1 Isotropic Covariance Functions

Let $\{Z(s)\}$ be a Gaussian process on $\mathbb{R}^n$, *i.e.*, a collection of jointly normal random variables $Z(s)$ associated with n-dimensional locations $s \in \mathbb{R}^n$. The joint distribution of $\{Z(s)\}$ depends only on the means $\mu(s) = \mathsf{E}Z(s)$ and the covariances $C(s,t) = \mathsf{E}\big(Z(s) - \mu(s)\big)\big(Z(t) - \mu(t)\big)$.

The process is called *stationary* or *translation invariant* if the distribution wouldn't change under a rigid translation of the entire collection of locations, *i.e.*, if $\mu(s) = \mu(s+h)$ and $C(s+h, t+h) = C(s,t)$ for all h; in this case $\mu(s) \equiv \mu$ is constant and $C(s,t) = C(s-t, 0)$ can only depend on the difference $h = (s-t)$ between the two locations, so must be of the form $C(s,t) = C_0(s-t)$ for some function $C_0(h) = C(h,0)$ on $\mathbb{R}^n$. Not just any function $C_0(h)$ can be a covariance function; let's see what the choices are.

It's easy to see that the function C_0 must be *even*, *i.e.*, must satisfy $C_0(h) = C_0(-h)$, since $C(s-t) = \mathsf{E}\big(Z(s) - \mu(s)\big)\big(Z(t) - \mu(t)\big) = C(t-s)$. But more is true: if $\{s_j\}$ any collection of locations, then complex linear combinations $a^\intercal(Z - \mu) = \sum a_j(Z_j - \mu_j)$ of the centered random variables $Z_j = Z(s_j)$ (with means $\mu_j = \mu(s_j)$) must have nonnegative squared modulus $\mathsf{E}\big|\sum a_j(Z_j - \mu_j)\big|^2 = \sum a_j C(s_j - s_k)\bar{a}_k \geq 0$ for every set of complex numbers $\{a_j\} \subset \mathbb{C}$. A function $C_0(h)$ is called *positive semi-definite* if it always satisfies the inequality $\sum_{jk} a_j C(s_j - s_k)\bar{a}_k \geq 0$ for any locations s_j and complex numbers a_j; this is equivalent to asking that $C(h) = C(-h)$ for every $h \in \mathbb{R}^n$ and that $\sum a_j C(s_j - s_k) a_k \geq 0$ for all *real* numbers $a_j \in \mathbb{R}$. One way to get a symmetric positive semi-definite function $C_0(h)$ is by taking the Fourier transform

$$C_0(h) = \int_{\mathbb{R}^n} e^{ih\cdot\omega} G(\omega)\, d^n\omega$$

of any positive function $G(\omega)$ on $\mathbb{R}^n$ or, more generally, of any finite positive measure $G(d\omega)$, because then

$$\begin{aligned}
\sum_{jk} a_j C(s_j - s_k)\bar{a}_k &= \int_{\mathbb{R}^n} \sum_{jk} (a_j e^{s_j\cdot\omega})\overline{(a_k e^{s_k\cdot\omega})} G(d\omega) \\
&= \int_{\mathbb{R}^n} \Big|\sum_j a_j e^{s_j\cdot\omega}\Big|^2 G(d\omega) \geq 0.
\end{aligned}$$

It turns out that this is the *only* way to get one— that every positive semi-definite function can be written in this form for some finite positive measure

$G(d\omega)$, called the *spectral measure* (if $G(d\omega) = G(\omega)\,d\omega$ is absolutely continuous, $G(\omega)$ is called the *spectral density*). Known as "Bochner's Theorem,' this result is really just the Fourier inversion formula in an unfamiliar setting:

$$G(\omega) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{-ih\cdot\omega} C_0(h)\, d^n h.$$

Since the process $\{Z(s)\}$ is real-valued, the spectral density $G(\omega) = G(-\omega)$ must be an even function and so we can write

$$\begin{aligned} C_0(h) &= \int_{\mathbb{R}^n} \cos(h\cdot\omega) G(\omega)\, d^n\omega \\ G(\omega) &= (2\pi)^{-n} \int_{\mathbb{R}^n} \cos(h\cdot\omega) C_0(h)\, d^n\omega \end{aligned}$$

If the Gaussian process is also *isotropic*, or invariant under rotations, then $G(\omega) = g(|\omega|)$ must also be invariant under rotations and depend only on the length $r = |\omega|$ of the vector $\omega \in \mathbb{R}^n$. In this case we can simplify these integrals by transforming to polar coordinates.

1.1 Polar Coordinates for Probabilists

Polar coordinates are a familiar tool in two-dimensional integrals, where the change of variables from $x \in \mathbb{R}^2$ to $r = \sqrt{x_1^2 + x_2^2}$ and $\theta = \arctan x_2/x_1$ (so $x_1 = r\cos\theta$, $x_2 = r\sin\theta$) and a change from d^2x to $r\,dr\,d\theta$ lead to simple expressions for the integrals of radial functions. Equivalently, we can let σ have a uniform probability distribution (denoted by $d\sigma$) over the unit circle $S^1 = \{x : x_1^2 + x_2^2 = 1\}$, and change variables from $x = (x_1, x_2)$ to (r, σ), with $d^2x = dx_1\,dx_2$ replaced by $2\pi r\,dr\,d\sigma$.

In three dimensions the first polar approach has its analogue in the Euler angles, while the second is simpler with uniform measure for σ on the unit sphere $S^2 \subset \mathbb{R}^3$, with $d^3x = dx_1\,dx_2\,dx_3$ replaced by $4\pi r^2\,dr\,d\sigma$. Notice that $2\pi r$ and $4\pi r^2$ are the circumference of the circle and the area of the sphere of radius r, respectively. In any number n of dimensions the sphere S^{n-1} has area $2\pi^{n/2} r^{n-1}/\Gamma(n/2)$, and we can again again evaluate integrals in polar coordinates with the uniform probability distribution $d\sigma$ for $\sigma \in S^{n-1} \subset \mathbb{R}^n$, and $d^nx = \frac{2\pi^{n/2}}{\Gamma(n/2)} r^{n-1}\,dr\,d\sigma$. This makes it easy to compute integrals of radial functions; for functions that also depend on one or more of the components x_j, it is sometimes helpful to note that the squares $\{{\sigma_j}^2\}$ have a Dirichlet $\mathsf{Di}(\frac{1}{2}, ..., \frac{1}{2})$ joint distribution, so each σ_j is distributed as the square root of a $\mathsf{Be}(\frac{1}{2}, \frac{n-1}{2})$ random variable.

1.2 Evaluating $C_0(h)$

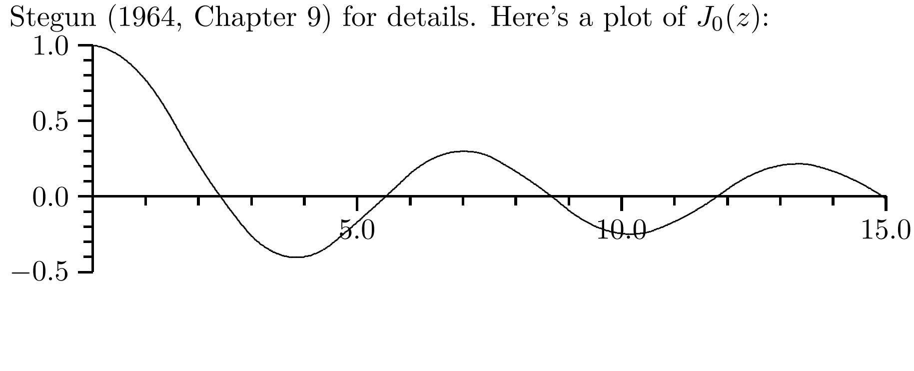
Switching to polar coordinates $r = |\omega| \geq 0$ and $\sigma = \omega/|\omega| \in S^{n-1}$ (where $d\sigma$ denotes the uniform probability measure on the unit sphere S^{n-1} in $\mathbb{R}^n$), and noting that the component $\sigma_h = \sigma \cdot h/|h|$ of $\sigma \in S^{n-1}$ in the direction h again has the same distribution as the square root of a $\mathsf{Be}(\frac{1}{2}, \frac{n-1}{2})$ random variable, writing ρ for $|h|$,

$$\begin{aligned}
C_0(h) &= \int_{\mathbb{R}^n} \cos\big(h \cdot \omega\big) g(|\omega|)\, d^n\omega \\
&= \iint_{\mathbb{R}_+ \times S^{n-1}} \cos\big(r\rho\sigma_h\big) g(r) \frac{2\pi^{n/2}\, r^{n-1}}{\Gamma(n/2)}\, dr\, d\sigma \\
&= \int_{\mathbb{R}_+} \int_0^1 \cos\big(r\rho\sqrt{u}\big) g(r) \frac{2\pi^{n/2}\, r^{n-1}}{\Gamma(n/2)} \frac{\Gamma(n/2)}{\Gamma(\frac{1}{2})\,\Gamma(\frac{n-1}{2})} u^{1/2-1}(1-u)^{(n-1)/2-1}\, dr\, du \\
&= \int_0^\infty \rho\,(2\pi r/\rho)^{\nu+1}\, J_\nu(r\rho)\, g(r)\, dr, \qquad \nu \equiv \frac{n}{2} - 1 \qquad (1) \\
&= \int_0^\infty (r\rho/2)^{-\nu}\Gamma(\nu+1) J_\nu(r\rho)\, \gamma(dr) \qquad (2) \\
&= \begin{cases} \int_0^\infty 2\cos(r\rho) g(r)\, dr & \text{if } n = 1 \\ \int_0^\infty 2\pi r\, J_0(r\rho)\, g(r)\, dr & \text{if } n = 2 \\ \int_0^\infty \rho(2\pi r/\rho)^{3/2} J_{1/2}(r\rho)\, g(r)\, dr & \text{if } n = 3 \end{cases}
\end{aligned}$$

where

$$J_\nu(z) = \frac{(z/2)^\nu}{\sqrt{\pi}\,\Gamma(\nu + 1/2)} \int_0^\pi \cos(z\cos\theta)\, \sin(\theta)^{2\nu}\, d\theta$$

is the Bessel function of the first kind of order ν (see Watson, 1944). Bessel functions aren't as familiar as sines and cosines, but they're common in engineering and physics and are in the standard C library, the GNU Scientific library (GSL), Maple and Mathematica, MatLab, *etc.*; see Abramowitz and Stegun (1964, Chapter 9) for details. Here's a plot of $J_0(z)$:



The plot of $J_0(z)$ looks a little like a sine or cosine, but falls off like $1/\sqrt{z}$ as $z \to \infty$.

The most general isotropic covariance is given in (2), with the absolutely continuous measure $g(r)\,\frac{2\pi^{n/2}}{\Gamma(n/2)}\,r^{n-1}dr$ replaced by an arbitrary positive finite measure $\gamma(dr)$ on $[0,\infty)$. Any isotropic covariance function may be approximated by one with a discrete spectral measure $\gamma(dr) = \sum \gamma_j \delta_{r_j}(dr)$ assigning mass γ_j to finitely many points r_j:

$$
\begin{aligned}
C(\rho) &\approx \sum_j (2/r_j\rho)^{\nu}\Gamma(\nu+1)J_{\nu}(r_j\rho)\gamma_j \qquad (3)\\
&= \begin{cases} \sum_j \gamma_j \cos(r_j\rho) & \text{if } n=1 \\ \sum_j \gamma_j J_0(r_j\rho) & \text{if } n=2 \\ \sum_j \gamma_j \sqrt{\pi/2r_j\rho}\,J_{1/2}(r_j\rho) & \text{if } n=3 \end{cases}
\end{aligned}
$$

but a more common approach is to choose small parametric families of densities $g^{\theta}(r)$ or measures $g^{\theta}(dr)$.

We can recover the spectral density $g(r) = G(\omega)$ (for $r = |\omega|$) through the Fourier inversion formula, using polar coordinates with $\rho = |h| \in \mathbb{R}_+$ and $\sigma = h/|h| \in S^{n-1}$:

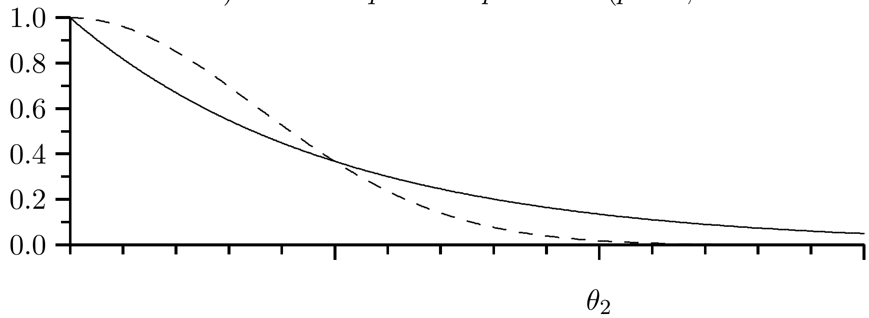
$$
\begin{aligned}
g(r) = G(\omega) &= \frac{1}{(2\pi)^n}\int \cos\big(-h\cdot\omega\big)C_0(h)\,d^n h\\
&= \frac{1}{(2\pi)^n}\iint_{\mathbb{R}_+\times S^{n-1}} \cos\big(-r\rho\,\sigma_{\omega}\big)C(\rho)\frac{2\pi^{n/2}\,\rho^{n-1}}{\Gamma(n/2)}\,d\rho\,d\sigma\\
&= \int_0^{\infty} r(\rho/2\pi r)^{n/2}J_{\nu}(r\rho)C(\rho)\,d\rho, \qquad \nu \equiv \frac{n}{2}-1 \qquad (4)\\
&= \begin{cases} \int_0^{\infty} \frac{2}{\pi}\cos(r\rho)C(\rho)\,d\rho & \text{if } n=1 \\ \int_0^{\infty} (\rho/2\pi)J_0(r\rho)\,C(\rho)\,d\rho & \text{if } n=2 \\ \int_0^{\infty} r(\rho/2\pi r)^{3/2}J_{1/2}(r\rho)\,C(\rho)\,d\rho & \text{if } n=3 \end{cases} \qquad (5)
\end{aligned}
$$

It is hard to imagine what $C_0(h)$ would look like for different choices of $g(r)$; a simple approach is to take whatever symmetric functions $G(u)$ whose Fourier transforms we can find, and see what we get. Here are some commonly used covariance families, in $n = 2$ dimensions; in each case $\theta_1 = C(0)$ is an overall level parameter and θ_2 is a distance scale parameter:

- Exponential Power family

$$C(\rho \mid \theta, p) = \theta_1 \exp\{-|\rho/\theta_2|^p\},\ 0 < p \le 2$$

Two notable covariograms in this family are the *exponential* ($p = 1$, solid below) and the *squared exponential* ($p = 2$, dashed below):

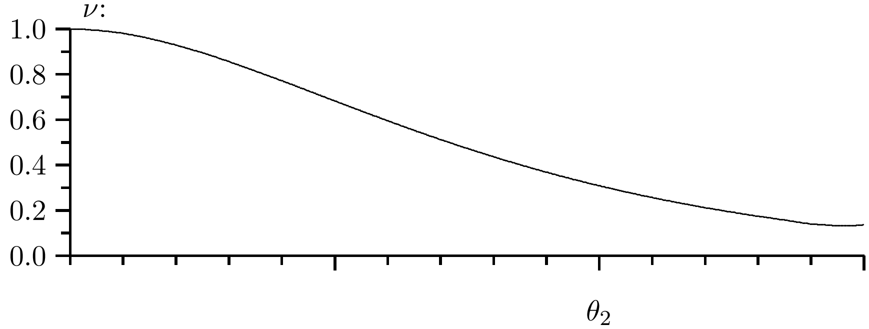


Notice that the exponential has a negative derivative at $z = 0$, so it falls off quickly at first, then slowly levels off, while the squared exponential has zero derivative near $z = 0$ then falls off very quickly. From (5) it follows that the exponential has spectral density function $g(r) = (\theta_1 {\theta_2}^2/2\pi)/\big(1 + r^2 {\theta_2}^2\big)^{3/2}$, proportional to a bivariate Cauchy density function, while the squared exponential has spectral density $g(r) = (\theta_1 {\theta_2}^2/4\pi) \exp\big(-r^2 {\theta_2}^2/4\big)$, proportional to a normal density.

- Matérn

$$C(\rho \mid \theta) = \frac{2\,\theta_1}{\Gamma(\theta_3)} \left(\frac{\rho}{2\theta_2}\right)^{\theta_3} K_{\theta_3}(\rho/\theta_2)$$

where $K_\nu(z)$ is the modified Bessel function of the third kind of order ν:



The displayed plot has shape parameter $\theta_3 = 2$. The Matérn class is quite flexible and includes the exponential family (with $\theta_3 = \frac{1}{2}$), the squared exponential family (in the limit as $\theta_3 \to \infty$), and many others. In n dimensions its spectral density function is

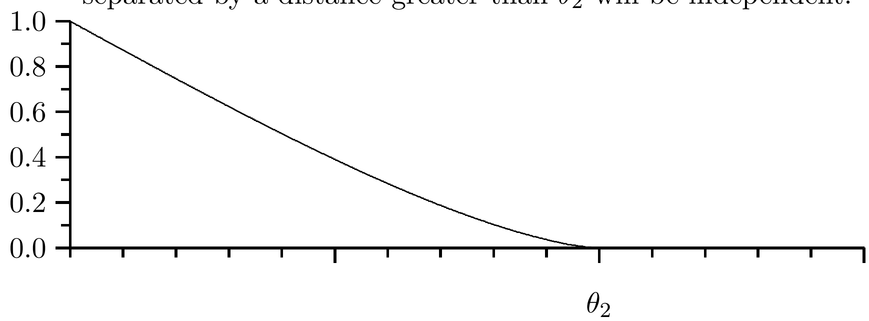
$$g(r) = \frac{\theta_1 {\theta_2}^n}{\Gamma(\theta_3)\pi^{n/2}} \big(1 + {\theta_2}^2 r^2\big)^{-\theta_3 - n/2},$$

proportional to the familiar n-variate Student's t density function with $2\theta_3$ degrees of freedom and variance scale $\sigma^2 = 1/2\theta_2{}^2\theta_3$. This lends more insight into how the Matérn reduces to the exponential when $\theta_3 = 1/2$ and to the squared exponential when $\theta_3 \to \infty$.

- Spherical

$$C(\rho \mid \theta) = \begin{cases} \theta_1 \left[1 - \frac{2}{\pi}\left(\frac{\rho}{\theta_2}\sqrt{1-(\frac{\rho}{\theta_2})^2} + \sin^{-1}\frac{\rho}{\theta_2}\right)\right] & \text{for } \rho < \theta_2 \\ 0 & \text{for } \rho \geq \theta_2 \end{cases}$$

The spherical covariance function is proportional to the area of intersection for two discs of diameter θ_2 with centers separated by distance ρ. In this model the Gaussian quantities Z_j and Z_k at loci s_j and s_k separated by a distance greater than θ_2 will be independent.



This is not quite linear. Like the exponential, it has a negative slope at $z = 0$ and falls off rapidly at first; like the squared exponential, it falls off rapidly later and in fact reaches zero. The spectral density, while available in closed form, isn't illuminating; it's best to think of the spherical process as a convolution or moving average of Gaussian white noise, integrated at each locus over the surrounding ball of diameter θ_2.

A variety of processes may be constructed similarly as kernel integrals of standard Gaussian white noise,

$$Z(h) = \int_{\mathbb{R}^n} k(h-s)\,\zeta(ds);$$

where "standard" means that $\mathsf{E}[\zeta(ds)] = 0$ and $\mathsf{E}[\zeta(ds)^2] = ds$. The covariance is

$$C_0(h) = \mathsf{E}\big[Z(0)\overline{Z(h)}\big] = \int_{\mathbb{R}^n} k(h-s)\,\overline{k(-s)}\,ds$$

with spectral density

$$\begin{aligned} G(\omega) &= (2\pi)^{-n} \int e^{-i\omega\cdot h} C_0(h)\, dh \\ &= (2\pi)^{-n} \iint e^{-i\omega\cdot h} k(h-s)\, \overline{k(-s)}\, ds\, dh \\ &= (2\pi)^{-n} \left| \int e^{-i\omega\cdot x} k(x)\, dx \right|^2 \end{aligned}$$

so that an isotropic kernel may be computed from the spectral density as

$$k(x) = (2\pi)^{-n/2} \int e^{i\omega\cdot x} G(\omega)^{1/2}\, d^n\omega$$

or, in polar coordinates,

$$\begin{aligned} k(\rho) &= \int_0^\infty r^{\nu+1} \rho^{-\nu} J_\nu(r\rho) g(r)^{1/2}\, dr \\ &= \begin{cases} \int_0^\infty \sqrt{\frac{2}{\pi}} \cos(r\rho) \sqrt{g(r)}\, dr & \text{if } n=1 \\ \int_0^\infty J_0(r\rho)\, r\, \sqrt{g(r)}\, dr & \text{if } n=2 \\ \int_0^\infty J_{1/2}(r\rho)\, r^{3/2} \rho^{-1/2}\, \sqrt{g(r)}\, d\rho & \text{if } n=3 \end{cases} \end{aligned}$$

provided that the square root of the spectral density *is* the Fourier transform of a finite positive function, *i.e.*, is itself positive semidefinite. For the Matérn class, the root spectral density $\sqrt{g(r)} \propto \left(1+{\theta_2}^2 r^2\right)^{-(\theta_3+n/2)/2}$ will be another n-variate t density provided $\theta_3 > n/2$ and in this case, setting $\epsilon = (2\theta_3 - n)/4 > 0$, we find

$$k(\rho) = \frac{2{\theta_1}^{1/2} (2\rho\theta_2)^{-\epsilon-n/2}}{\Gamma(\epsilon+n/2)\sqrt{\Gamma(2\epsilon+n/2)}\pi^{n/4}} K_\epsilon(\rho/\theta_2)$$

leads to a moving-average kernel representation for the Matérn covariance class. In any number $n \geq 1$ of dimensions the restriction $\epsilon > 0$ entails $\theta_3 > n/2 \geq 1/2$, ruling out the exponential covariance, but the squared exponential covariance (the limiting case as $\theta_3 \to \infty$) is available in any number of dimensions, with

$$k(\rho) = {\theta_1}^{1/2} (\pi {\theta_2}^2/4)^{-n/2} e^{-2\rho^2/{\theta_2}^2}.$$

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