Models for Spatial-Temporal Covariances

Michael Stein and Mikyoung Jun

Department of Statistics, University of Chicago

This research is funded by
U.S. EPA - Science To Achieve Results (STAR) Program
Grant # R-82940201-0

Based on: http://www.stat.uchicago.edu/~cises/research/cises-tr4.pdf

Spatial-temporal covariances

$Z(\mathbf{x}, t)$ stationary spatial-temporal process, so that

$$\begin{aligned}\mathrm{cov}\{Z(\mathbf{x}_1, t_1), Z(\mathbf{x}_2, t_2)\} &= K(\mathbf{x}_1 - \mathbf{x}_2, t_1 - t_2)\\ \gamma(\mathbf{x}, t) &= K(\mathbf{0}, 0) - K(\mathbf{x}, t).\end{aligned}$$

GOAL: $K(\mathbf{x}, t)$ should accurately describe the variances and correlations of all linear combinations of Z.

Monitoring data often collected at $(\mathbf{x}_i, t)$ for $i = 1, \ldots, n$ and $t = 1, \ldots, T$.

Does K accurately describe

$$\mathrm{var}\{Z(\mathbf{x}_1, t) - Z(\mathbf{x}_2, t) - Z(\mathbf{x}_1, t+1) + Z(\mathbf{x}_2, t+1)\}?$$

Example: Isotropic v. separable models

Suppose Z process on plane with

$$K(x,y) = \exp\left\{-(x^2+y^2)^{1/2}/10\right\}$$

(isotropic), but fit the separable model

$$K(x,y) = \theta_1 \exp\left\{-(|x|+|y|)/\theta_2\right\}.$$

Simulate isotropic process on 20×20 square grid with spacing 1.

MLE: $(\hat\theta_1, \hat\theta_2) = (0.656, 2.93)$.

Visual fit to empirical variogram: $(\hat\theta_1, \hat\theta_2) = (1.725, 20.8)$.

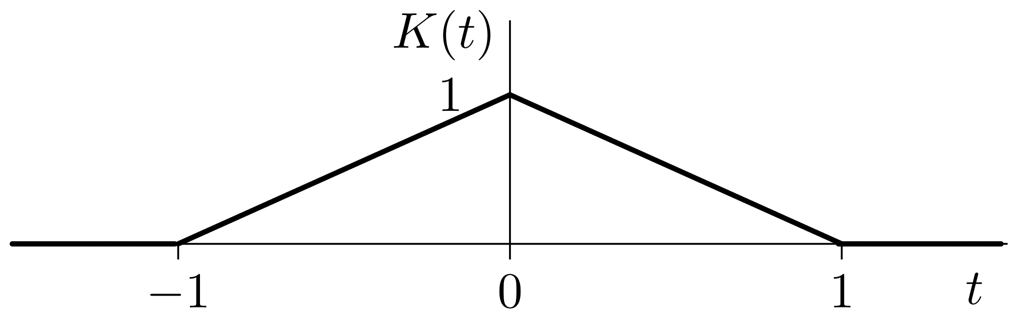
Consider $\mathrm{var}\big\{Z(0,0) - Z(1,0)\big\} = 2\gamma(1,0)$:

Truth: 0.190 MLE: 0.379 Visual: 0.162

Consider $\mathrm{var}\big\{Z(0,0) - Z(1,0) - Z(0,1) + Z(1,1)\big\}$:

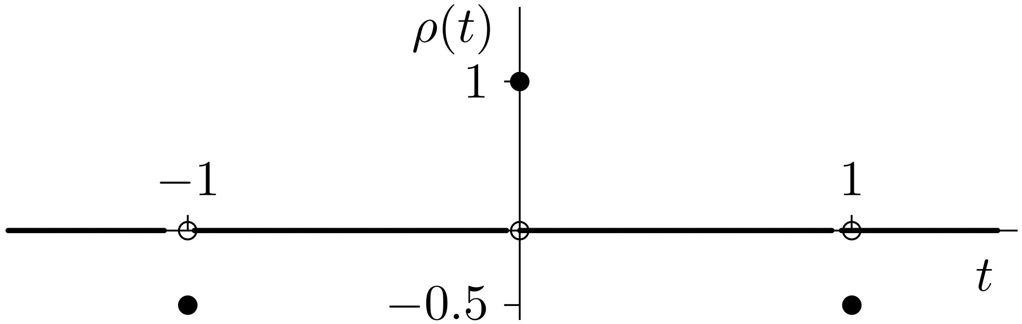
Truth: 0.234 MLE: 0.219 Visual: 0.0152

Triangular Covariance Function



Define $\rho_\epsilon(t) = \text{corr}\{Z(\epsilon) - Z(0), Z(t+\epsilon) - Z(t)\}$.

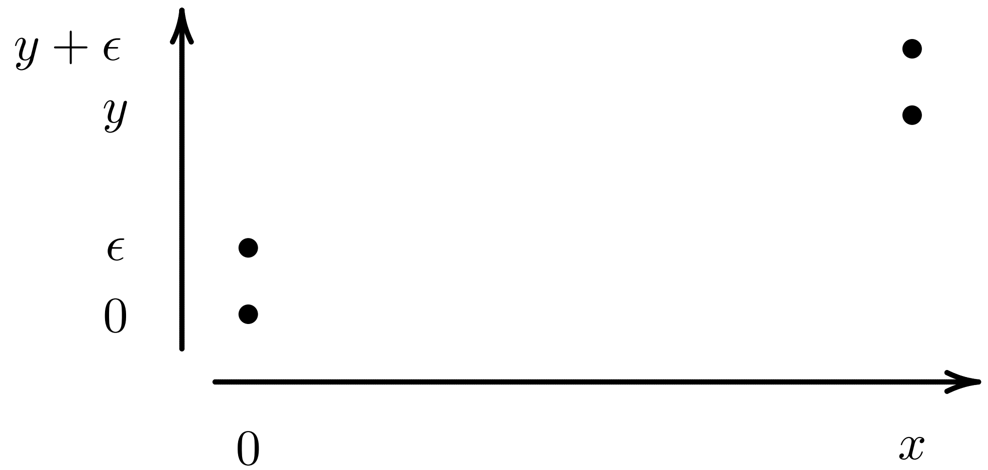
For all t, $\rho(t) = \lim_{\epsilon \to 0} \rho_\epsilon(t)$ exists.



Separable Covariance Function

Suppose $K(x, y) = e^{-|x|-|y|}$.

Define $\rho_\epsilon(x, y) = \mathrm{corr}\{Z(0, \epsilon) - Z(0, 0), Z(x, y + \epsilon) - Z(x, y)\}$.



For all x, y, $\rho(x, y) = \lim_{\epsilon \to 0} \rho_\epsilon(x, y)$ exists.

- $\rho(x, 0) = e^{-|x|}$
- $\rho(x, y) = 0$ otherwise

Ridges and Covariance Functions

Can show it is the presence of the ridges along axes that lead to

- Very small value for $\mathrm{var}\big\{Z(0,0) - Z(1,0) - Z(0,1) + Z(1,1)\big\}$
- Discontinuity in $\rho(x,y)$ at $y = 0$

Many proposed spatial-temporal covariance models have similar ridges (Cressie and Huang (1999), Gneiting (2002)).

Models without ridges:

- $K(\mathbf{x},t) = K\big((|\mathbf{x}|^2 + \beta^2 t^2)^{1/2}\big)$

But these models are equally smooth in space and time.

Can we get arbitrary and different smoothness in space and time and avoid ridges?

YES!

Consider the spectral density

$$f(\mathbf{w}, v) = \left\{c_1(a_1^2 + |\mathbf{w}|^2)^{\alpha_1} + c_2(a_2^2 + v^2)^{\alpha_2}\right\}^{-\nu}$$

and the corresponding covariance function

$$K(\mathbf{x}, t) = \int_{\Re^d \times \Re} e^{i\mathbf{x}'\mathbf{w} + itv} f(\mathbf{w}, v)\, \mathbf{dw}\, dv.$$

- K is an allowable covariance function
- Can get any degree of smoothness in space
- Can get any degree of smoothness in time
- K is infinitely differentiable away from origin

Can only carry out Fourier inversion for some very special cases.

Moments of spectral densities and smoothness of covariance functions

Well-known results ($d = 1$):

- f has mth moment $\Longrightarrow K^{(m)}$ exists
- $K^{(2m)}(0)$ exists $\Longleftrightarrow K^{(2m)}$ exists $\Longleftrightarrow f$ has $2m$th moment $\Longleftrightarrow Z$ is m-times mean square differentiable

Less well-known result:

- $\lim_{x\to\infty} x \int_x^\infty w f(w) dw = 0 \Longleftrightarrow K'(0)$ exists

If f doesn't have moments, can we say anything about derivatives of K other than at the origin?

Moments of derivatives of f

Derivatives away from $\mathbf{0}$ of $K \iff$ Smoothness of $f(\mathbf{w})$ for large $|\mathbf{w}|$

One dimension: If f' integrable, $x \neq 0$, then integrating by parts,

$$K(x) = ix^{-1} \int e^{iwx} f'(w) dw.$$

If $wf'(w)$ integrable, for $x \neq 0$,

$$K'(x) = -\frac{i}{x^2} \int e^{iwx} f'(w) dw - \frac{1}{x} \int w e^{iwx} f'(w) dw.$$

Examples:

- $K(x) = e^{-|x|}$, $f(w) = \frac{1}{\pi(1+w^2)} \Longrightarrow wf'(w) = -\frac{2w^2}{\pi(1+w^2)^2}$
- $K(x) = (1-|x|)^+$, $f(w) = \frac{1-\cos(w)}{\pi w^2} \Longrightarrow wf'(w) = \frac{\sin(w)}{\pi w} + O(|w|^{-2})$

More than one dimension

Derivatives away from $\mathbf{0}$ of $K \iff$ Smoothness of $f(\mathbf{w})$ for $|\mathbf{w}|$ large

Suppose $|\mathbf{w}|^m \frac{\partial^k}{\partial w_j^k} f(\mathbf{w})$ is integrable for $j = 1, \ldots, d$.

Then for all $\mathbf{x} \neq \mathbf{0}$, $\frac{\partial^{q_1+\cdots+q_d}}{\partial x_1^{q_1} \cdots \partial x_d^{q_d}} K(\mathbf{x})$ exists when $q_1 + \cdots + q_d \leq m$.

Examples:

- $f(\mathbf{w}, v) = \left\{c_1(a_1^2 + |\mathbf{w}|^2)^{\alpha_1} + c_2(a_2^2 + v^2)^{\alpha_2}\right\}^{-\nu}$
  $\Longrightarrow \left(|\mathbf{w}|^m + |v|^m\right) \frac{\partial^k}{\partial w_j^k} f(\mathbf{w})$ is integrable for k sufficiently large.

- $K(x) = e^{-|x|-|y|}$, $f(w) \propto (1 + w_1^2)^{-1}(1 + w_2^2)^{-1}$
  $\Longrightarrow w_2 \frac{\partial^k}{\partial w_1^k} f(\mathbf{w}) = \frac{w_2}{1+w_2^2} \times$ function of w_1. Not integrable.

Asymmetry in space-time covariances

Often find $K(\mathbf{x},t) \neq K(-\mathbf{x},t)$.

Examples:

- N-S and E-W components of wind vector
- Measured sulfate concentrations
- CMAQ sulfate concentrations
- Differences between measured and CMAQ sulfate

Asymmetries in correlations weaker for differences sign that CMAQ is working (?)

Explicit models with asymmetry

If $K(\mathbf{x}, t)$ is symmetric, then $K(\mathbf{x} - t\mathbf{v}, t)$ is not.

If K is Fourier transform of $\Psi(|\mathbf{w}|, |v|)$ and K is twice differentiable, then Fourier transform of

$$f(\mathbf{w}, v) = \left\{a + b(\mathbf{w}'\mathbf{z})v + c_1|\mathbf{w}|^2 + c_2 v^2\right\}\Psi(|\mathbf{w}|, |v|)$$

can be written in terms of derivatives of K.

If $|\mathbf{z}| = 1$, a, c_1, c_2 nonnegative and $b^2 \leq 4c_1c_2$, then f is nonnegative and integrable.

Example: Let $\mathcal{M}_\nu(y) = y^\nu \mathcal{K}_\nu(y)$ (Matérn class), then

$$K(\mathbf{x}, t) = (2\nu + d + 1)\mathcal{M}_\nu(y) - 2\tau(\beta_1\mathbf{x}'\mathbf{z})\beta_2 t\mathcal{M}_{\nu-1}(y),$$

is covariance function on $\Re^d \times \Re$ for $y = (\beta_1^2|\mathbf{x}|^2 + \beta_2^2 t^2)^{1/2}$, ν, β_1, β_2 positive and $0 \leq \tau \leq 1$.

Summary and look ahead

Little is known about modeling and analysis of space-time processes

- Space-time covariance functions and space-time interactions
- Methods for studying space-time interactions, especially for fixed monitoring networks

Other big issues:

- More sophisticated methods for combining monitoring data and physical models
- Nonstationary, non-Gaussian processes