Modelling of Spatio-Temporal Processes

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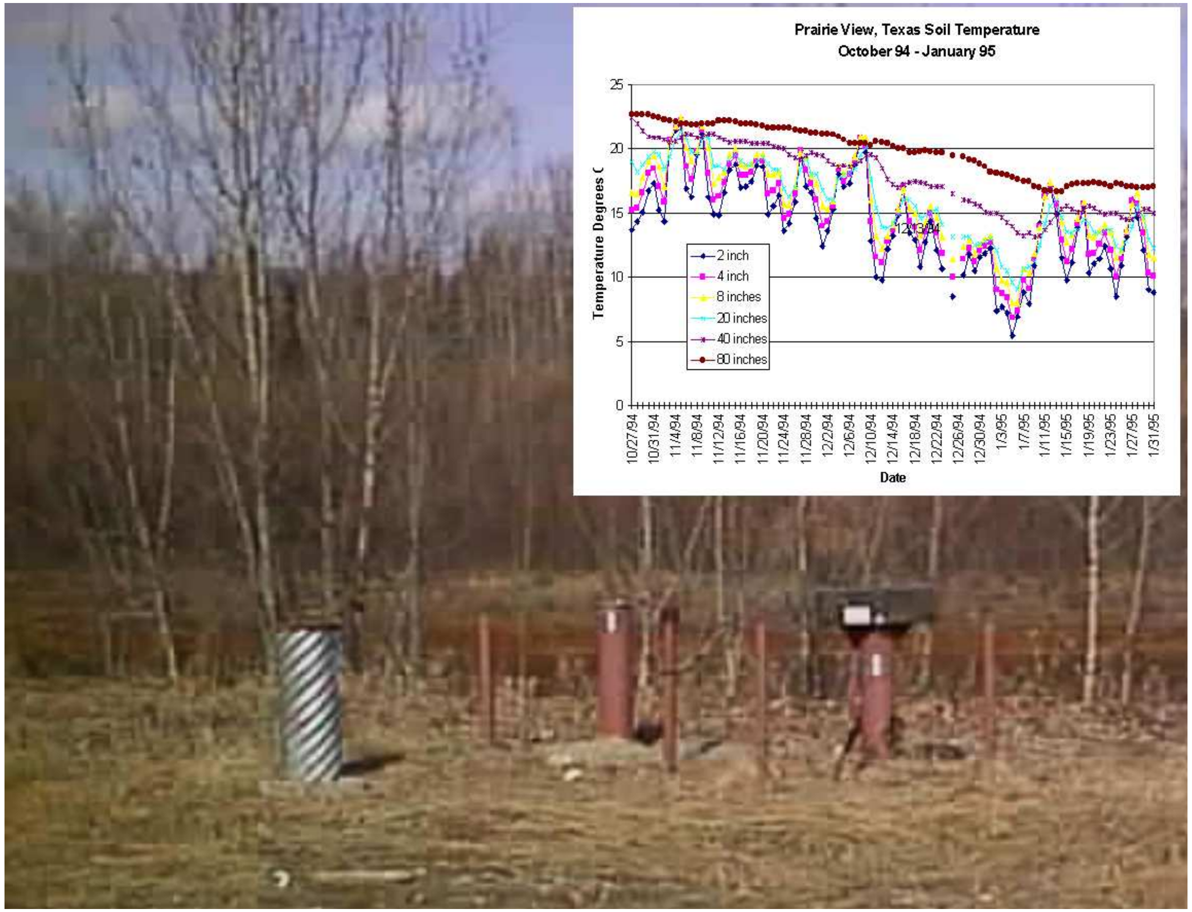
Collection of soil physical data



Ref: `http://www.wcc.nrcs.usda.gov/publications/Briefing-Book/bb21.html`
`http://www.uaf.edu/water/projects/ftww/gwdata/gwdatasm.html`

- real-valued data
- case dependent space-time modelling

Multivariate time series approach

Example: water fluxes in drain pipes

- longer times series at a small number of locations
- prediction sufficient for the given locations

Approches: (i) space-time Kalman filtering (Wikle and Cressie, 1999)

$$Y(x,t) = \int w_x(y) Y(y, t-1)\,\mathrm{d}y + \eta(x,t)$$

- $\left|\int w_x(y)\,\mathrm{d}y\right| < 1$
- $\eta(x,t)$ spatially dependent error process, independent in time
- approximation of w_x by a weighted some of orthogonal functions
- weights are estimated and used for prediction

(ii) STARMAX (Stoffer, 1986)

$$z_t = \sum_{j=1}^{q} D_j \Lambda_j z_{t-j} + \sum_{l=0}^{k} \theta_l y_{t-l} + \eta_t$$

$z_t = (z_t(x_1), \ldots, z_t(x_n))$: data at time t at location $x_1, \ldots, x_n$

D_j : inverse "distance" matrix, e.g. covariance

Λ_j : regression parameter, diagonal matrix

y_t : covariates: linear, zero-mean process, $y_t = \sum_{j=0}^{\infty} A_j \varepsilon_{t-j}$

ε_t, η_t, $t \in \mathbb{Z}$: independent variables

Parameter estimation by Yule-Waker-type equation;
prediction only for the given temporal grid and the given locations

Multivariate random field approach

Example: change of soil properties after treatment (ploughing, harrowing)

- modelling of spatial variability at a few instances
- only spatial prediction required at the given instances

Approach: Papritz and Flühler (1994)

- temporal data at given location modelled as multivariate vector
- temporal stationarity not required

Spatial parameter field approach

Example: Extreme metereological events

Approach: (Casson and Coles, 1999)

- spatial random fields provides parameters of time series
- example: extreme value field where the parameters of the marginal distribution at each site are given by stationary Gaussian random field

Geostatistical approach

Examples: soil temperature, soil moisture

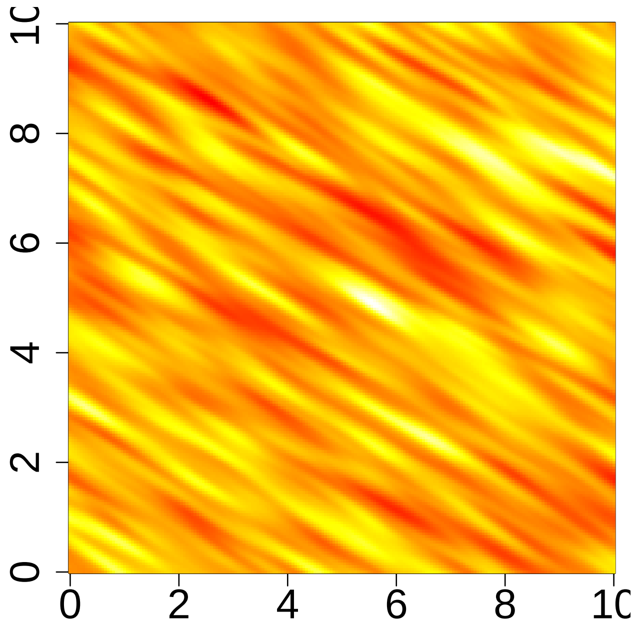
- modelling of the spatial and the temporal variability

Random field Z:
$Z(x)$ real valued random quantity for all $x \in \mathbb{R}^d$
(based on the same probability space)

Gaussian Random field Z in $\mathbb{R}^d$:
Z is called Gaussian if the distribution of $(Z(x_1), \ldots Z(x_n))$ is multivariate Gaussian for all $x_1, \ldots, x_n \in \mathbb{R}^d$ and $n \in \mathbb{N}$.

Stationary random fields

$\mathbb{E}\, Z(x)$ and $\mathrm{Cov}(Z(h+x), Z(x))$ independent of x for all $h \in \mathbb{R}^d$



stationary Gaussian random field completely characterised by

- the expectation $\mathbb{E}\, Z(0)$ and
- $C(h) = \mathrm{Cov}(Z(h+x), Z(x))$

Covariance function

Covariance function of a stationary random field

$$C(x) = \mathrm{Cov}(Z(x), Z(0)), \qquad x \in \mathbb{R}^d$$

A symmetric function C is called positive definite if

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i C(x_i - x_j) a_j \geq 0$$

for all $a_i \in \mathbb{R}$, $x_i \in \mathbb{R}^d$, $n \in \mathbb{N}$

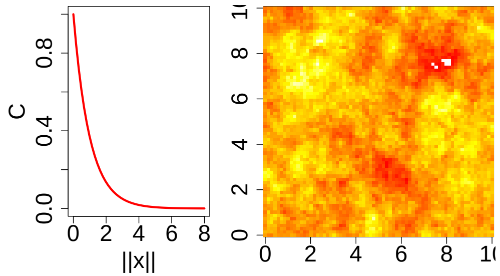
A function $C : \mathbb{R}^d \to \mathbb{R}$ is a covariance function if and only if C is positive definite.

Whittle-Matern class

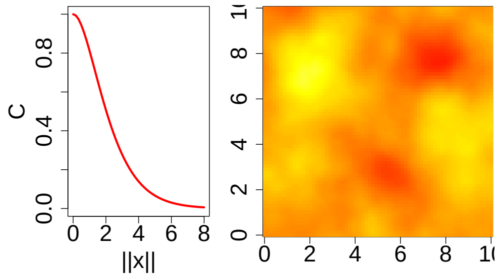
$$W_\nu(x) = \frac{2^{1-\nu}}{\Gamma(\nu)} \|x\|^\nu K_\nu(\|x\|)$$

$\nu > 0$

K_ν : modified Bessel function



$\nu = 0.5$

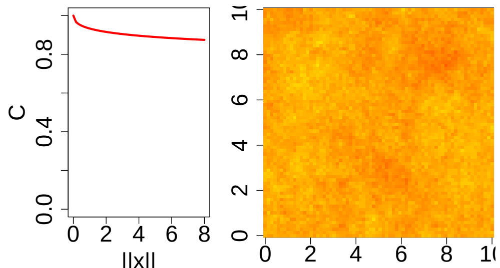


$\nu = 2$

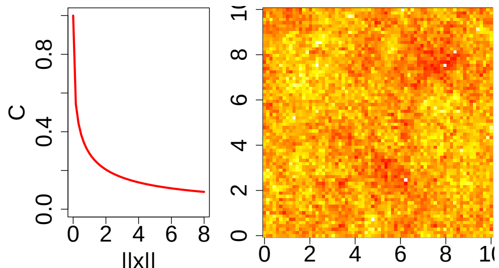
Generalised Cauchy class

$$C(x) = (1 + \|x\|^a)^{-b/a}$$

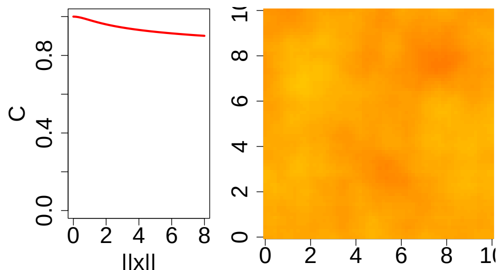
$a \in (0, 2], \quad b > 0$



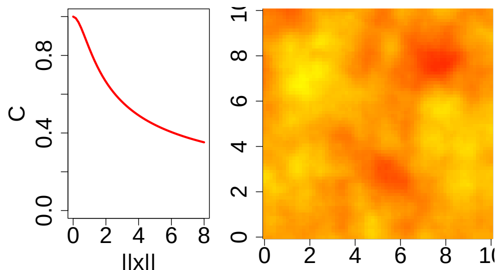
$a = 0.5$, $b = 0.05$



$a = 0.5$, $b = 0.9$



$a = 1.9$, $b = 0.05$

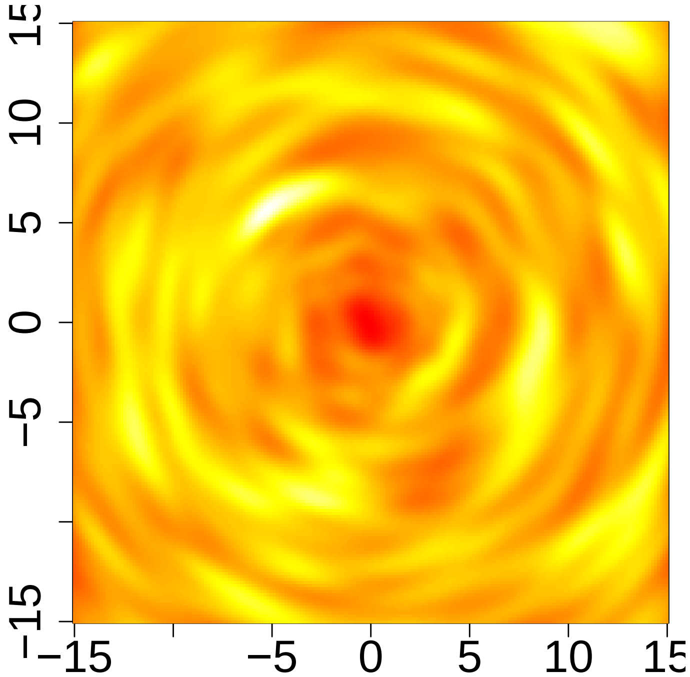


$a = 1.9$, $b = 0.9$

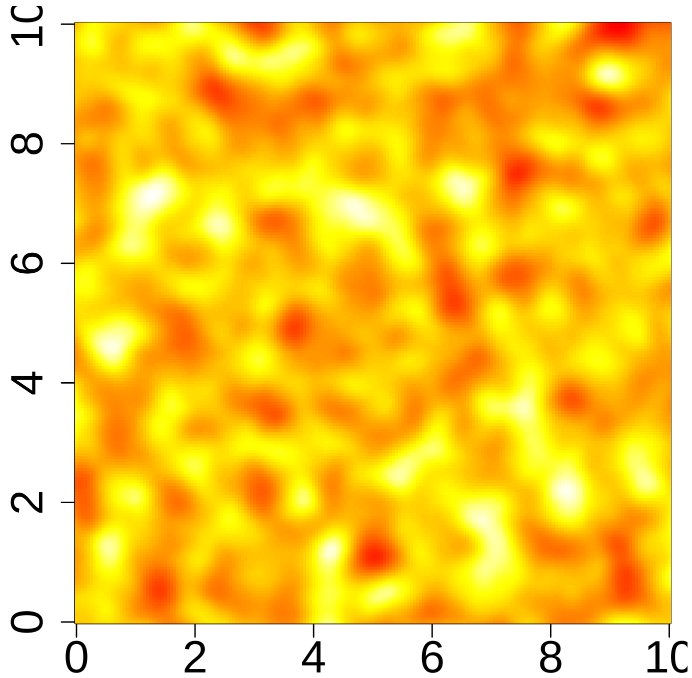
Isotropy

$$\mathrm{Cov}(Z(Ax), Z(Ay)) \;=\; \mathrm{Cov}(Z(x), Z(y))$$

for all $x, y \in \mathbb{R}^d$ and all rotation matrices A



Stationary and isotropic random field



Covariance function C is rotationinvariant, i.e.

$$C(x) = \varphi(\|x\|)$$

for some function $\varphi : [0, \infty) \to \mathbb{R}$.

Characterisation of covariance functions

C : continuous covariance function. Then (Bochner, 1932, 1933, 1955)

$$C(x) = \int \exp(ix^\top w_x)\,\mathrm{d}F(w_x), \qquad x \in \mathbb{R}^d$$

for some finite measure F on $\mathbb{R}^d$.

If C is integrable then

$$\frac{\mathrm{d}F}{\mathrm{d}w_x} = f(w_x) = \frac{1}{(2\pi)^d}\int \exp(-ix^\top w_x)C(x)\,\mathrm{d}x, \qquad w_x \in \mathbb{R}^d$$

C : measurable rotationinvariant covariance function in $\mathbb{R}^d$, $d > 2$. Then (Gneiting and Sasvári, 1999)

$$C(x) = c1_{\{0\}}(x) + C_c(x)$$

for some $c \geq 0$ and a continuous covariance function C_c.

Separable models

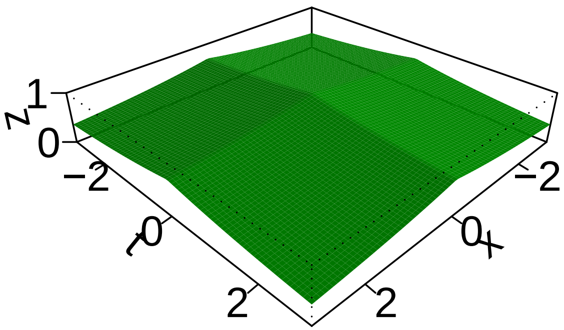
(i) $$C(x,t) = C_x(x) + C_t(t)$$

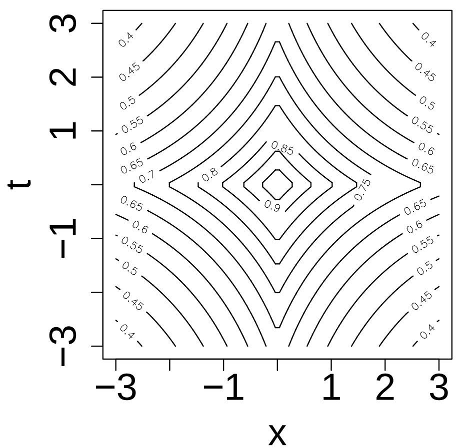
Construction:

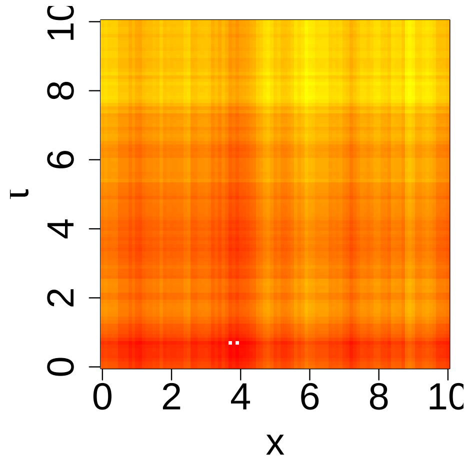
$Z_x(x)$ and $Z_t(t)$ independent random fields

let $Z(x,t) = Z_x(x) + Z_t(t)$

Example: $$C(x,t) = \frac{1}{2}\left[\exp(-\|x\|/3) + \exp(-|t|/3)\right]$$







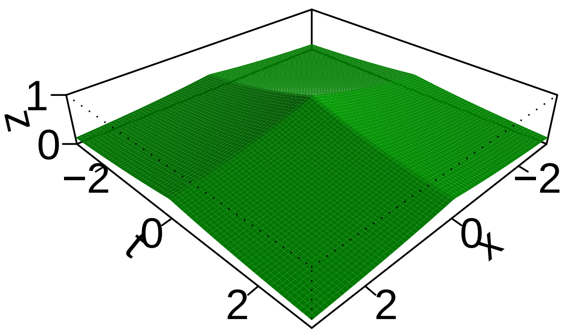
(ii) $$C(x,t) = C_x(x)C_t(t)$$

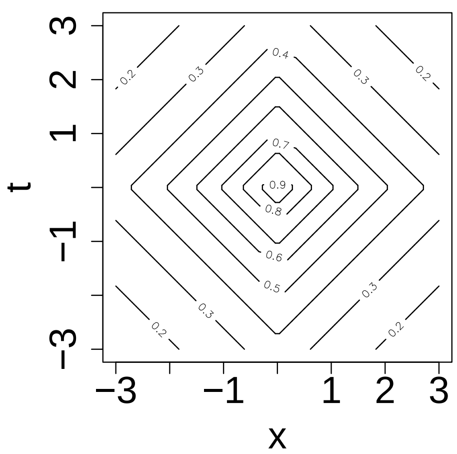
Construction:

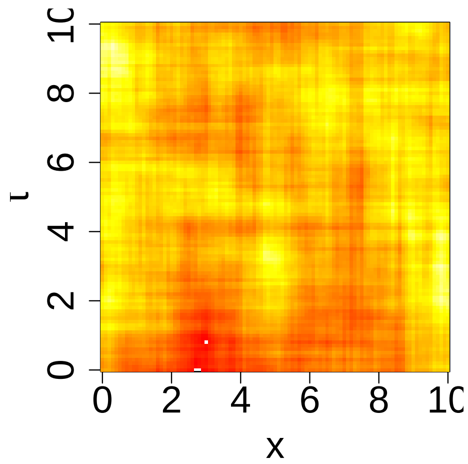
$Z_x(x)/$ and $Z_t(t)$ independent random fields

let $Z(x,t) = Z_x(x)Z_t(t)$

Example: $$C(x,t) = \exp(-\|x\| - |t|)$$



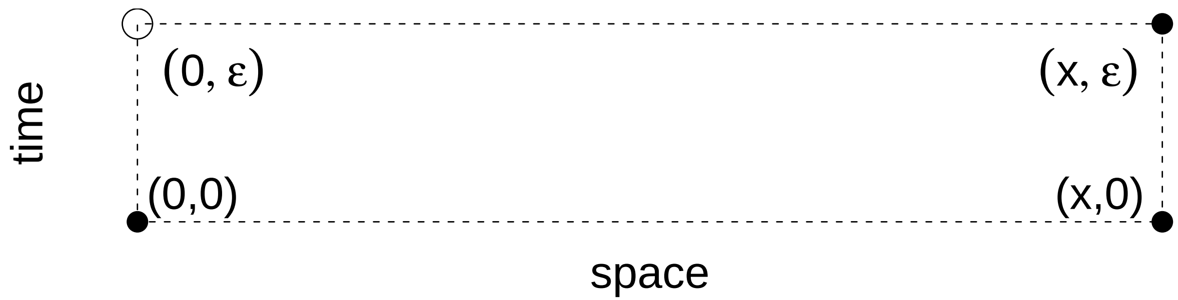




All other models are called non-separable.

Problems with separable models

- lack of interaction of time and space, no guideline how to separate the two component structures (Kyriakidis and Journel, 1999)
- singular kriging systems (Rouhani and Myers, 1990)
- Let $C(x,t) = C(x) + C_0(x)|t|^\alpha + o(|t|^\alpha)$.



The variance of ordinary kriging predictor for $Z(\varepsilon, 0)$ is (Stein, 2005)

$$2C_0(0)\varepsilon^\alpha + o(\varepsilon^\alpha), \quad \text{given } Z(0,0)$$

$$2\left(C_0(0) - \frac{C_0^2(x)}{C_0(0)}\right)\varepsilon^\alpha + o(\varepsilon^\alpha), \quad \text{given } Z(0,0), Z(0,x), Z(\varepsilon,x)$$

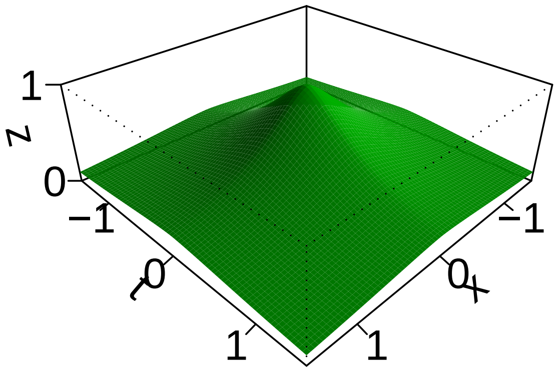
Product-sum models

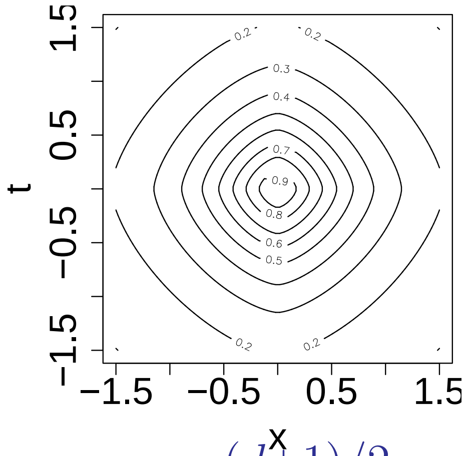
Idea:

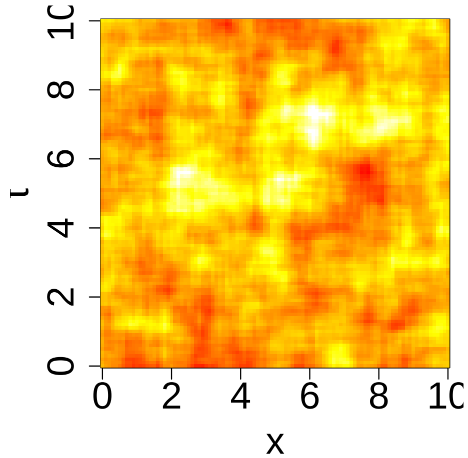
$$C(x,t) = \lim_{n\to\infty} \sum_{i=1}^{n} C_{x,i}(x) C_{t,i}(t), \qquad n \geq 2$$

Example (de Iaco et al., 2002; de Cesare et al., 2002)

$$C(x,t) \;=\; \int_0^\infty C_x(\xi x) C_t(\xi t)\,\mathrm{d}F(\xi)$$







$$C(x,t) = \left(1 + \|x\|^\alpha + |t|^\delta\right)^{-(d+1)/2}, \qquad 1 \leq \alpha, \delta \leq 2$$

Isotropic Models

Kyriakidis and Journel (1999)

Isotropy is well defined in space, while it has no meaning in a space-time context due to the intrinsic ordering and nonreversibility of time. Scales and distance units are different between space and time and cannot be directly compared in a physical sense.

Anisotropic Models

Let $\varphi(\|\cdot\|)$ be a model valid in $\mathbb{R}^4$ and

$$M : (x,t) \mapsto \begin{pmatrix} A & -v \\ a & \tau \end{pmatrix} \begin{pmatrix} x \\ t \end{pmatrix}$$

Then a valid space-time model is

$$C(x,t) = \varphi(\|M(x,t)^\top\|)$$

Examples in rainfall modelling

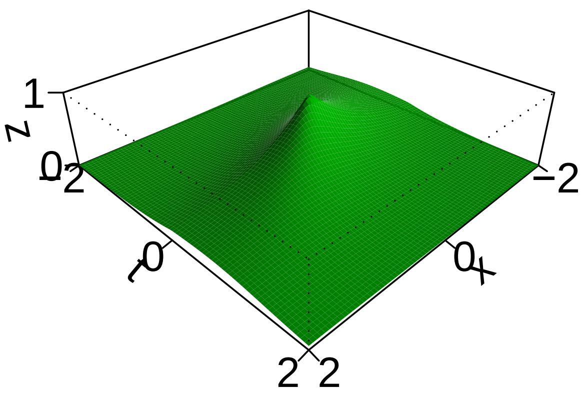
- Armstrong et al. (1993)
  $a = v = 0$, $C(x,t) = \varphi(\|(Ax, \tau t)\|)$
- frozen model (Gupta and Waymire, 1987)
  $A = \mathrm{id}$, $a = \tau = 0$, $C(x,t) = \varphi(\|x - vt\|)$
- Cox and Isham (1988)
  $A = \mathrm{id}$, $a = \tau = 0$, $v = RV$, R and V random variables

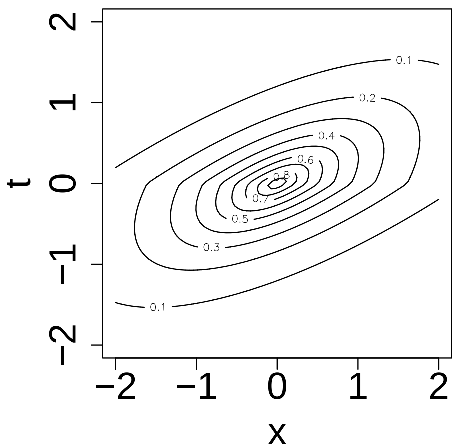
Example Cox-Isham-Model

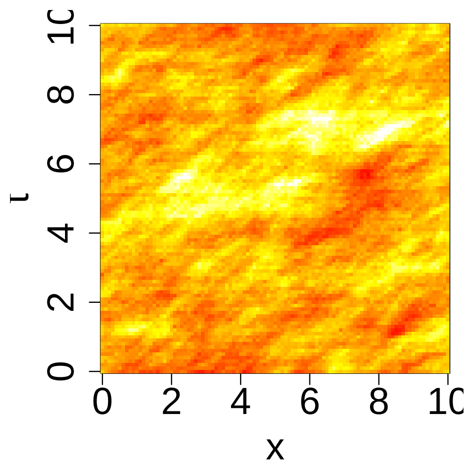
$$C(x,t) = e^{-a|t|}\varphi(\|x - vt\|), \qquad a > 0$$

For instance, in $\mathbb{R}^2$,

$$C(x,t) = e^{-|t|/2}e^{-\|x-(1,1)t\|}$$







Non-Separable Models

C is called fully symmetric (Gneiting, 2002) if

$$C(x,t) = C(x,-t) \quad (= C(-x,t) = C(-x,-t)), \quad (x,t) \in \mathbb{R}^d \times \mathbb{R}$$

C is fully symmetric if and only if

$$C(x,t) = \iint \cos(x^\top w_x)\cos(tw_t)\,\mathrm{d}F(x,t), \qquad x \in \mathbb{R}^d, t \in \mathbb{R}$$

Examples

- product-sum models
- anisotropic model with $M : (x,t) \mapsto \begin{pmatrix} A & -v \\ a & \tau \end{pmatrix}\begin{pmatrix} x \\ t \end{pmatrix}$ if and only if $a = 0$ and $v = 0$

Fully symmetric models based on completely monotone functions

Fully symmetric model (Gneiting, 2002)

- Fourier-free implementation of Cressie and Huang's 1999 approach

$$C(x,t) = \frac{\sigma^2}{\psi(|t|^2)^{d/2}}\, \varphi\left(\frac{\|x\|^2}{\psi(|t|^2)}\right), \qquad (x,t) \in \mathbb{R}^d \times \mathbb{R},$$

$\varphi(t) : [0,\infty) \longrightarrow \mathbb{R}$ completely monotone, i.e.,

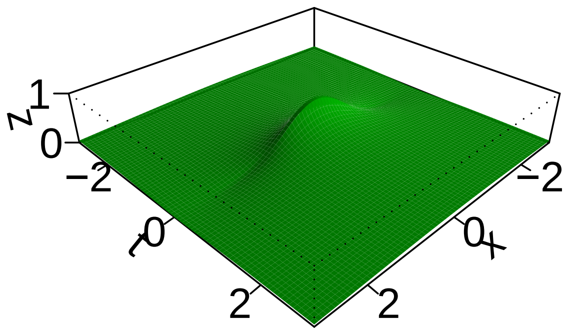
$$(-1)^n \varphi^{(n)}(t) \geq 0, \qquad n \in \mathbb{N}$$

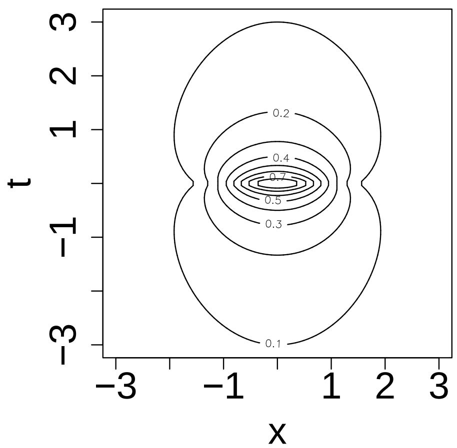
$\psi(t) : [0,\infty) \longrightarrow \mathbb{R}$ positive, completely monotone derivative

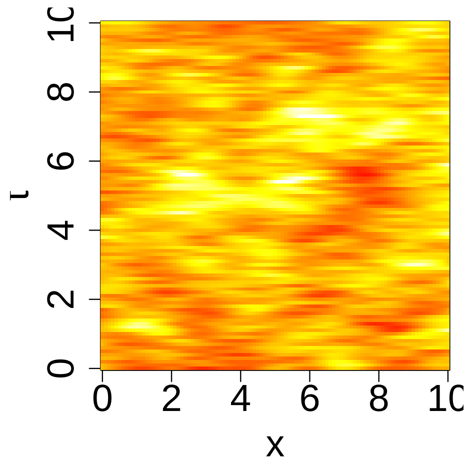
Examples

Function	Parameters
$\varphi(u) = \exp(-cu^\gamma)$	$c > 0, \quad \gamma \in (0,1]$
$\varphi(u) = (1 + cu^\gamma)^{-\nu}$	$c > 0, \quad \gamma \in (0,1], \quad \nu > 0$
$\varphi(u) = W_\nu(c\sqrt{u})$	$c > 0, \quad \nu > 0$
$\psi(u) = (au^\alpha + 1)^\beta$	$a > 0, \quad \alpha \in (0,1], \quad \beta \in (0,1]$
$\psi(u) = (au^\alpha + b)/(au^\alpha + 1)$	$a > 0, \quad b \in (0,1], \quad \alpha \in (0,1]$

Example: $C(x,t) = (|3t| + 1)^{-1} \exp\left(-\|x\|^2/(|3t|+1)\right)$







Fourier-Transform Approach (Stein, 2005)

Fourier density

$$f(w_1, w_2) = g(w_1, w_2)\left[c_1(a_1^2 + |w_1|^2)^{\alpha_1} + c_2(a_2^2 + |w_2|^2)^{\alpha_2}\right]^{-\nu}$$

$c_i, a_i, \alpha_i \in (0, \infty)$, $d_1/(\alpha_1 \nu) + d_2/(\alpha_2 \nu) < 2$

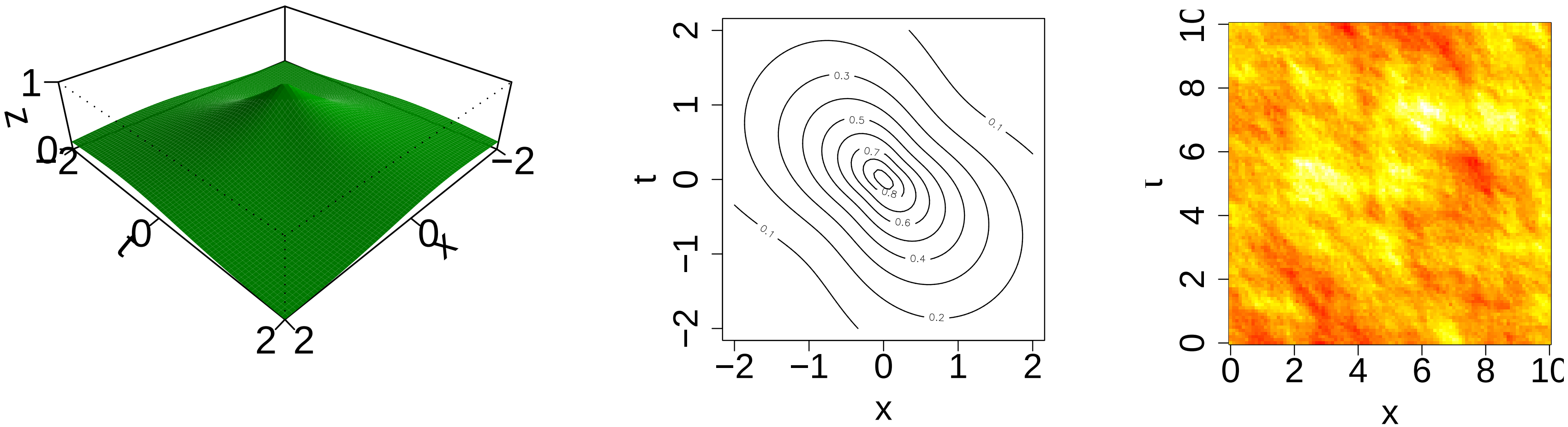
Examples of non-separabel models

- full symmetry if $g(w_1, w_2) \equiv 1$
- lack of full symmetry on $\mathbb{R}^d \times \mathbb{R}$

$$g(w_1, w_2) = a + b(w^\top z)w_2 + c_1|w_1|^2 + c_2|w_2|^2$$

$a, c_2 \in (0, \infty)$, $b^2 < 4c_1c_2$

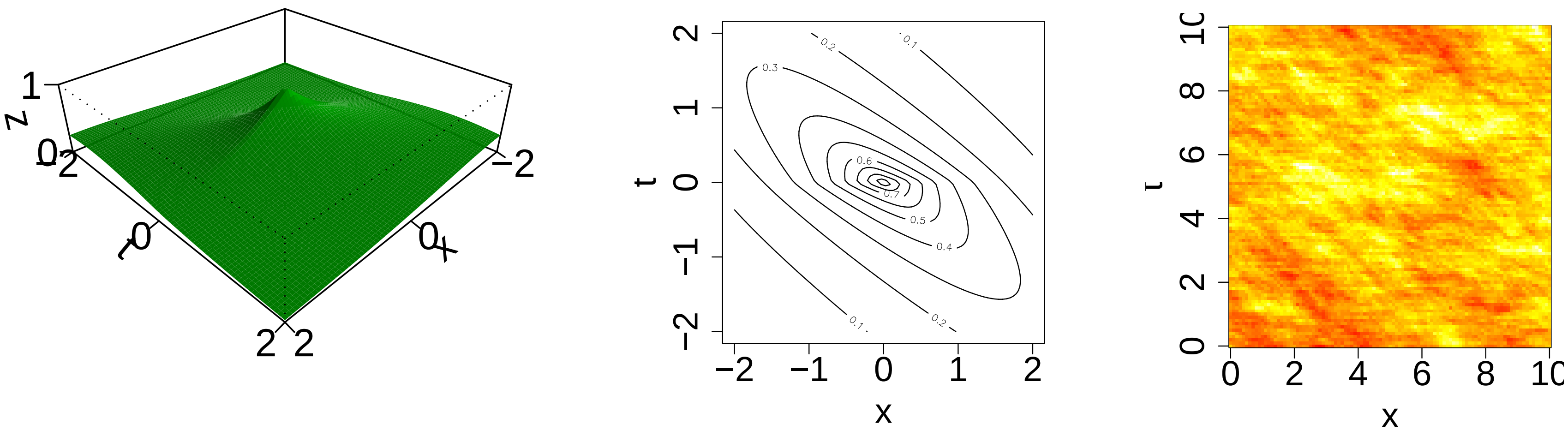
$$
\begin{aligned}
C(x,t) &= W_\nu(y) - 2(x^\top z)tW_{\nu-1}(y)/[2(\nu-1)(2\nu+3)] \\
y &= \|(x_1, x_2, t)\|, \qquad \nu = 0.5, \quad z = (\sqrt{2}, 0)
\end{aligned}
$$



- (Ma, 2003a; Stein, 2005)

$$
C(x,t) = \Gamma(\nu+\gamma(t))\,\{\Gamma(\nu+\gamma(t)+d/2)\}^{-1}\,W_{\nu+\gamma(t)}(\|x - Vt\|)
$$

$$
\nu = 0.5, \qquad \gamma(t) = 1 - e^{-|t|}, \qquad V = (-\tfrac{1}{2}, -\tfrac{1}{2})
$$



Covariance models based on PDE

For instance: heat conduction equation (Jones and Zhang, 1997)

$$\left(\frac{\partial^2}{\partial x^2} - a\frac{\partial}{\partial t} - b^2\right) Y(x,t)\,\mathrm{d}t = \mathrm{d}B(x,t), x, t \in \mathbb{R}$$

$\mathrm{d}B(s,t)$: uncorrelated Brownian motion

$$C(x,t) = \frac{1}{2}\left\{e^{-br}\mathrm{erfc}\left(\frac{2bt-cx}{2\sqrt{ct}}\right) + e^{br}\mathrm{erfc}\left(\frac{2bt+cx}{2\sqrt{ct}}\right)\right\}, \qquad x,t \geq 0$$

Generalisation (Brown et al., 2000)

$$\mathrm{d}Y(x,t) = \left[-\mu\nabla_x Y(x,t) + \frac{1}{2}\mathrm{trace}\left\{\nabla_x(\nabla_x Y)^\top \Sigma_1\right\} - Y(x,t)\right]\mathrm{d}t + \mathrm{d}B(s,t)$$

$\mathrm{d}B(s,t)$: BM, spatially correlated with cov. functn $g(h,0,\Sigma_2)$, the Gaussian pdf

$$C(x,t) = \int_0^\infty e^{-\lambda(2v+|t|)}\, g(x, t\mu, (2v+|t|)\Sigma_1 + \Sigma_2)\,\mathrm{d}v, \quad (x,t) \in \mathbb{R}^d \times \mathbb{R}$$

Often: covariance function only given in implicite form (Kolovos et al., 2004)

Simulation

Space-time grid on $\mathbb{R}^2 \times \mathbb{R}$

- circulant embedding (Wood and Chan, 1994)

(An-)isotropic model for $\mathbb{R}^2 \times \mathbb{R}$, arbitrary locations and instances

- turning bands

(An-)isotropic model for $\mathbb{R}^d \times \mathbb{R}$, $d \in \{2, 3\}$, instances on a grid

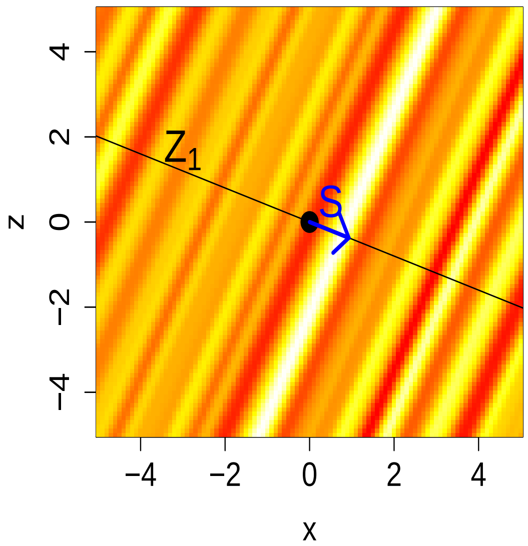
- turning layers (Schlather, 2005)

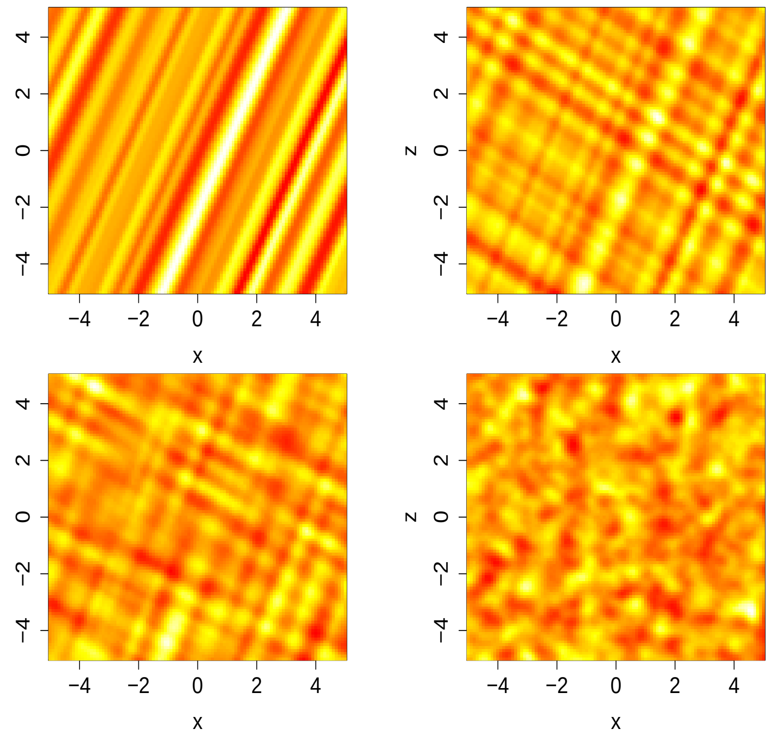
Software

- extension package `RandomFields` (Schlather, 2001-5) for `R`

Turning bands (Matheron, 1973)

Method to simulate isotropic random fields.





Let $C(x) = \varphi(\|x\|)$. Then $C_1(x) = \varphi_1(\|x\|)$ of Z_1 is given by

$$\varphi_1(u) = \frac{\mathrm{d}}{\mathrm{d}u}(u\varphi(u)), \qquad u > 0$$

Estimation and prediction

Estimation

- (generalized/weighted) least squares (Chilès and Delfiner, 1999)
- (Pseudo-) MLE (Chilès and Delfiner, 1999)
- (generalized) method of moments (Hansen, 1982)
- cross-validation type (Carroll et al., 1997)
- sequential fit (Gneiting, 2002)

Prediction

- kriging approaches (moving neighbourhood)

Conclusions

- main model choice
  typically case specific (Kyriakidis and Journel, 1999)
- choice of submodels (i.e. covariance function)
  away from case specific models, towards general parametric ones
- estimation
  standard estimators borrowed from time series analysis and geo-statistics
- simulation
  oversimplified models (e.g. separabel models) are easy to simulate and vice versa
- software
  extension package `RandomFields` for `R`

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