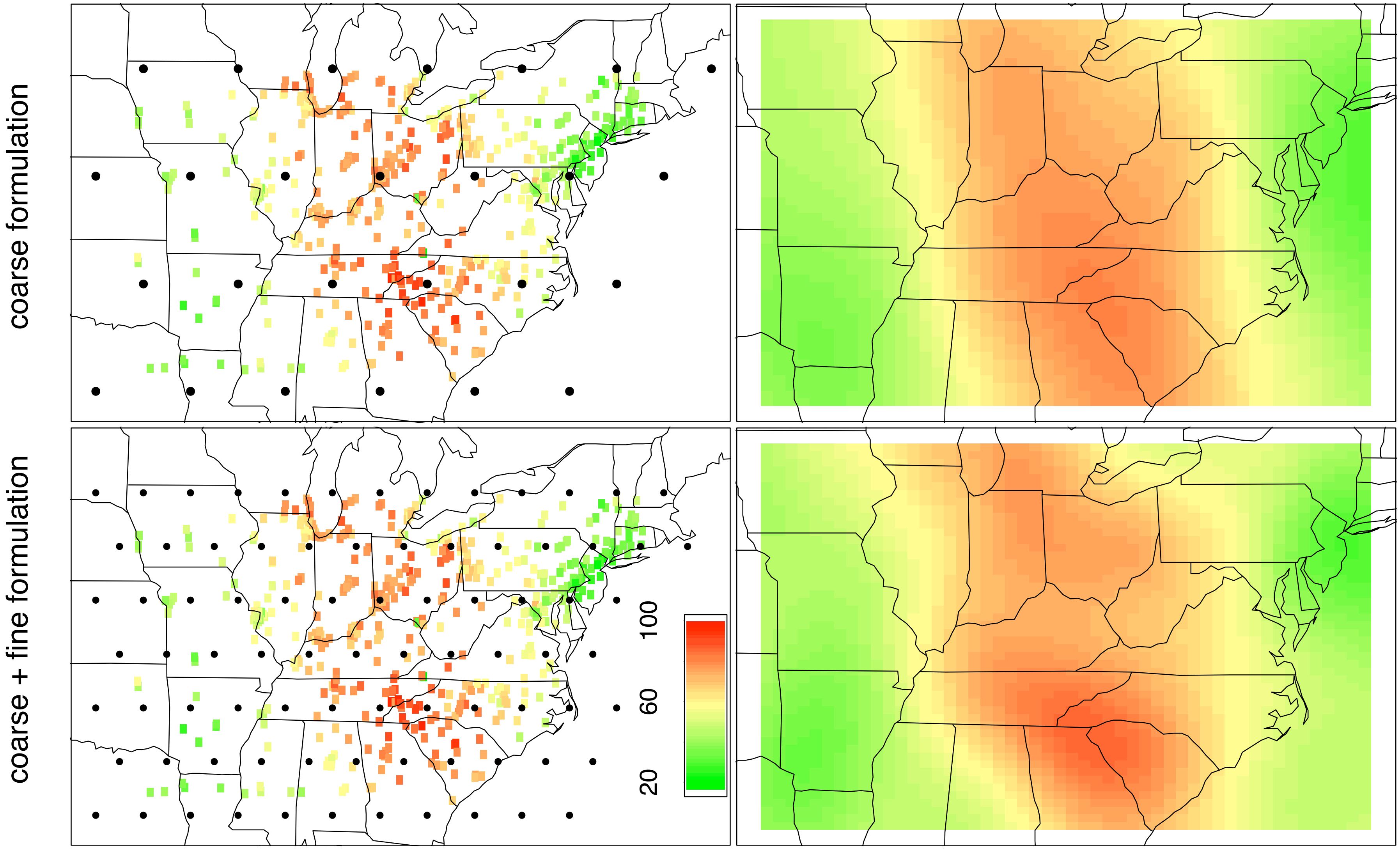
$$
W_x = \begin{pmatrix} \lambda_c I_{m_c} & 0 \\ 0 & \lambda_f I_{m_f} \end{pmatrix}
$$



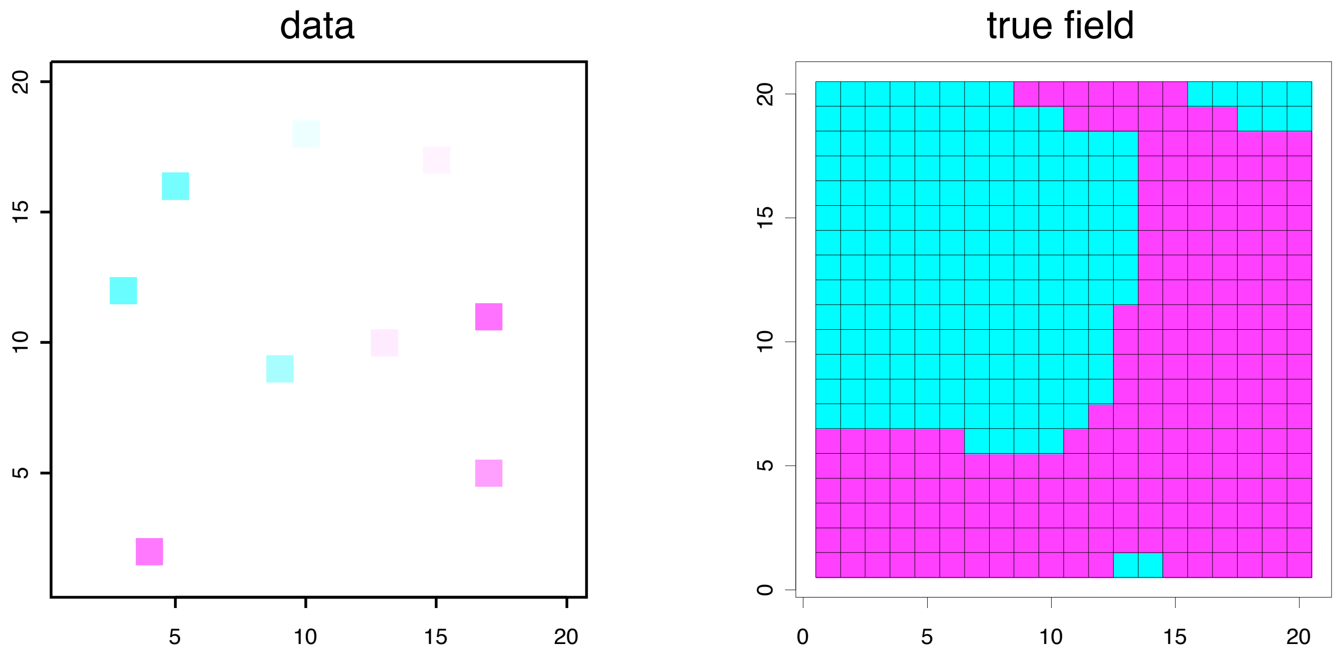
Gibbs sampler implementation then becomes

$$
\begin{aligned}
x|\cdots &\sim N((\lambda_y K^T K + W_x)^{-1}\lambda_y K^T y, (\lambda_y K^T K + W_x)^{-1}) \\
\lambda_c|\cdots &\sim \Gamma(a_x + \frac{m_c}{2}, b_x + .5 x_c^T x_c) \\
\lambda_f|\cdots &\sim \Gamma(a_x + \frac{m_f}{2}, b_x + .5 x_f^T x_f) \\
\lambda_y|\cdots &\sim \Gamma(a_y + \frac{n}{2}, b_y + .5(y - Kx)^T(y - Kx))
\end{aligned}
$$

Multiresolution model for 8 hour max ozone



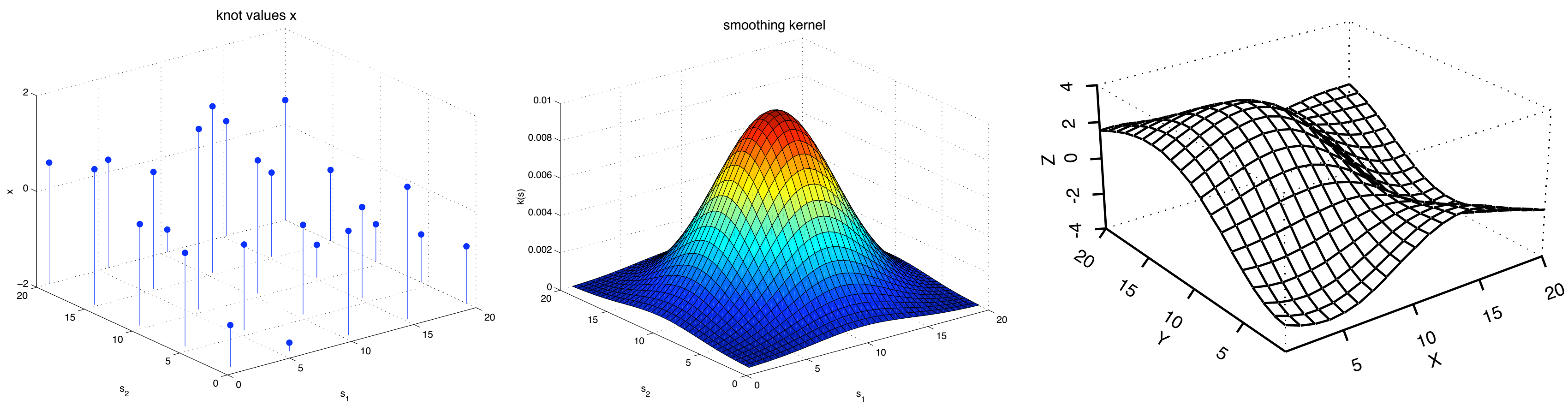
# Basic binary classification example




- binary spatial process $z^*(s)$
- spatial area partitioned into two regions: $z^*(s) = 1$ and $z^*(s) = 0$.
- $n = 10$ measurements $y = (y_1, \ldots, y_n)^T$ taken at spatial locations $s_1, \ldots, s_n$.

$$y_i = z^*(s_i) + \epsilon_i, \quad i = 1, \ldots, n; \quad \epsilon_i \overset{iid}{\sim} N(0,1), \quad i = 1, \ldots, n$$

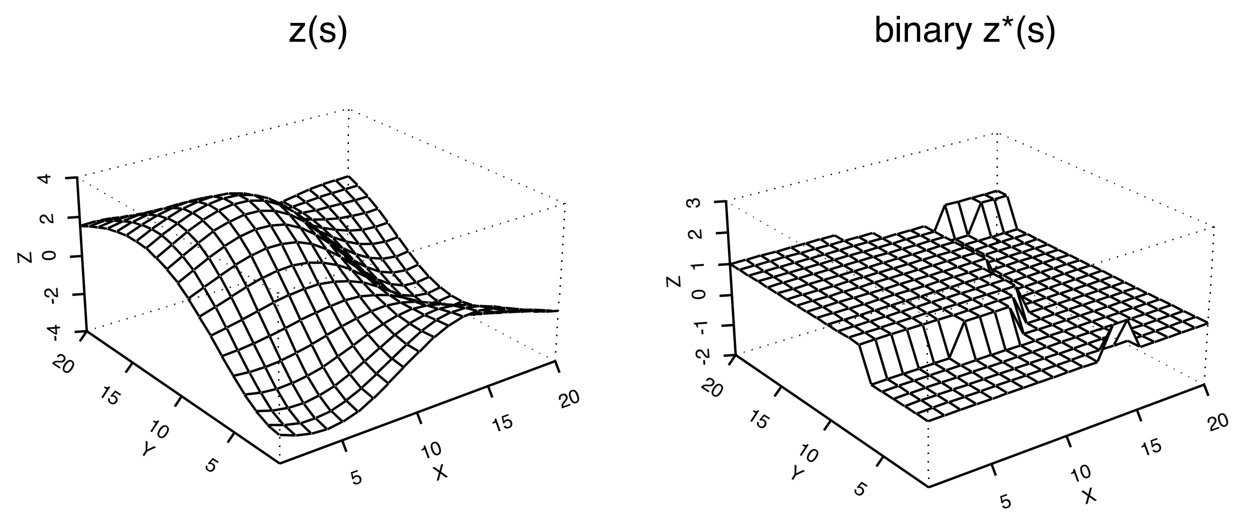
# Constructing a binary spatial process $z^*(s)$




$x$ convolved with $k(s)$ gives $z(s)$

$$x \sim N(0, I_m) \text{ where each } x_j \text{ is located at } \omega_j; \;\; z(s) = \sum_{j=1}^{m} x_j k(s - \omega_j)$$






Now define the binary field $z^*(s)$ by "clipping" $z(s)$: $z^*(s) = I[z(s) > 0]$.

# Model Formulation

Define $n = 10$ observations $y = (y(s_1), \ldots, y(s_n))^T$.

Define $z^* = (z^*(s_1), \ldots, z^*(s_n))^T$.

Define $x = (x(\omega_1), \ldots, x(\omega_m))^T$ to be the $m = 25$-vector of white noise knot values at spatial grid sites $\omega_1, \ldots, \omega_m$.

Recall $z^*(s)$ and the vector $z^*$ are determined by the knot values $x$.

Likelihood

$$L(y|z^*) \propto \exp\{-\frac{1}{2}(y - z^*)^T(y - z^*)\}$$

Independent normal prior for $x$

$$\pi(x) \propto \exp\{-\frac{1}{2}x^T x\}$$

Posterior distribution

$$\pi(x|y) \propto \exp\{-\frac{1}{2}(y - z^*)^T(y - z^*) - \frac{1}{2}x^T x\}$$

# Sampling the posterior via Metropolis

Full conditional distributions

$$\pi(x_j|x_{-j}, y) \propto \exp\{-\frac{1}{2}(y - z^*)^T(y - z^*) - \frac{1}{2}x_j^2\},\ j = 1, \ldots, m$$

Metropolis implementation for sampling from $\pi(x|y)$:

Initialize $x$ at $x = 0$.

Cycle thru full conditionals updating each $x_j$ according to Metropolis rules.

- generate proposal $x_j^* \sim U[x_j - r, x_j + r]$.
- compute acceptance probability

$$\alpha = \min\left\{1, \frac{\pi(x_j^*|x_{-j}, y)}{\pi(x_j|x_{-j}, y)}\right\}$$

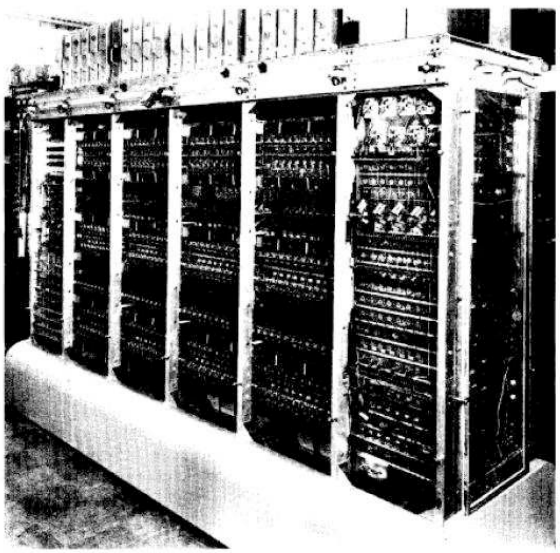
- update $x_j$ to new value:

$$x_j^{\text{new}} = \begin{cases} x_j^* & \text{with probability } \alpha \\ x_j & \text{with probability } 1 - \alpha \end{cases}$$

Here we ran for $T = 1000$ scans, giving realizations $x^1, \ldots, x^T$ from the posterior. Discarded the first 100 for burn in.

Note: proposal width $r$ tuned so that $x_j^*$ is accepted about half the time.

# Sampling from non-standard multivariate distributions



Nick Metropolis – Computing pioneer at Los Alamos National Laboratory

– inventor of the Monte Carlo method

– inventor of Markov chain Monte Carlo:

Equation of State Calculations by Fast Computing Machines (1953) by N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller and E. Teller, *Journal of Chemical Physics*.

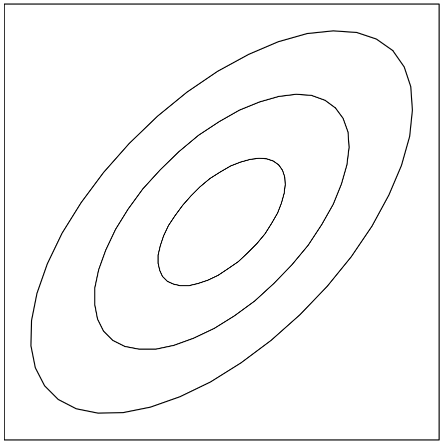
Originally implemented on the MANIAC1 computer at LANL

Algorithm constructs a Markov chain whose realizations are draws from the target (posterior) distribution.

Constructs steps that maintain detailed balance.

# Gibbs Sampling and Metropolis for a bivariate normal density

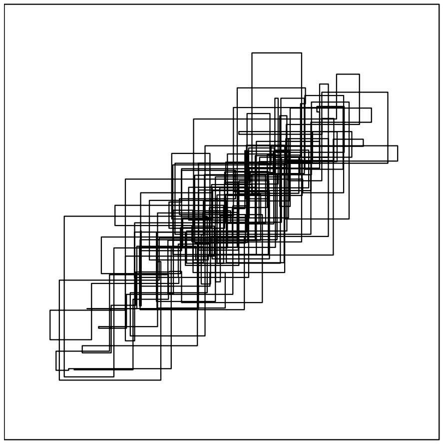
$$\pi(z_1, z_2) \propto \begin{vmatrix} 1 & \rho \\ \rho & 1 \end{vmatrix}^{-\frac{1}{2}} \exp\left\{-\frac{1}{2} \begin{pmatrix} z_1 & z_2 \end{pmatrix} \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}^{-1} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}\right\}$$



sampling from the full conditionals

$$\begin{aligned} z_1 | z_2 &\sim N(\rho z_2, 1-\rho^2) \\ z_2 | z_1 &\sim N(\rho z_1, 1-\rho^2) \end{aligned}$$

also called heat bath

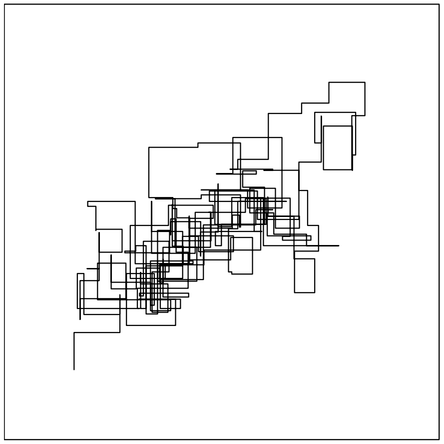


Metropolis updating:

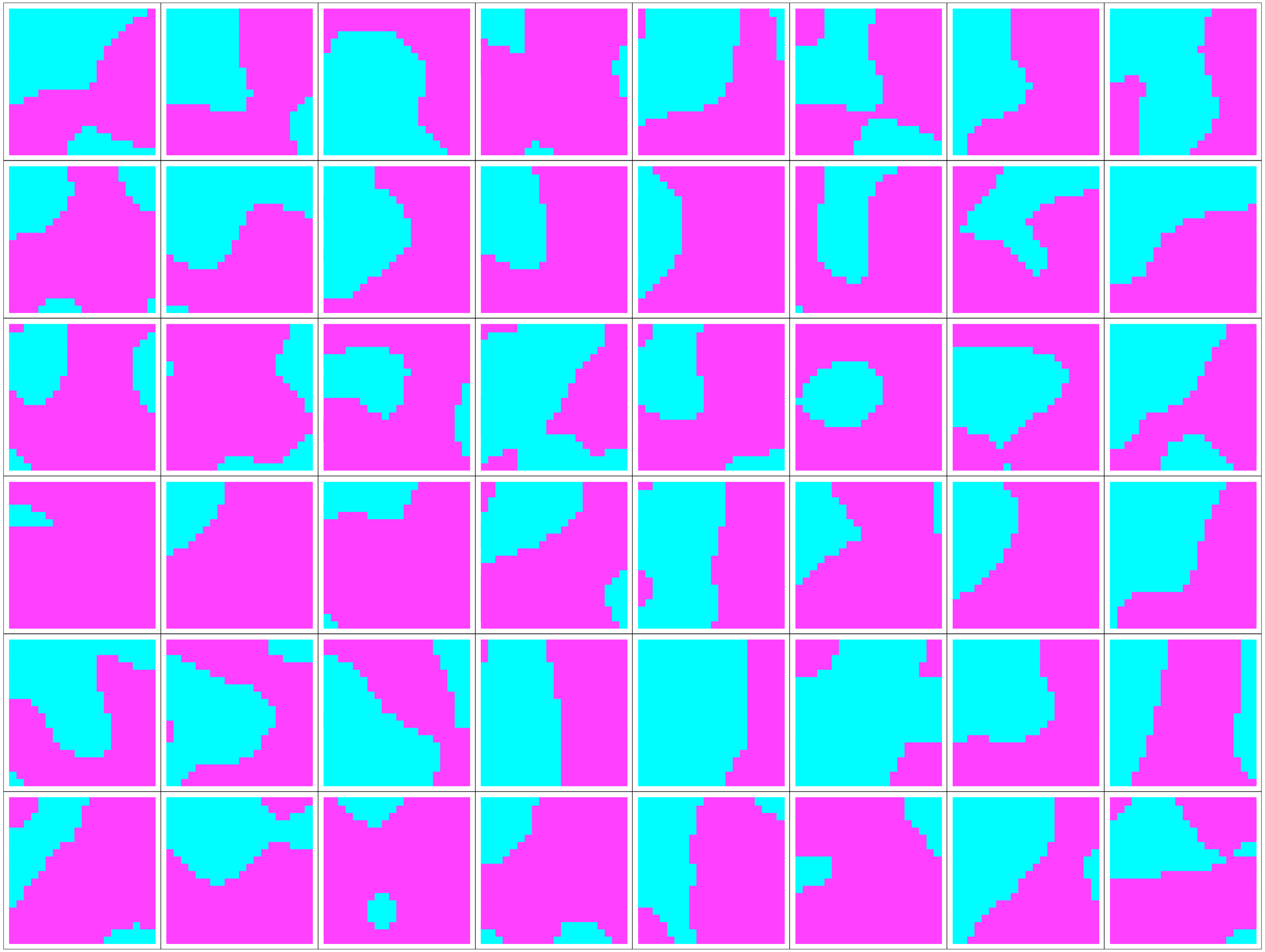
generate $z_1^* \sim U[z_1 - r, z_1 + r]$

calculate $\alpha = \min\{1, \frac{\pi(z_1^*, z_2)}{\pi(z_1, z_2)} = \frac{\pi(z_1^* | z_2)}{\pi(z_1 | z_2)}\}$

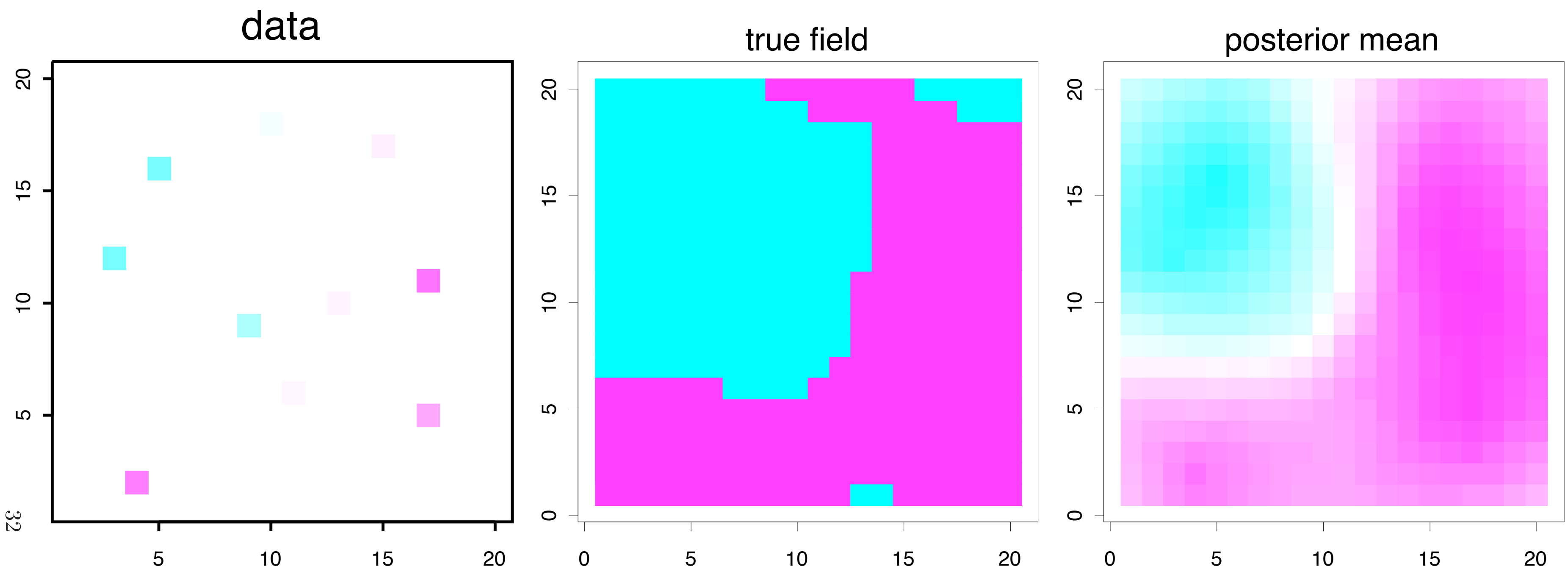
set $z_1^{\text{new}} = \begin{cases} z_1^* \text{ with probability } \alpha \\ z_1 \text{ with probability } 1-\alpha \end{cases}$



# Posterior realizations of $z^*(s) = I[z(s) > 0]$

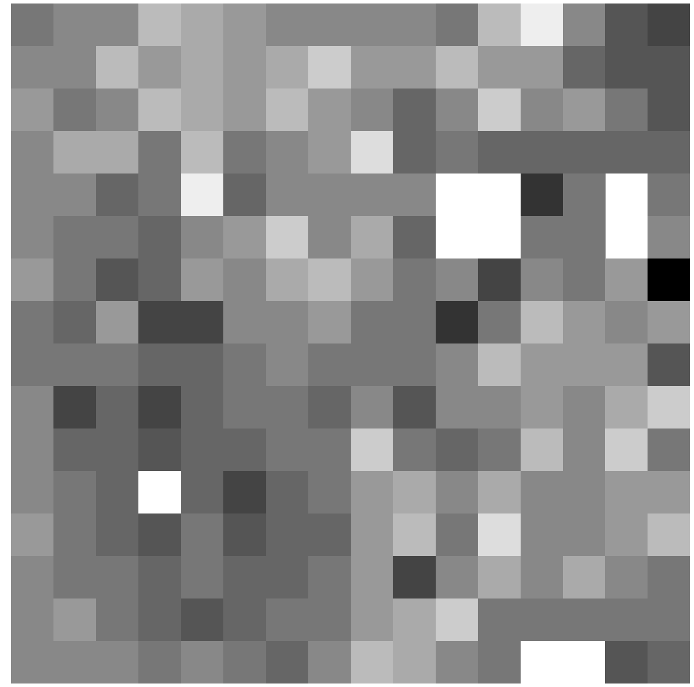


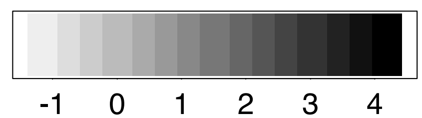
# Posterior mean of $z^*(s) = I[z(s) > 0]$



# Application – locating archeological sites

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.7 | 1.1 | 1.0 | -0.1 | 0.2 | 0.6 | 1.2 | 1.3 | 1.3 | 1.0 | 1.6 | -0.1 | -1.3 | 1.3 | 2.4 | 2.6 |
| 1.2 | 1.0 | 0.1 | 0.6 | 0.4 | 0.7 | 0.3 | -0.3 | 0.6 | 0.9 | 0.0 | 0.7 | 0.9 | 1.8 | 2.2 | 2.4 |
| 0.6 | 1.4 | 1.3 | 0.1 | 0.3 | 0.7 | -0.1 | 0.6 | 1.3 | 1.8 | 1.2 | -0.4 | 1.2 | 0.8 | 1.6 | 2.4 |
| 1.0 | 0.4 | 0.4 | 1.4 | 0.2 | 1.4 | 1.0 | 0.6 | -0.9 | 1.8 | 1.4 | 2.0 | 2.0 | 2.0 | 1.8 | 2.0 |
| 1.2 | 1.1 | 1.8 | 1.5 | -1.1 | 1.8 | 1.2 | 1.2 | 1.2 | 1.3 | ? | ? | 3.2 | 1.7 | ? | 1.4 |
| 1.2 | 1.4 | 1.6 | 1.9 | 1.1 | 0.6 | -0.2 | 1.3 | 0.3 | 2.0 | ? | ? | 1.4 | 1.7 | ? | 1.2 |
| 0.7 | 1.6 | 2.2 | 1.8 | 0.7 | 1.3 | 0.4 | 0.1 | 0.7 | 1.5 | 1.3 | 2.5 | 1.2 | 1.6 | 0.9 | 4.4 |
| 1.4 | 1.8 | 0.8 | 2.6 | 2.8 | 1.3 | 1.2 | 0.7 | 1.7 | 1.4 | 2.9 | 1.4 | -0.1 | 0.8 | 1.0 | 0.8 |
| 1.5 | 1.5 | 1.5 | 2.0 | 1.8 | 1.4 | 1.1 | 1.6 | 1.6 | 1.7 | 1.2 | 0.1 | 0.7 | 0.8 | 0.8 | 2.2 |
| 1.1 | 2.7 | 2.0 | 2.8 | 1.8 | 1.4 | 1.5 | 1.8 | 1.3 | 2.3 | 1.3 | 1.3 | 0.6 | 1.2 | 0.4 | -0.4 |
| 1.2 | 1.8 | 2.1 | 2.4 | 1.8 | 2.0 | 1.4 | 1.5 | -0.4 | 1.6 | 1.8 | 1.7 | 0.1 | 1.1 | -0.2 | 1.5 |
| 1.0 | 1.4 | 2.1 | ? | 2.0 | 2.5 | 1.8 | 1.7 | 0.6 | 0.4 | 1.2 | 0.4 | 1.1 | 1.0 | 0.7 | 0.7 |
| 0.9 | 1.7 | 2.0 | 2.4 | 1.6 | 2.4 | 1.9 | 1.8 | 0.9 | 0.0 | 1.6 | -0.7 | 1.2 | 1.1 | 0.7 | 0.2 |
| 1.1 | 1.5 | 1.6 | 1.8 | 1.6 | 1.9 | 1.9 | 1.6 | 0.9 | 2.8 | 1.1 | 0.3 | 1.3 | 0.3 | 1.0 | 1.5 |
| 1.3 | 0.7 | 1.4 | 1.8 | 2.1 | 2.0 | 1.7 | 1.7 | 0.9 | 0.4 | -0.4 | 1.4 | 1.4 | 1.5 | 1.6 | 1.4 |
| 1.3 | 1.0 | 1.2 | 1.6 | 1.3 | 1.6 | 1.8 | 1.2 | 0.2 | 0.2 | 1.1 | 1.4 | ? | ? | 2.4 | 1.8 |








Data at $16 \times 16 - 9$ locations over 10 $m^2$ area

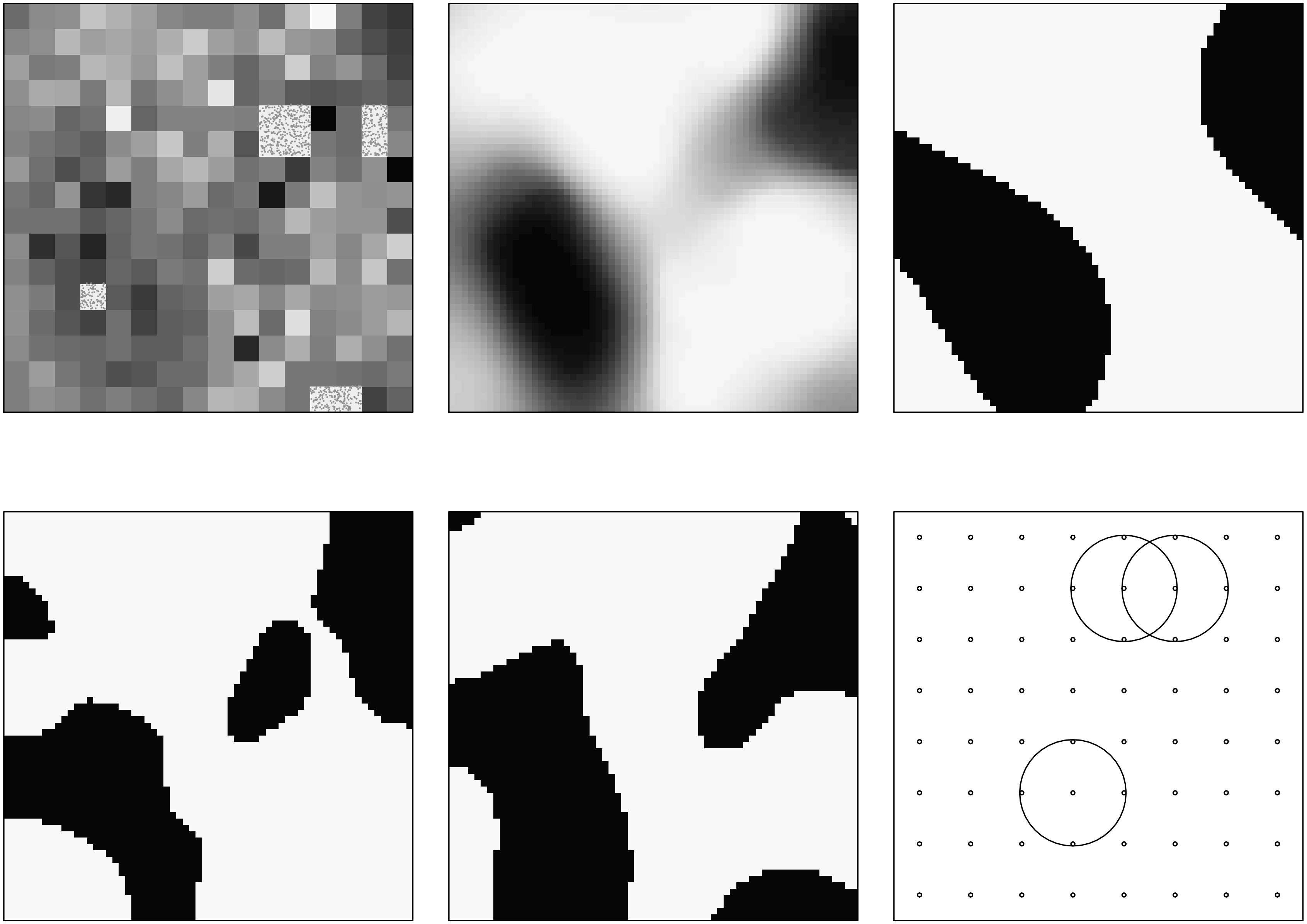
Assume $y(s_i)|z^*(s_i) \sim N(\mu(z^*(s_i)), 1)$ – $\mu(0) = 1$, $\mu(1) = 2$.

Recall $z(s) = \Sigma_{j=1}^{m} x_j k(s - \omega_j)$ and $z^*(s) = I[z(s) > 0]$.

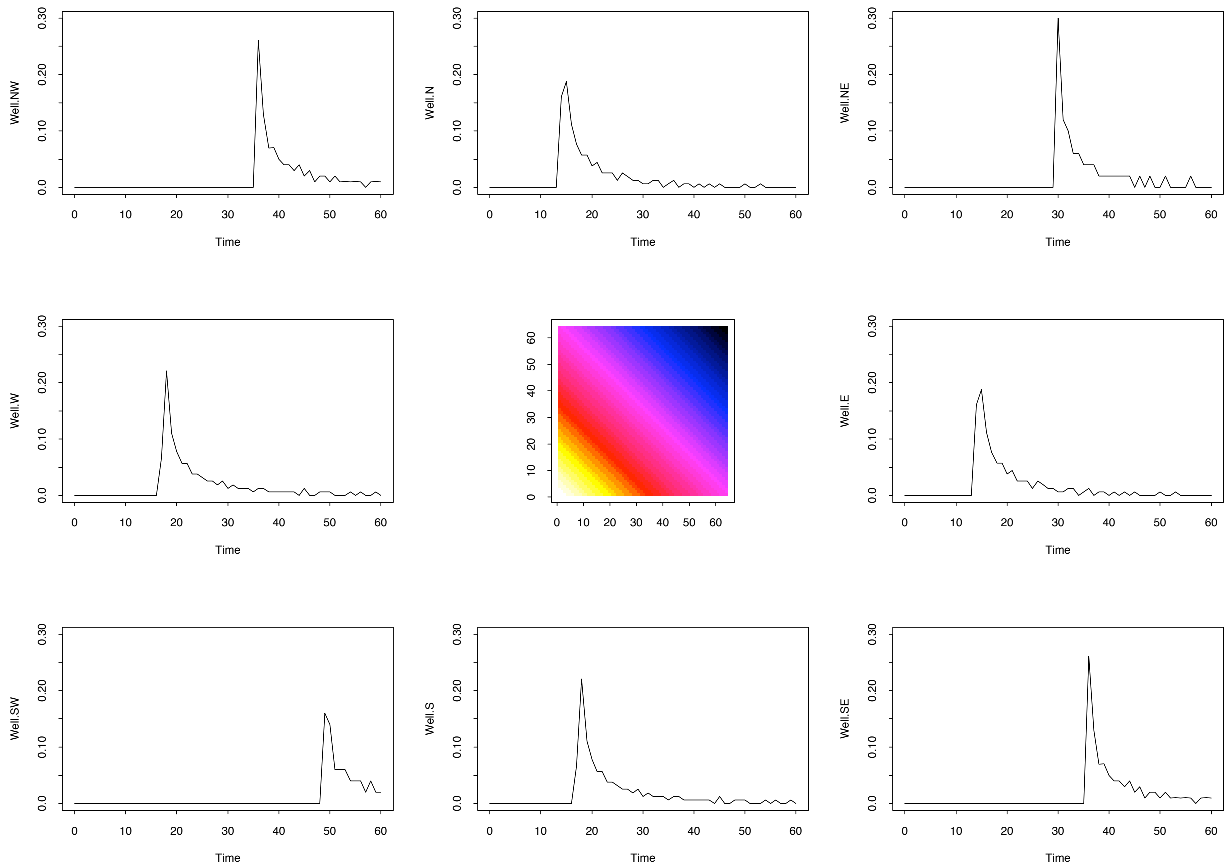
$m = 8 \times 8$ lattice of knot locations $\omega_1, \ldots, \omega_m$;

sd of $k(s)$ equal to knot spacings.

# Posterior mean and realizations for $z^*(s) = I[z(s) > 0]$



# Bayesian formulation



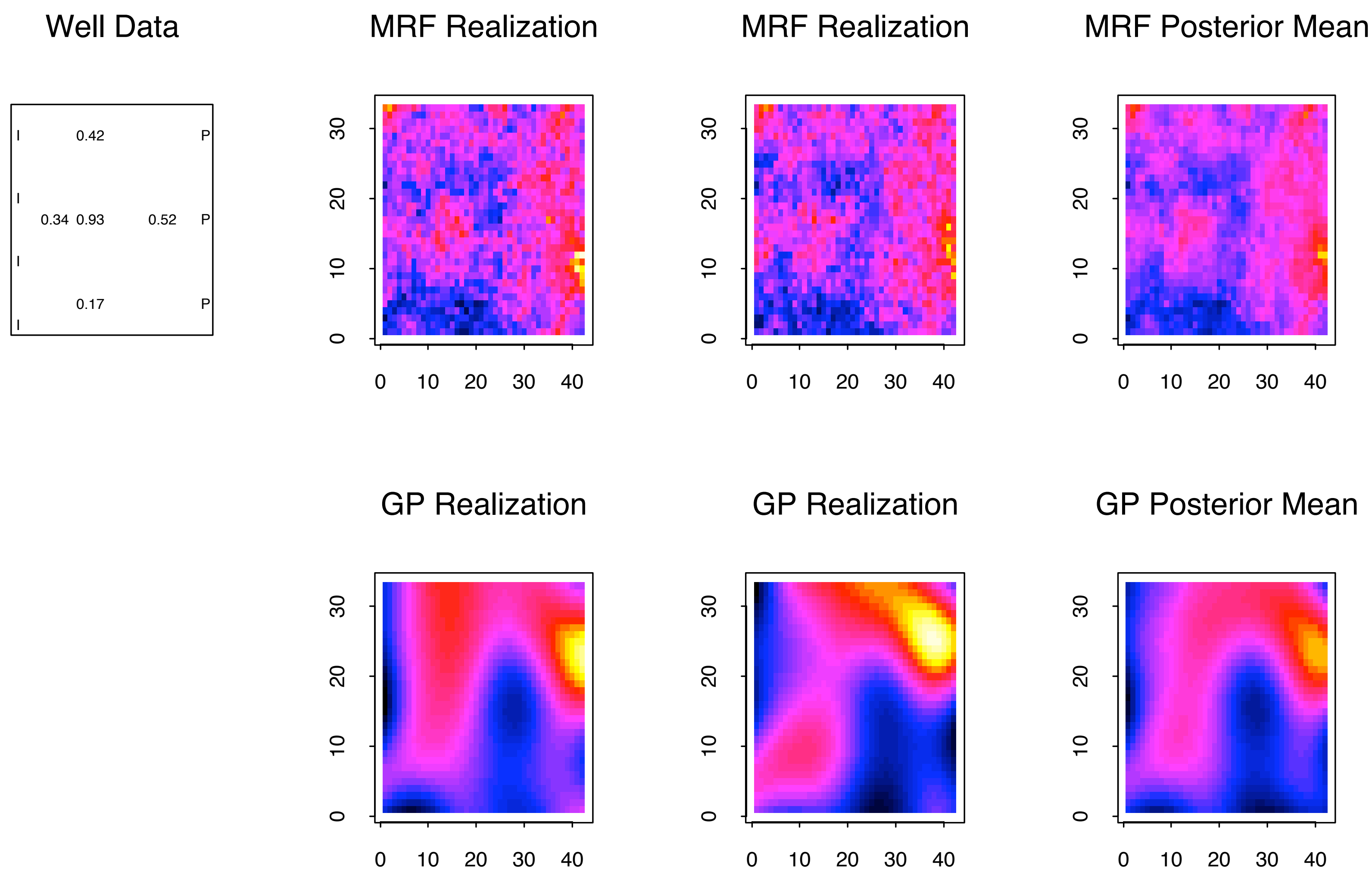

$$L(y|\eta(z)) \;\propto\; |\Sigma|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}(y-\eta(z))^T\Sigma^{-1}(y-\eta(z))\right\}$$

$$\pi(z|\lambda_z) \;\propto\; \lambda_z^{\frac{m}{2}} \exp\left\{-\frac{1}{2}z^T W_z z\right\}$$

$$\pi(\lambda_z) \;\propto\; \lambda_z^{a_z-1} \exp\left\{b_z\lambda_z\right\}$$

$$\pi(z,\lambda_z|y) \;\propto\; L(y|\eta(z)) \times \pi(z|\lambda_z) \times \pi(\lambda_z)$$

# Posterior realizations of $z$ under MRF and moving average priors

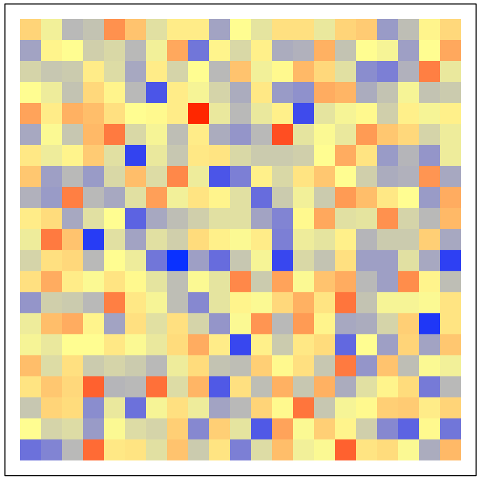


# References


- D. Higdon (1998) A process-convolution approach to modeling temperatures in the North Atlantic Ocean (with discussion), *Environmental and Ecological Statistics*, 5:173–190.
- D. Higdon (2002) Space and space-time modeling using process convolutions, in *Quantitative Methods for Current Environmental Issues* (C. Anderson and V. Barnett and P. C. Chatwin and A. H. El-Shaarawi, eds),37–56.
- D. Higdon, H. Lee and C. Holloman (2003) Markov chain Monte Carlo approaches for inference in computationally intensive inverse problems, in *Bayesian Statistics 7, Proceedings of the Seventh Valencia International Meeting* (Bernardo, Bayarri, Berger, Dawid, Heckerman, Smith and West, eds).

# NON-STATIONARY SPATIAL CONVOLUTION MODELS

# A convolution-based approach for building non-stationary spatial models



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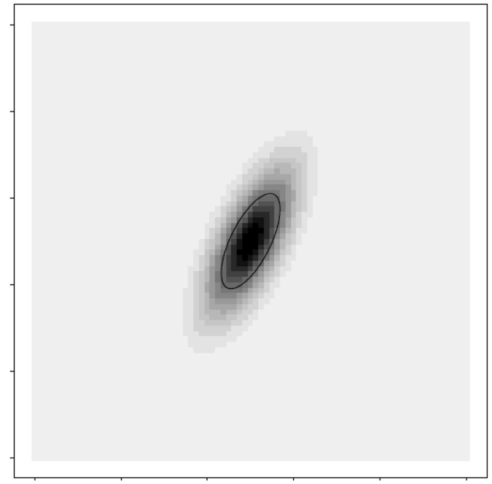

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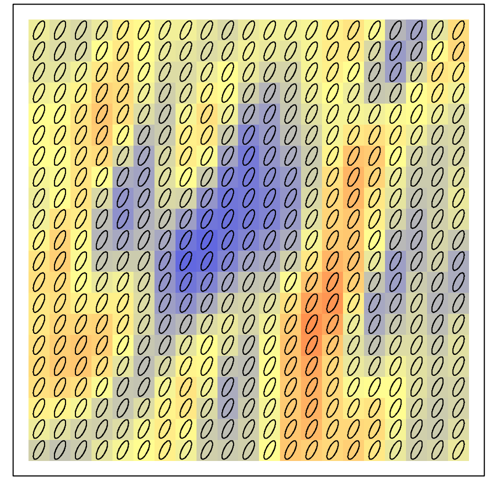


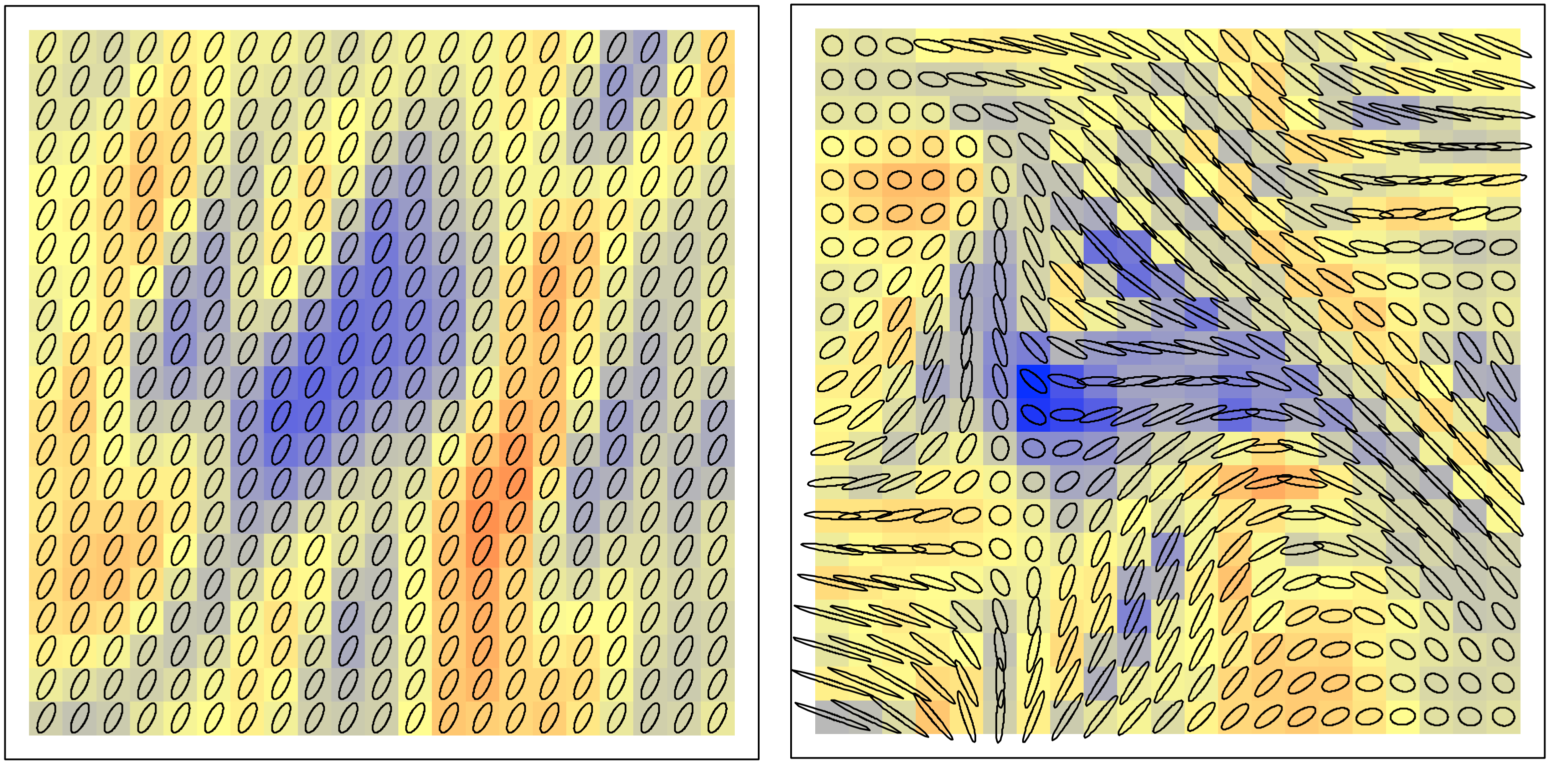
white noise smoothing kernel spatial field



$$z(s) = \sum_{j=1}^{m} x_j k(\omega_j - s) = \sum_{j=1}^{m} x_j k_s(\omega_j)$$

$x \sim N(0, I_m)$ where each $x_j$ is located at $\omega_j$ over a regular 2-d grid.

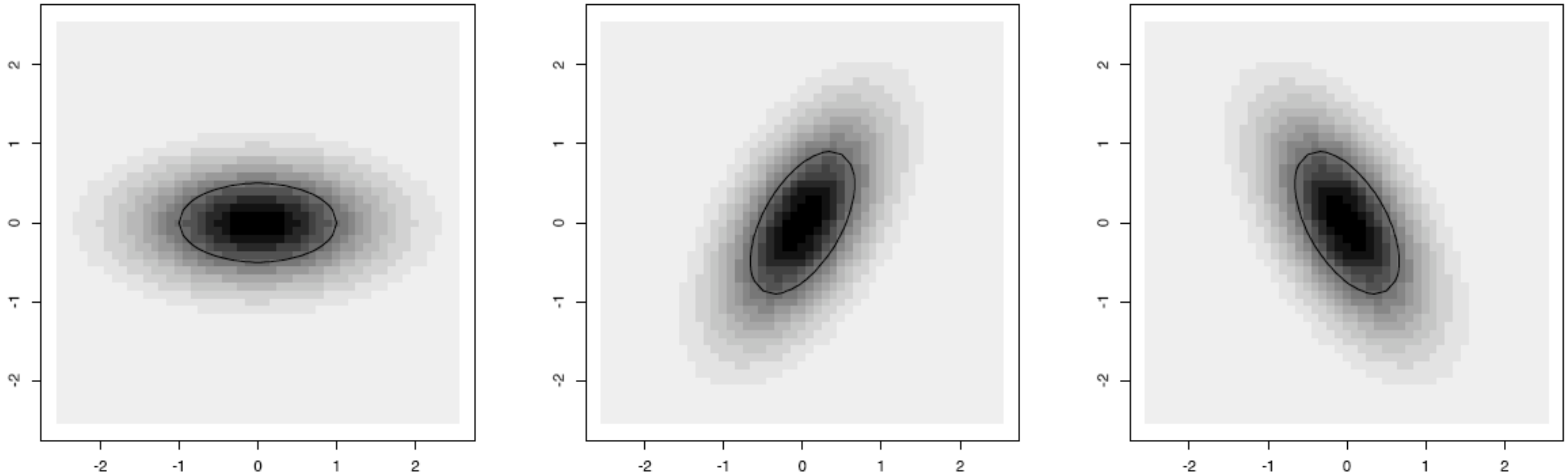
# Convolutions for constructing non-stationary spatial models



$$
\begin{aligned}
z(s) &= \sum_{j=1}^{m} x_j k_s(\omega_j) \\
x &\sim N(0, \lambda_x^{-1} I_m) \text{ at regular 2-d lattice locations } \omega_1, \ldots, \omega_m. \\
&\Rightarrow z(s) \sim GP(0, C(s_1, s_2) \text{ where } C(s_1, s_2) = \lambda_x^{-1} \sum_{j=1}^{m} k_{s_1}(\omega_j) k_{s_2}(\omega_j)
\end{aligned}
$$

smoothing kernel $k_s(\cdot)$ changes smoothly over spatial location

# Defining smoothly varying kernels via basis kernels




$k_1(\cdot)$ $k_2(\cdot)$ $k_3(\cdot)$

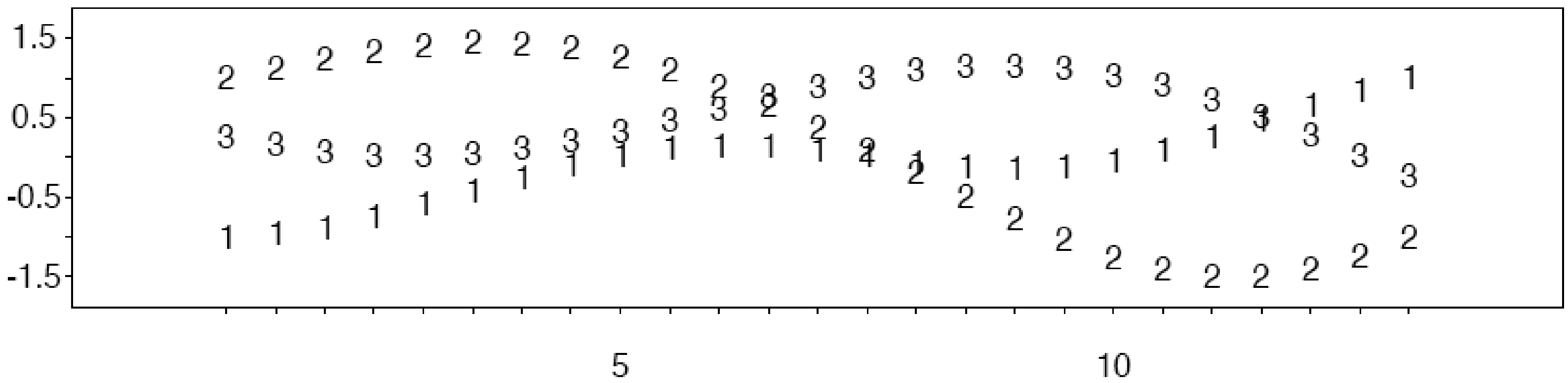


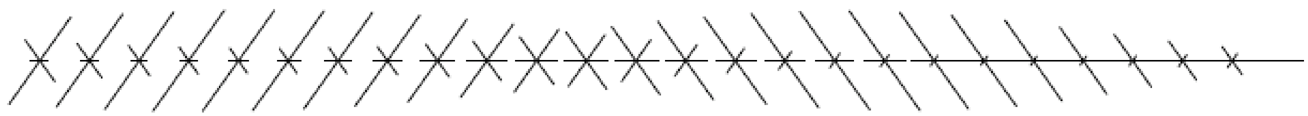
Define $k_s(\cdot) = w_1(s)k_1(\cdot - s) + w_2(s)k_2(\cdot - s) + w_3(s)k_3(\cdot - s)$

$k_s(\cdot)$ is a weighted combination of kernels centered at $s$.

Define weights that change smoothly over space.

# Defining smoothly varying kernels via basis kernels





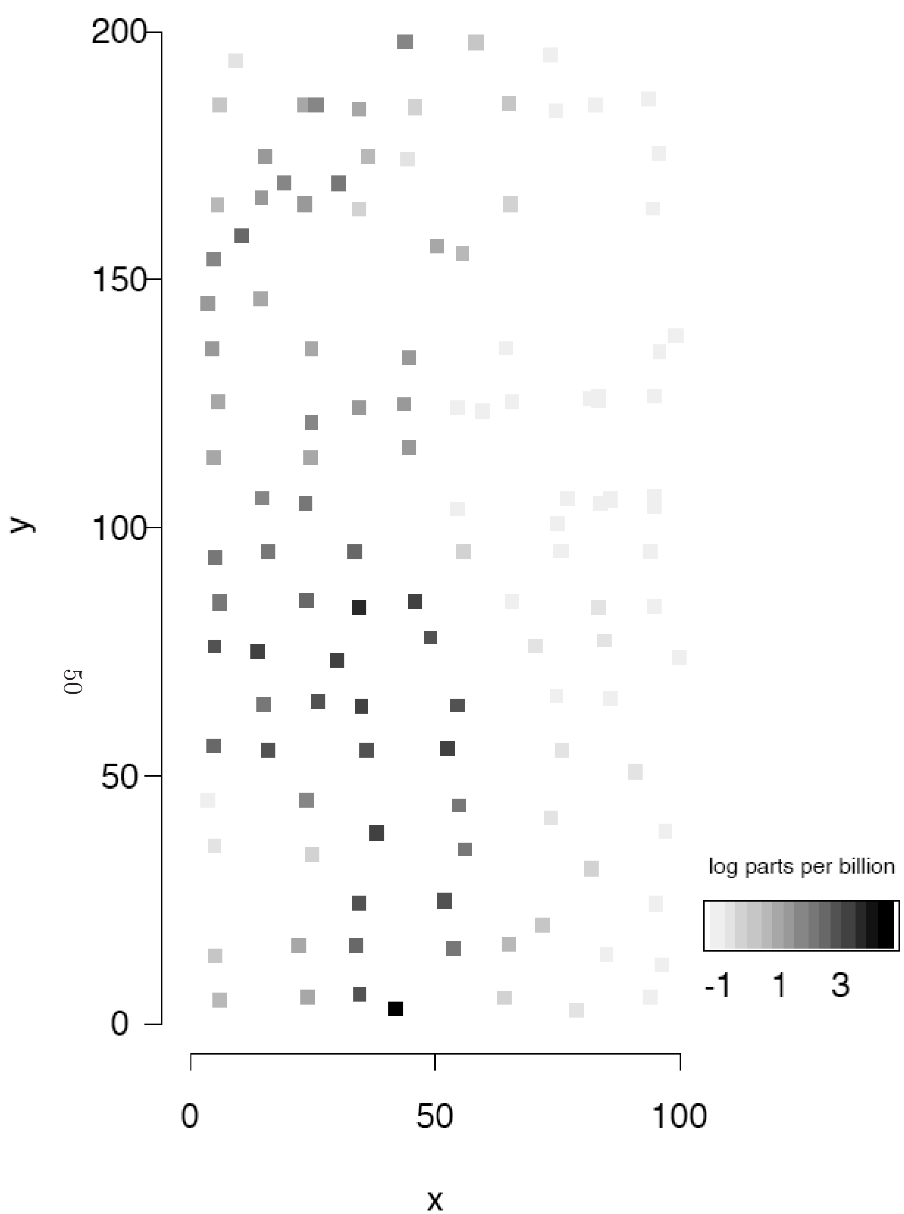
Define iid, mean 0 Gaussian Processes $\phi_1(s)$, $\phi_2(s)$ and $\phi_3(s)$

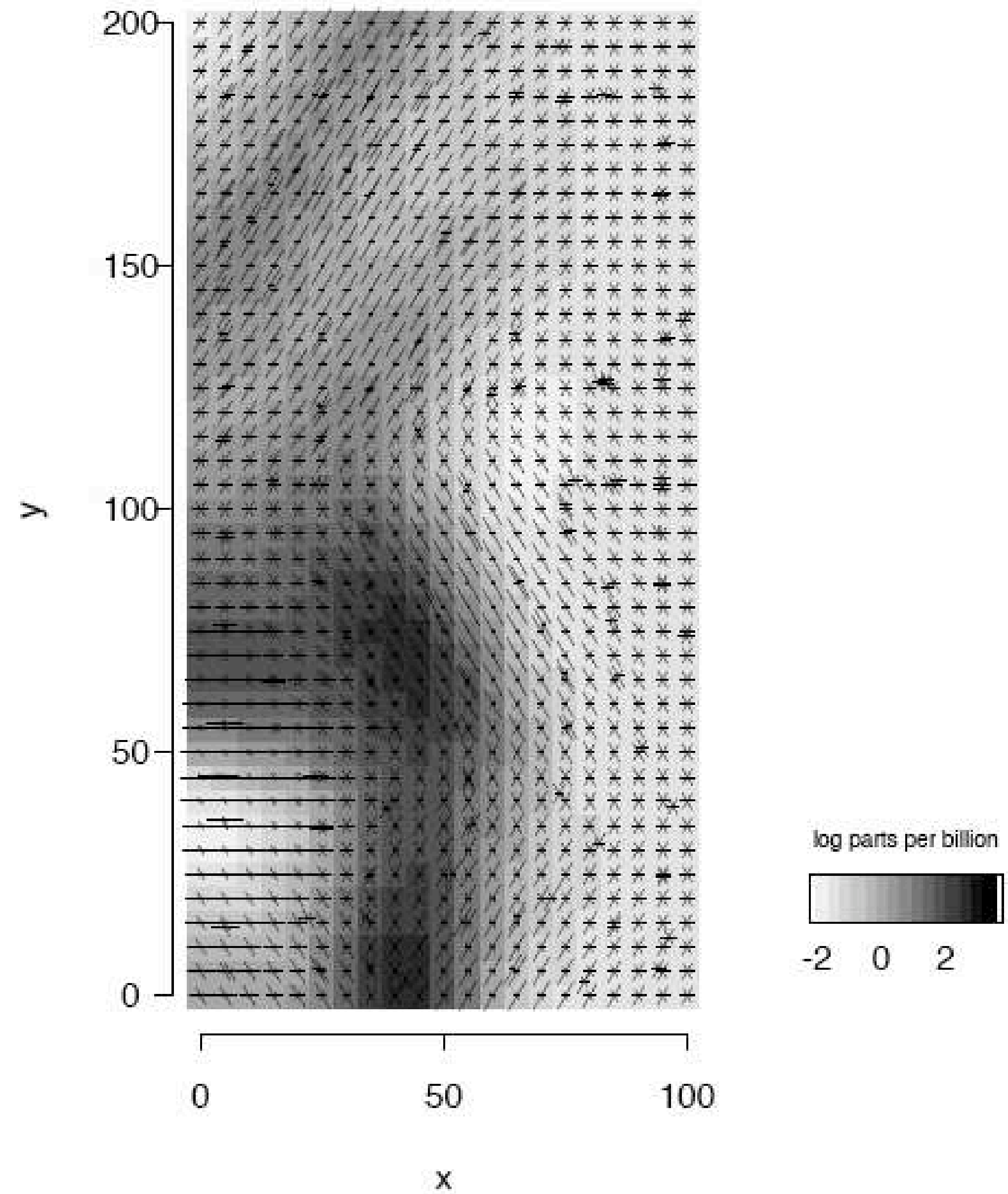
Set

$$w_i(s) = \frac{\exp\{\phi_i(s)\}}{\exp\{\phi_1(s)\} + \exp\{\phi_2(s)\} + \exp\{\phi_3(s)\}}$$

Estimate $\phi_i(s)$'s like any other parameter in the analysis.

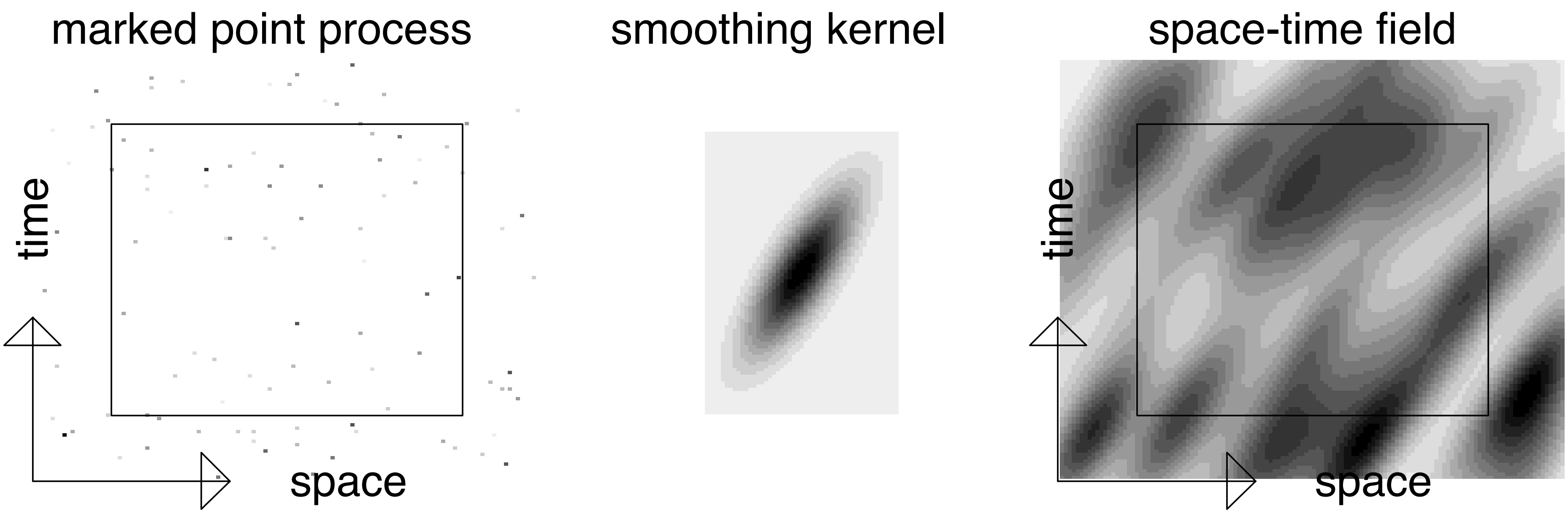
# An application to Piazza Road Superfund site



# MOVING AVERAGE/BASIS SPACE-TIME MODELS

# A convolution-based approach for building space-time models






Define space-time domain $\mathcal{S} \times \mathcal{T}$

Define discrete knot process $x(s,t)$ on $\{(\omega_1, \tau_1), \ldots, (\omega_m, \tau_m)\}$ within $\mathcal{S} \times \mathcal{T}$

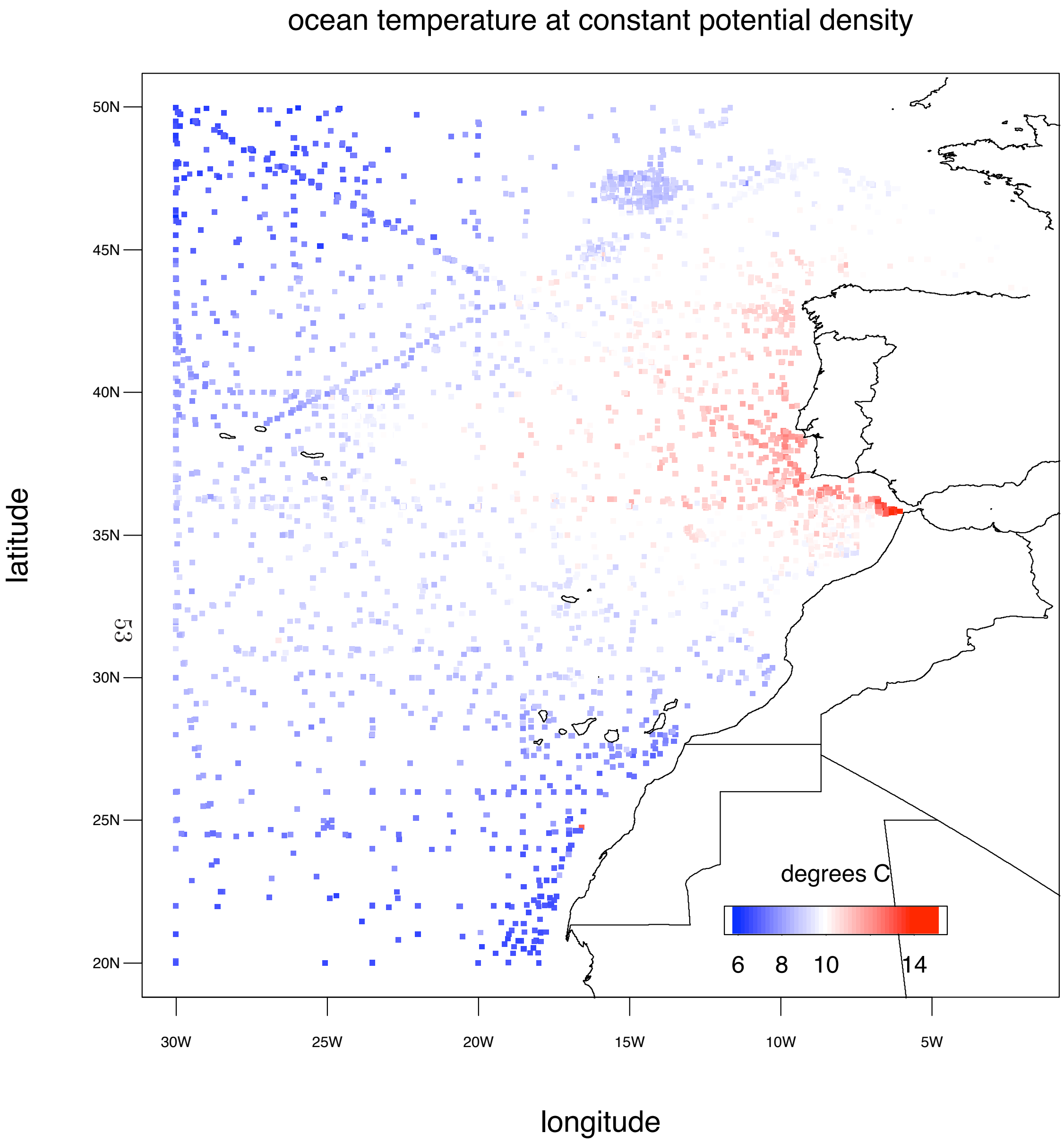
Define smoothing kernel $k(s,t)$

Construct space-time process $z(s,t)$

$$z(s,t) \;=\; \sum_{j=1}^{m} k((s,t) - (\omega_j, \tau_j))x(\omega_j, \tau_j) \quad \text{or with varying kernel}$$

$$z(s,t) \;=\; \sum_{j=1}^{m} k_{st}(\omega_j, \tau_j)x_j$$

# A Space-time model for ocean temperatures




Data:

$$y = (y_1, \ldots, y_n)^T$$

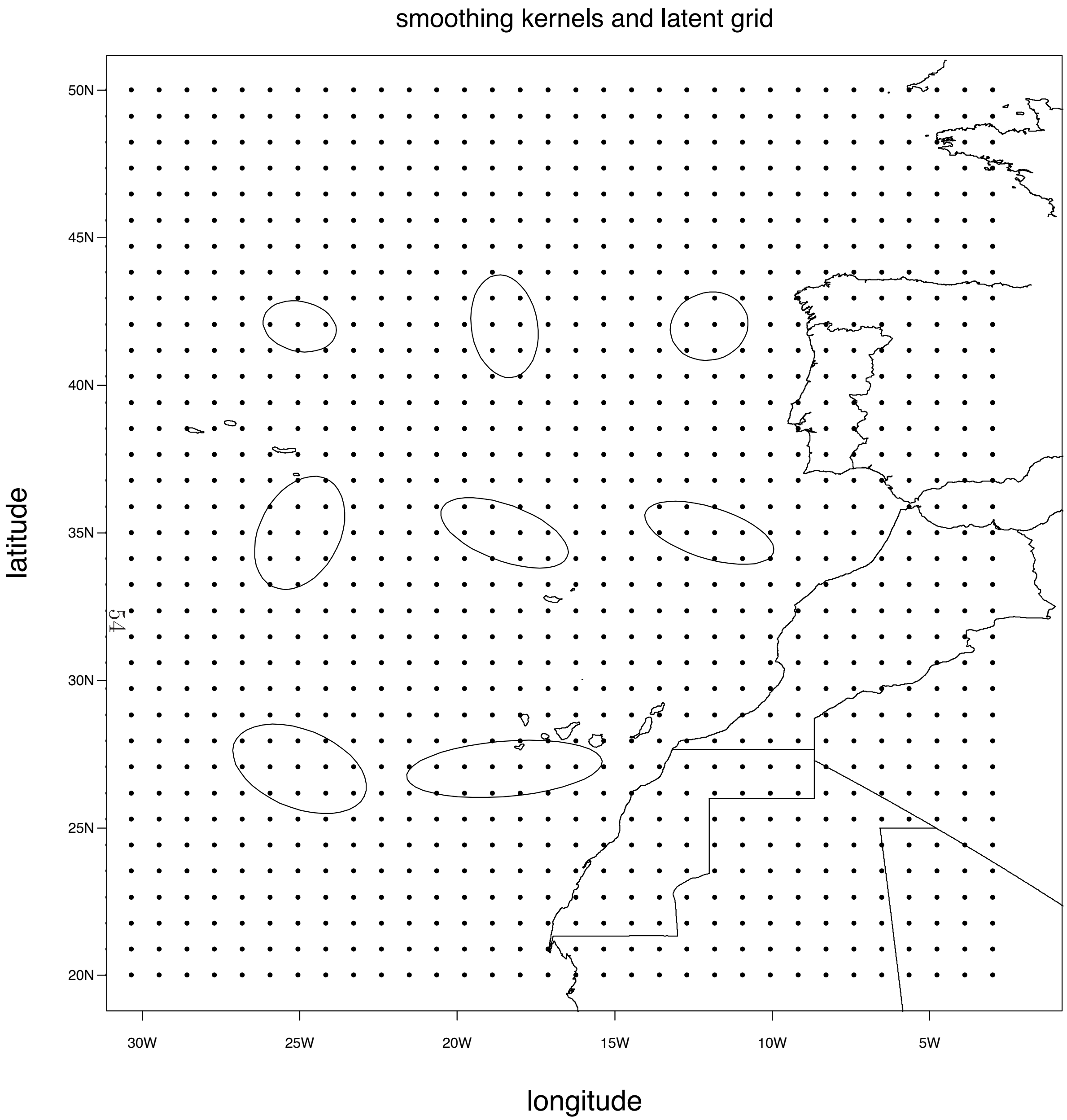
at space-time locations:

$$(s_1, t_1), \ldots, (s_n, t_n)$$

Times: 1910–1988

assume data are centered ($\bar{y} = 0$)

# Knot locations and kernels




$m$ knot locations over a space-time grid

$$(\omega_1, \tau_1), \ldots, (\omega_m, \tau_m)$$

Spatial knot locations shown;

Temporal knot spacing $\sim$ 7 years; 1900-1995;

Kernels vary with spatial location

$$k_{st}(\omega, \tau) = k_s(\omega, \tau)$$

use spatial mixture of normal "basis" kernels.

# Formulation for the ocean example

Likelihood:

$$L(y|x,\lambda_y) \propto \lambda_y^{\frac{n}{2}} \exp\left\{-\frac{1}{2}\lambda_y(y-Kx)^T(y-Kx)\right\}$$

where $K_{ij} = k_{s_i t_i}(\omega_j, \tau_j)x_j$.

Priors:

$$\begin{aligned}
\pi(x|\lambda_x) \;&\propto\; \lambda_x^{\frac{m}{2}} \exp\left\{-\frac{1}{2}\lambda_x x^T x\right\} \\
\pi(\lambda_x) \;&\propto\; \lambda_x^{a_x-1} \exp\{-b_x\lambda_x\} \\
\pi(\lambda_y) \;&\propto\; \lambda_y^{a_y-1} \exp\{-b_y\lambda_y\}
\end{aligned}$$

Posterior:

$$\pi(x,\lambda_x,\lambda_y|y) \;\propto\; \lambda_y^{a_y+\frac{n}{2}-1} \exp\left\{-\lambda_y[b_y + .5(y-Kx)^T(y-Kx)]\right\} \times \lambda_x^{a_x+\frac{m}{2}-1} \exp\left\{-\lambda_x[b_x + .5x^T x]\right\}$$

# Full conditionals for ocean formulation

Full conditionals:

$$\pi(x|\cdots) \propto \exp\{-\frac{1}{2}[\lambda_y x^T K^T K x - 2\lambda_y x^T K^T y + \lambda_x x^T x]\}$$

$$\pi(\lambda_x|\cdots) \propto \lambda_x^{a_x+\frac{m}{2}-1} \exp\left\{-\lambda_x[b_x + .5x^T x]\right\}$$

$$\pi(\lambda_y|\cdots) \propto \lambda_y^{a_y+\frac{n}{2}-1} \exp\left\{-\lambda_y[b_y + .5(y-Kx)^T(y-Kx)]\right\}$$

Gibbs sampler implementation



$$x|\cdots \sim N((\lambda_y K^T K + \lambda_x I_m)^{-1}\lambda_y K^T y, (\lambda_y K^T K + \lambda_x I_m)^{-1})$$

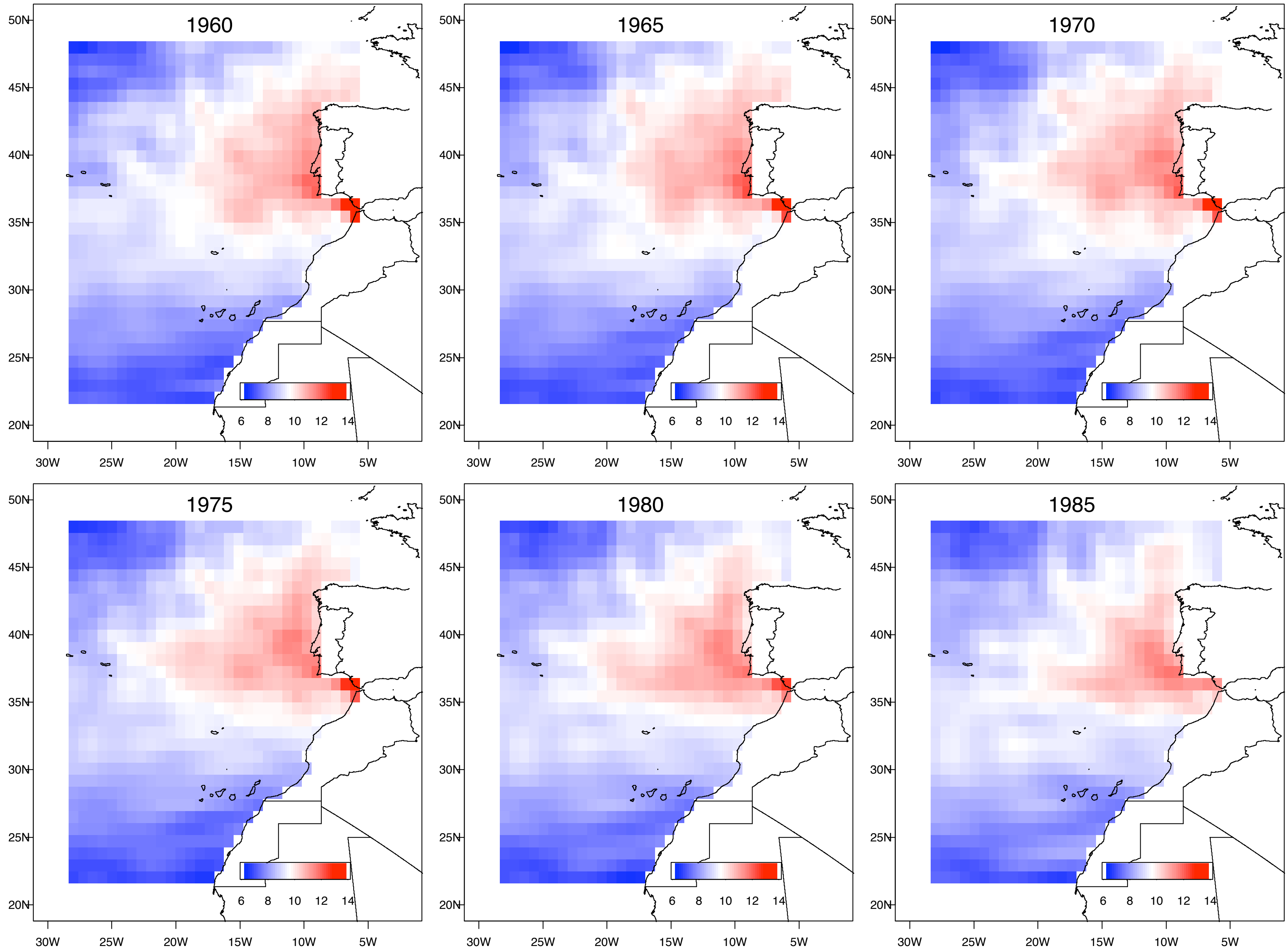
$$x_j|\cdots \sim N\left(\frac{\lambda_y r_j^T k_j}{\lambda_y k_j^T k_j + \lambda_x}, \frac{1}{\lambda_y k_j^T k_j + \lambda_x}\right)$$

$$\lambda_x|\cdots \sim \Gamma(a_x + \frac{m}{2}, b_x + .5x^T x)$$

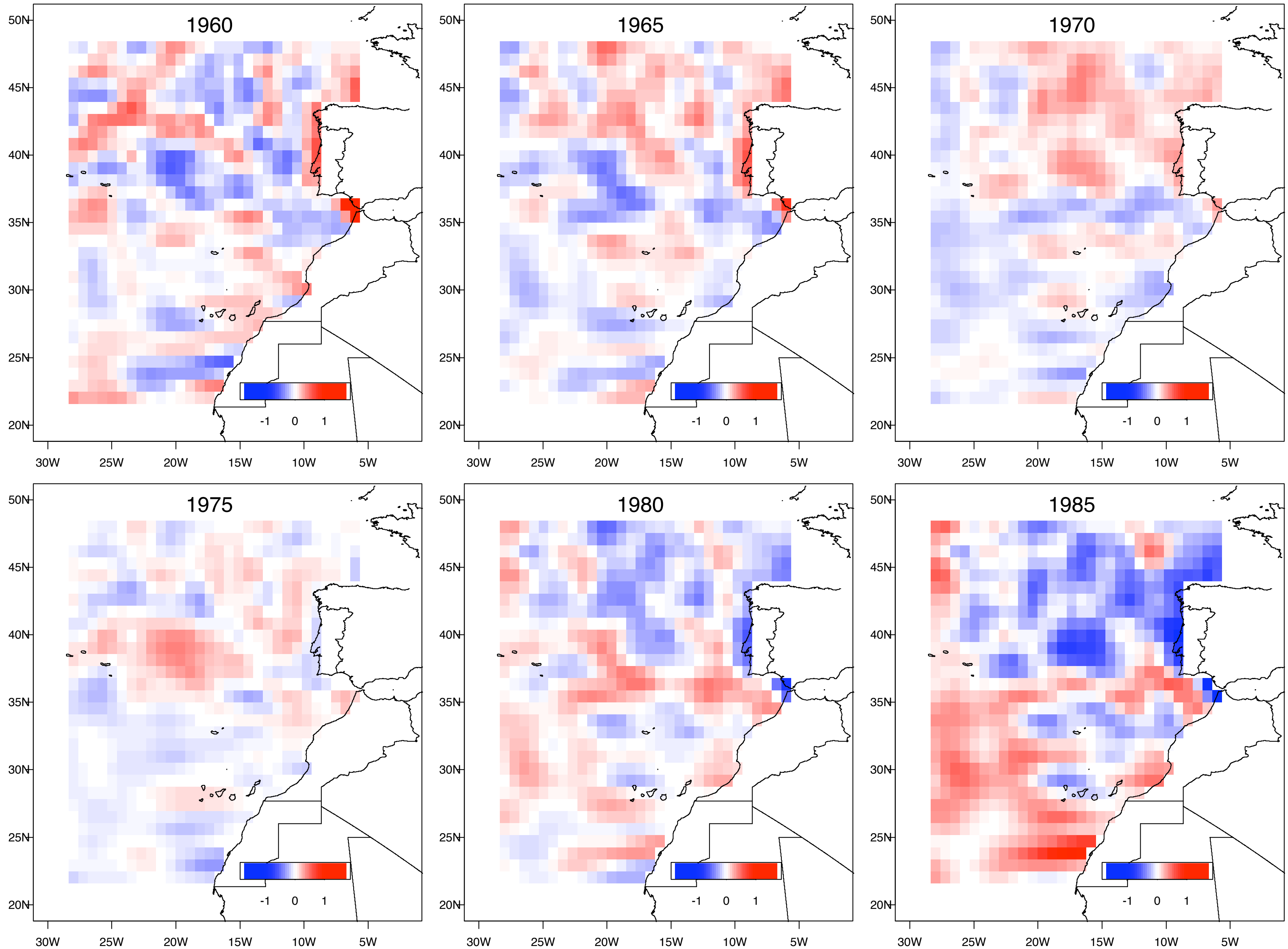
$$\lambda_y|\cdots \sim \Gamma(a_y + \frac{n}{2}, b_y + .5(y-Kx)^T(y-Kx))$$

where $k_j$ is $j$th column of $K$ and $r_j = y - \Sigma_{j' \neq j} k_{j'} x_{j'}$.

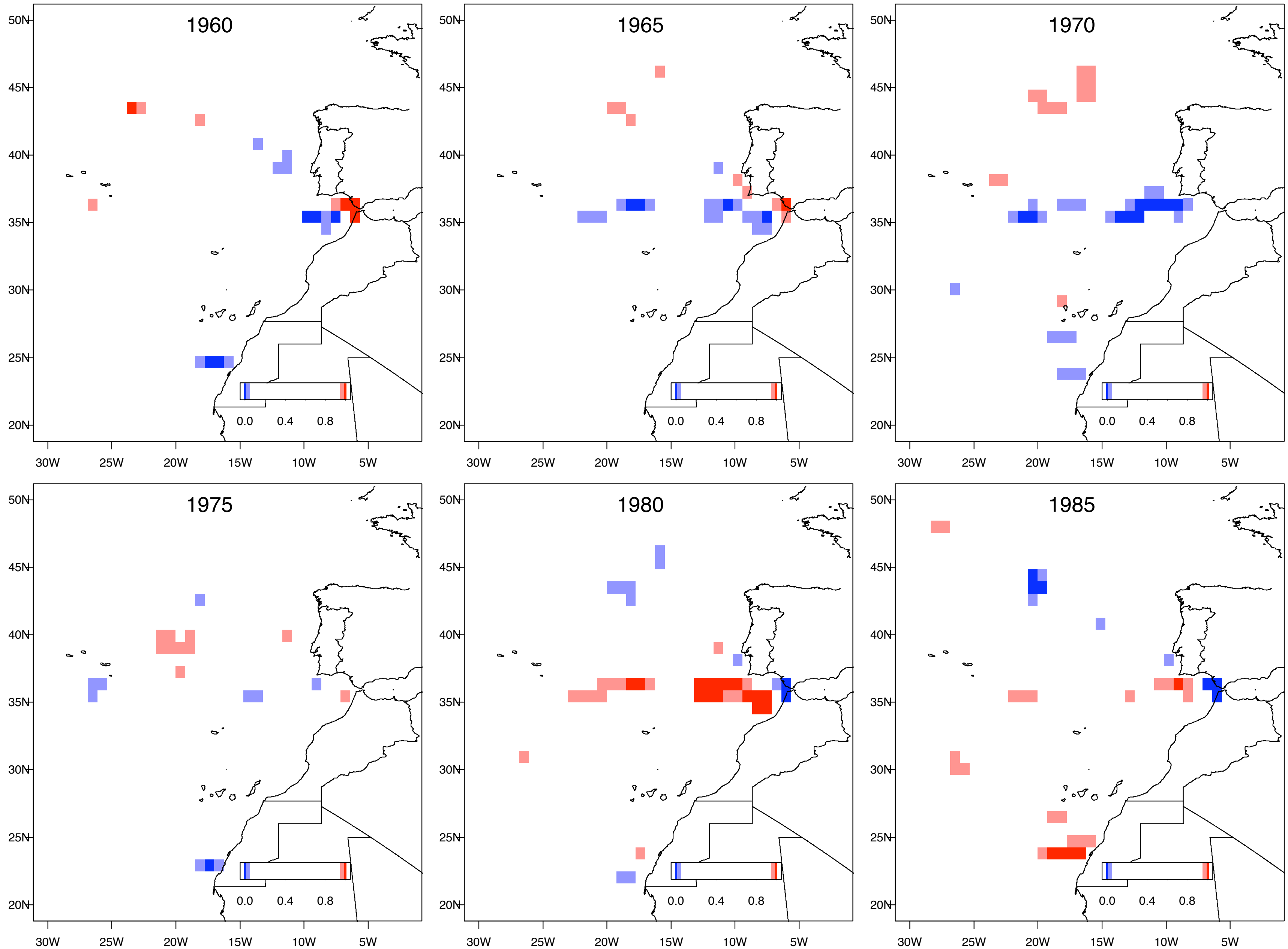
# Posterior mean of the space-time temperature field



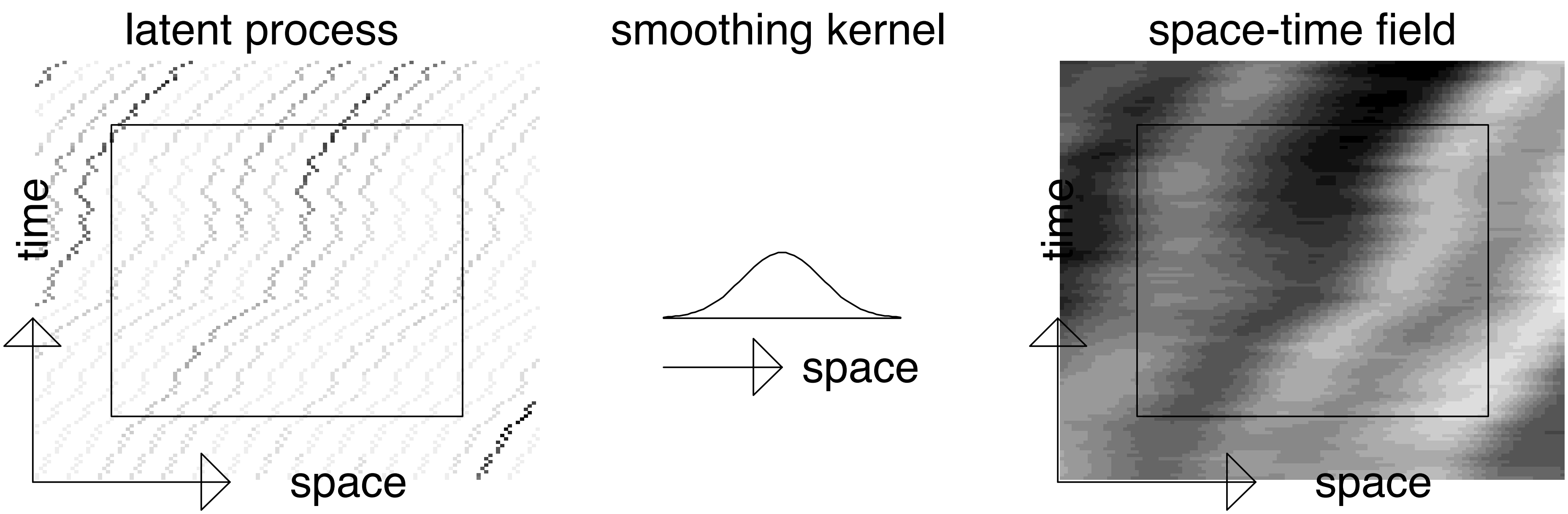
# Deviations from time-averaged mean temperature field



# Posterior probabilities of differing from time-averaged mean field



# Alternative approaches for building space-time models






Define space-time domain $\mathcal{S} \times \mathcal{T}$ with $\mathcal{T} = \{1, \ldots, n_t\}$

Discrete knot process $x(s,t)$ on $\{\omega_1, \ldots, \omega_{n_s}\} \times \{1, \ldots, n_t\}$, $n_t \cdot n_s = m$

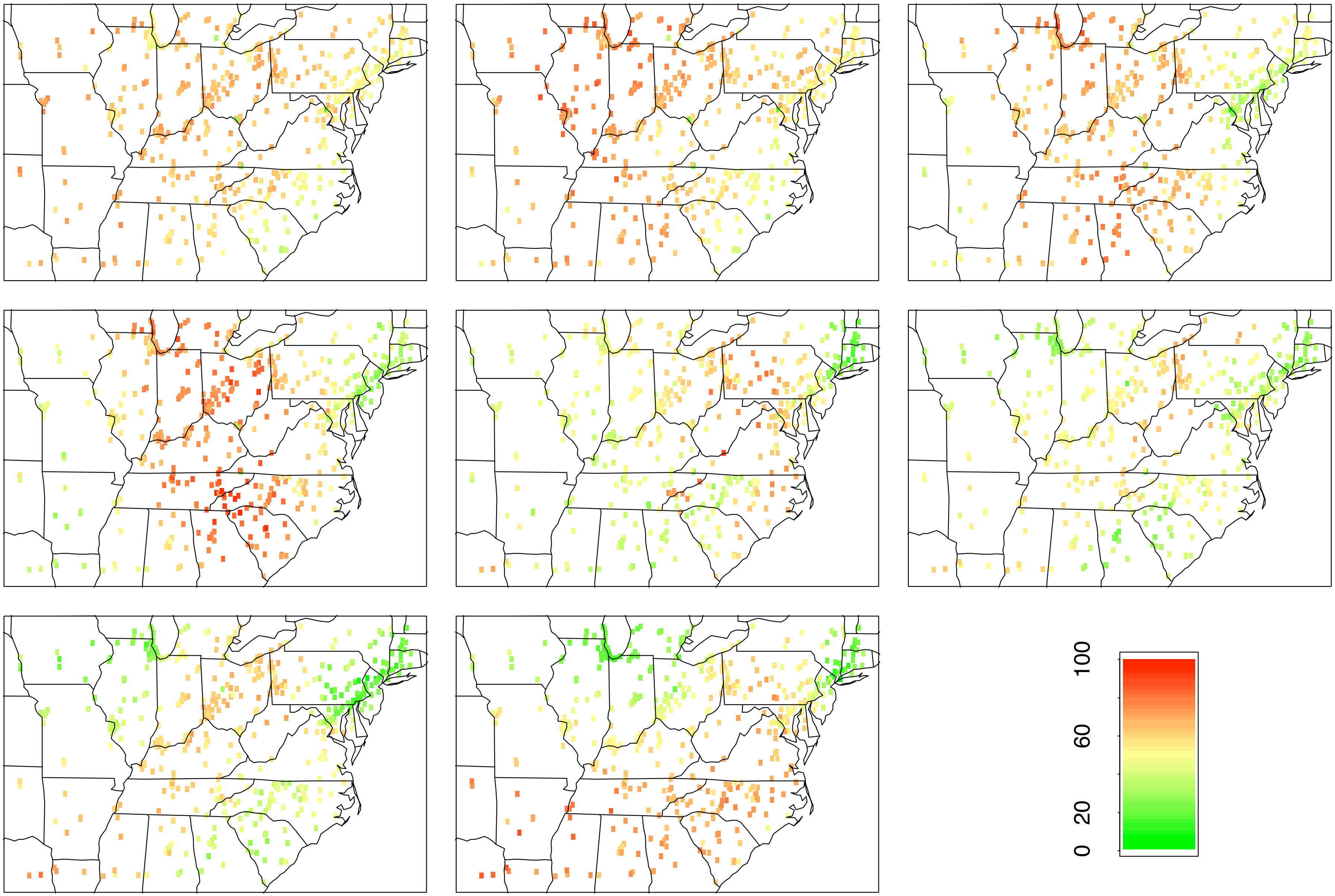
Define spatial smoothing kernel $k(s)$

Construct space-time process $z(s,t)$

$$z(s,t) \;=\; \sum_{j=1}^{n_s} k(s-\omega_j)x(\omega_j,t) \quad \text{or with varying kernel}$$

$$z(s,t) \;=\; \sum_{j=1}^{n_s} k_{st}(\omega_j)x_{jt}$$

# 8 hour max for ozone over summer days in the Eastern US




$n = 510$ ozone measurements each of 30 days

$\omega_k$'s laid out on same hexagonal lattice

# Temporally evolving latent $x(s,t)$ process

Times: $t \in \mathcal{T} = \{1, \ldots, n_t\}$, $n_t = 30$

spatial knot locations: $\mathcal{W} = \{\omega_1, \ldots, \omega_{n_s}\}$, $n_s = 27$

$x(s,t)$ defined on $\mathcal{W} \times \mathcal{T}$

Space-time process $z(s,t)$ obtained by convolving $x(s,t)$ with $k(s)$:

$$\begin{aligned} z(s,t) &= \sum_{j=1}^{n_s} k(\omega_j - s) x(\omega_j, t) \\ &= \sum_{j=1}^{n_s} k_s(\omega_j) x_{jt} \end{aligned}$$

Specify locally linear MRF priors for each $x_j = (x_{j1}, \ldots, x_{jn_t})^T$

$$\pi(x_j|\lambda_x) \propto \lambda^{\frac{n_t}{2}} \exp\left\{-\frac{1}{2}\lambda_x x_j^T W x_j\right\}$$

where

$$W_{ij} = \begin{cases} -1 & \text{if } |i-j| = 1 \\ 1 & \text{if } i = j = 1 \text{ or } i = j = n_t \\ 2 & \text{if } 1 < i = j < n_t \\ 0 & \text{otherwise} \end{cases}$$

So for $x = (x_{11}, x_{21} \ldots, x_{n_s 1}, x_{12}, \ldots, x_{n_s 2}, \ldots, x_{1n_t}, \ldots, x_{n_s n_t})^T$

$$\pi(x|\lambda_x) \propto \lambda^{\frac{n_t n_s}{2}} \exp\left\{-\frac{1}{2}\lambda_x x^T (W \otimes I_{n_s}) x\right\}$$

# Formulation for temporally evolving $z(s,t)$

Data: at each time $t$, observe $n$-vector $y_t = (y_{1t}, \ldots, y_{nt})^T$ at sites $s_1, \ldots, s_n$.

Likelihood for data observed at time $t$:

$$L(y_t|x_t, \lambda_y) \propto \lambda_y^{\frac{n}{2}} \exp\left\{-\frac{1}{2}\lambda_y (y_t - K^t x_t)^T (y - K^t x_t)\right\}$$

where $K^t_{ij} = k(\omega_j - s_i)$

Define $n \cdot n_t$-vector $y = (y_1^T, \ldots, y_{n_t}^T)^T$

Likelihood for entire data $y$:

$$L(y|x, \lambda_y) \propto \lambda_y^{\frac{nn_t}{2}} \exp\left\{-\frac{1}{2}\lambda_y (y - Kx)^T (y - Kx)\right\}$$

where $K = \text{diag}(K^1, \ldots, K^{n_t})$.

Priors:

$$\pi(x|\lambda_x) \;\propto\; \lambda_x^{\frac{m}{2}} \exp\left\{-\frac{1}{2}\lambda_x x^T W x\right\}$$

$$\pi(\lambda_x) \;\propto\; \lambda_x^{a_x - 1} \exp\{-b_x \lambda_x\}$$

$$\pi(\lambda_y) \;\propto\; \lambda_y^{a_y - 1} \exp\{-b_y \lambda_y\}$$

# Posterior and full conditionals

$$\pi(x, \lambda_x, \lambda_y | y) \propto \lambda_y^{a_y + \frac{nn_t}{2} - 1} \exp\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\} \times$$
$$\lambda_x^{a_x + \frac{n_S n_t}{2} - 1} \exp\{-\lambda_x [b_x + .5 x^T W x]\}$$

Full conditionals:

$$\pi(x | \cdots) \propto \exp\{-\frac{1}{2}[\lambda_y x^T K^T K x - 2\lambda_y x^T K^T y + \lambda_x x^T W x]\}$$
$$\pi(\lambda_x | \cdots) \propto \lambda_x^{a_x + \frac{m}{2} - 1} \exp\{-\lambda_x [b_x + .5 x^T W x]\}$$
$$\pi(\lambda_y | \cdots) \propto \lambda_y^{a_y + \frac{n}{2} - 1} \exp\{-\lambda_y [b_y + .5(y - Kx)^T (y - Kx)]\}$$

Gibbs sampler implementation



$$x | \cdots \sim N((\lambda_y K^T K + \lambda_x W)^{-1} \lambda_y K^T y, (\lambda_y K^T K + \lambda_x W)^{-1})$$
$$x_{jt} | \cdots \sim N\left(\frac{\lambda_y r_{tj}^T k_{tj} + n_j \bar{x}_{\partial j}}{\lambda_y k_{tj}^T k_{tj} + n_j \lambda_x}, \frac{1}{\lambda_y k_j^T k_j + n_j \lambda_x}\right)$$
$$\lambda_x | \cdots \sim \Gamma(a_x + \frac{m}{2}, b_x + .5 x^T x)$$
$$\lambda_y | \cdots \sim \Gamma(a_y + \frac{n}{2}, b_y + .5(y - Kx)^T (y - Kx))$$

where $k_{tj}$ is $j$th column of $K^t$, $r_{tj} = y_t - \Sigma_{j' \neq j} k_{tj'} x_{tj'}$, $n_j =$ number of neighbors of $x_{jt}$, and $x_{\partial jt} =$mean of neighbors of $x_{jt}$

# DLM setup for ozone example

Given latent process $x_t = (x_{1,t}, \ldots, x_{27,t})^T$, $t = 1, \ldots, 30$

$y_t = (y_{1t}, \ldots, y_{n_y t})^T$ at sites $s_{1t}, \ldots, s_{n_y t}$

$$
\begin{aligned}
y_t &= K^t x_t + \epsilon_t \\
x_t &= x_{t-1} + \nu_t
\end{aligned}
$$

where $K^t$ is the $n_y \times 27$ matrix given by:

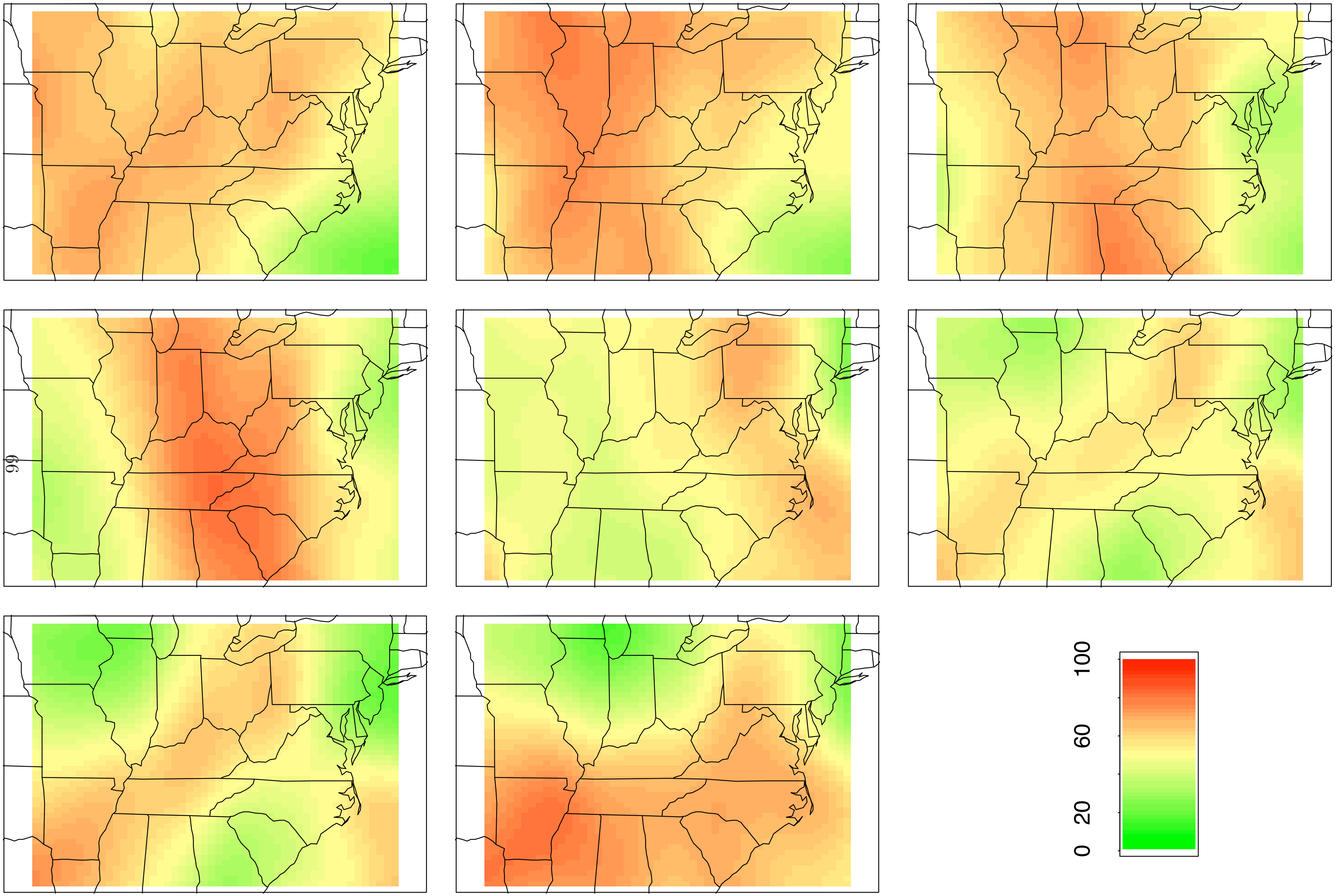
$$
\begin{aligned}
K^t_{ij} &= k(s_{it} - \omega_j),\ t = 1, \ldots, 30, \\
\epsilon_t &\overset{\text{i.i.d.}}{\sim} N(0, \sigma^2_\epsilon),\ t = 1, \ldots, 30, \\
\nu_t &\overset{\text{i.i.d.}}{\sim} N(0, \sigma^2_\nu),\ t = 1, \ldots, 30,\ \text{and} \\
x_1 &\sim N(0, \sigma^2_x I_{27}).
\end{aligned}
$$

can use dynamic linear model (DLM)/Kalman filter machinery

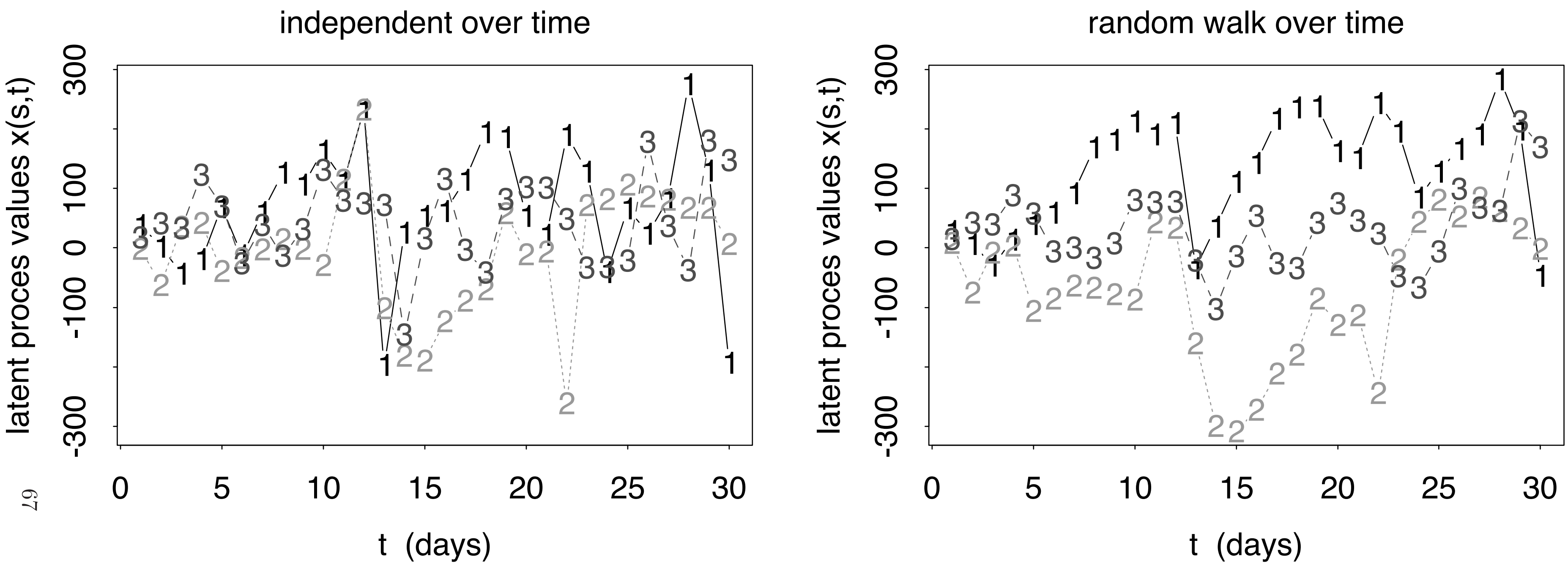
single site MCMC works too

See Stroud et.al. (1999) for alternative model.

# Posterior mean for first 9 days



# Posterior mean of selected $x_j$'s



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