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

$$C_0(h) = \int_{\mathbb{R}^n} e^{ih\cdot\omega} G(\omega)\, d^n\omega = \int_{\mathbb{R}^n} e^{ih\cdot\omega} G(d\omega) \tag{1}$$

of any positive function $G \in L_1(\mathbb{R}^n)$ or, more generally, of any finite positive Borel 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 $C_0(h)$

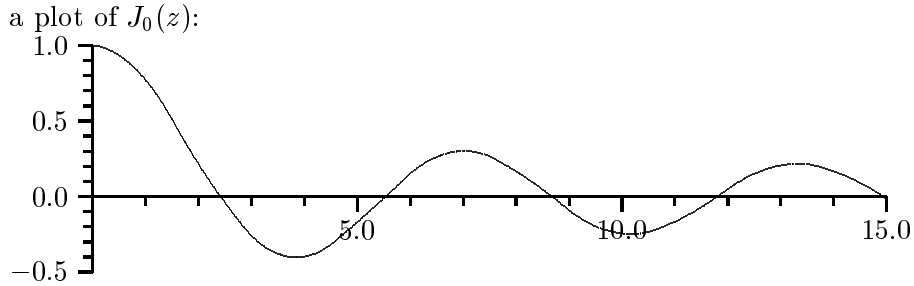
Switching to polar coordinates $r = |\omega| \geq 0$ and $\sigma = \omega/|\omega| \in S^{n-1}$ (where $d\sigma$ denotes the uniform probability measure on the unit sphere S^{n-1} in $\mathbb{R}^n$), and noting that the component $\sigma_h = \sigma \cdot h/|h|$ of $\sigma \in S^{n-1}$ in the direction 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 $|h|$,

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

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), `R`, Maple and Mathematica, MatLab, Python's SciPy library, *etc.*; for more details, see Abramowitz and Stegun (1964, Chapter 9). 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 (3), 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:

$$\begin{aligned} C_0(h) = C(\rho) \quad &\approx \quad \sum_j (2/r_j\rho)^\nu \Gamma(\nu+1) J_\nu(r_j\rho)\gamma_j \qquad (4) \\ &= \quad \begin{cases} \sum_j \gamma_j \cos(r_j\rho) & \text{if } n=1 \\ \sum_j \gamma_j J_0(r_j\rho) & \text{if } n=2 \\ \sum_j \gamma_j \sqrt{\pi/2r_j\rho}\, J_{1/2}(r_j\rho) & \text{if } n=3 \end{cases} \end{aligned}$$

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

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

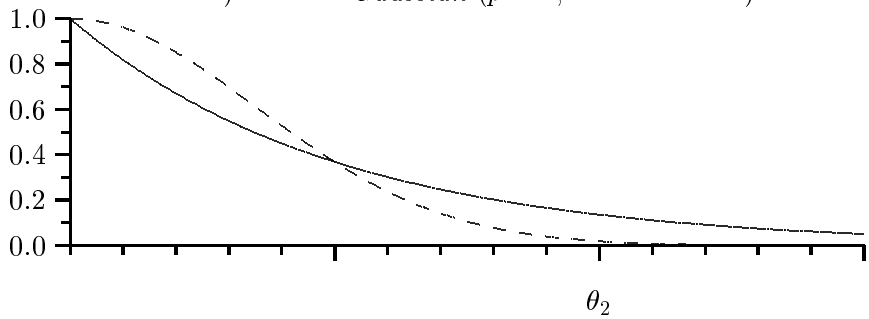
$$\begin{aligned} g(r) = G(\omega) \quad &= \quad \frac{1}{(2\pi)^n} \int \cos\big(-h\cdot\omega\big) C_0(h)\, d^n h \\ &= \quad \frac{1}{(2\pi)^n} \iint_{\mathbb{R}_+ \times S^{n-1}} \cos\big(-r\rho\,\sigma_\omega\big) C(\rho) \frac{2\pi^{n/2}\,\rho^{n-1}}{\Gamma(n/2)}\, d\rho\, d\sigma \\ &= \quad \int_0^\infty r(\rho/2\pi r)^{n/2} J_\nu(r\rho) C(\rho)\, d\rho, \qquad \nu \equiv \frac{n}{2} - 1 \qquad (5) \\ &= \quad \begin{cases} \int_0^\infty \frac{2}{\pi}\cos(r\rho) C(\rho)\, d\rho & \text{if } n=1 \\ \int_0^\infty (\rho/2\pi) J_0(r\rho)\, C(\rho)\, d\rho & \text{if } n=2 \\ \int_0^\infty r(\rho/2\pi r)^{3/2} J_{1/2}(r\rho)\, C(\rho)\, d\rho & \text{if } n=3 \end{cases} \qquad (6) \end{aligned}$$

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 $\theta_1 = C_0(0)$ is an overall level parameter and θ_2 is a distance scale parameter:

- Power Exponential 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 *Gaussian* ($p = 2$, dashed below):

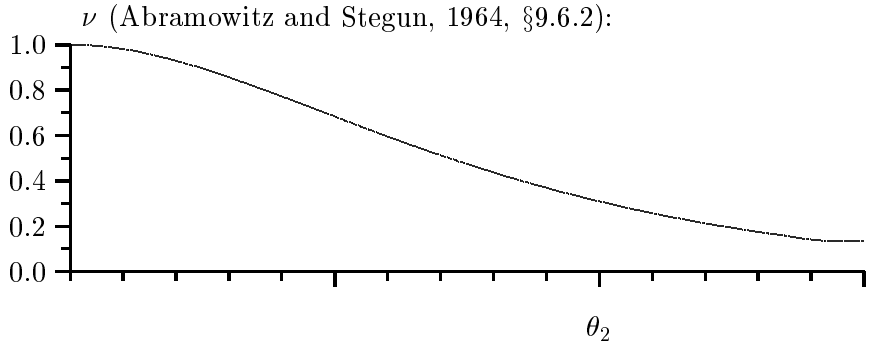


Notice that the exponential has a negative derivative at $z = 0$, so it falls off quickly at first, then slowly levels off, while the Gaussian has zero derivative near $z = 0$ then falls off very quickly. From (6) it follows that the exponential has spectral density function $g(r) = (\theta_1 {\theta_2}^2/2\pi)/\left(1 + r^2 {\theta_2}^2\right)^{3/2}$, proportional to a bivariate Cauchy density function, while the Gaussian has spectral density $g(r) = (\theta_1 {\theta_2}^2/4\pi) \exp\left(-r^2 {\theta_2}^2/4\right)$, 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 (Abramowitz and Stegun, 1964, §9.6.2):



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 Gaussian family (in the limit as $\theta_3 \to \infty$), and many others. In n dimensions its spectral density function is

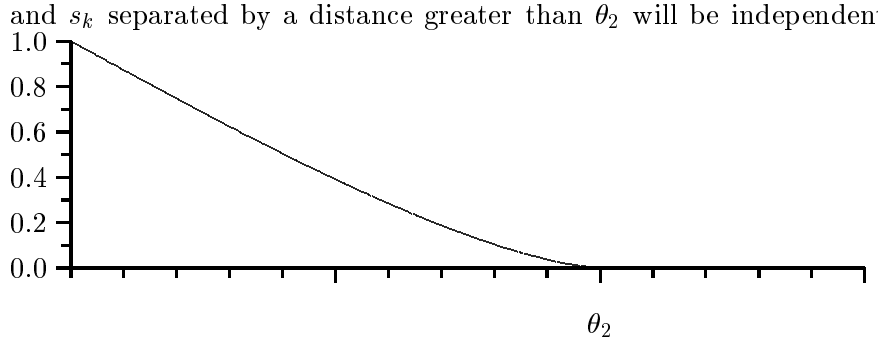
$$g(r) = \frac{\theta_1 {\theta_2}^n}{\Gamma(\theta_3)\pi^{n/2}} \left(1 + {\theta_2}^2 r^2\right)^{-\theta_3 - n/2},$$

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 Gaussian 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 Gaussian, 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.

The same idea works in any dimension d— a constant θ_1, times the volume of intersection of two balls of radius θ_2 whose centers are separated by a distance ρ, is a valid covariance function in dimensions $n \leq d$ (for any *real* $d \geq 1$, not just $d \in \mathbb{N}$):

$$C(\rho \mid \theta) = 2\theta_1 I_{(1-\rho/\theta_2)/2}\left(\tfrac{d+1}{2}, \tfrac{d+1}{2}\right), \quad 0 \leq \rho \leq \theta_2$$

where $I_z(\alpha, \beta)$ is the normalized incomplete Beta function (Abramowitz and Stegun, 1964, §6.6.2), the CDF at z of the $\mathsf{Be}(\alpha, \beta)$ distribution. For $d = 2$ this reduces to the equation above, and for $d = 3$ to $C(\rho \mid \theta) = \theta_1(\theta_2 - \rho)^2(2\theta_2 + \rho)/2\theta_2^2$ for $0 \leq \rho \leq \theta_2$.

2 Constructing GPs from their Spectral Measures

The integral representations of isotropic covariance functions can be exploited to *construct* random fields with specified covariance structure, in at least two different ways.

2.1 White-Noise Convolutions

Many 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 $\mathsf{E}[\zeta(ds)^2] = ds$ (more formally, that ζ is countably additive with $\zeta(A) \sim \mathsf{No}(0, |A|)$ for Borel $A \subset \mathbb{R}^n$ of finite Lebesgue measure $|A|$). 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

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

Thus 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 Gaussian covariance (the limiting case as $\theta_3 \to \infty$) is available in any number of dimensions, with

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

2.2 Spectral Representation

We generalize Hida and Hitsuda (1993, §III.2, *pp.* 42 ff). Let $\Theta \subseteq \mathbb{R}^n$ be the *spectrum*, the support of the spectral measure $G(d\omega)$ (see (1)), and let $\zeta(d\omega)$ be a Gaussian random measure on the Borel sets of Ω with control measure $G(d\omega)$ (so $\zeta(A) \sim \mathsf{No}\big(0, G(A)\big)$ for Borel sets $A \subset \Omega$ of finite G-measure). For $t \in \mathbb{R}$ set

$$Z_s := \int_\Omega e^{is\cdot\omega}\, \zeta(d\omega).$$

Then Z is a complex-valued Gaussian stochastic process with mean zero and autocovariance

$$\mathsf{E} Z_s \bar{Z}_t = \int_\Omega e^{i(s-t)\cdot\omega}\, G(d\omega) = C_0(s-t)$$

I think we can arrange for Z to be real-valued, but probably not ζ since if ζ were real then we would have $Z_{-t} \equiv \bar{Z}_t$.

For the special case of $n = 1$, we can start with independent real-valued Gaussian random measures $\zeta_0(d\omega)$ and $\zeta_1(d\omega)$ on $\Omega_+ = \Omega \cap \mathbb{R}_+$, each with control measure $\frac{1}{2}G(d\omega)$ restricted to Ω_+, and set

$$\zeta(A) = \left[\zeta_0(A_+) + \zeta_0(A_-)\right] + i\left[\zeta_1(A_+) - \zeta_1(A_-)\right]$$

(where of course $A_+ = A \cap \mathbb{R}_+$ and $A_- = A \cap \mathbb{R}_-$). Then ζ is a complex Gaussian measure on $\mathbb{R}$ with mean zero and covariance

$$\mathsf{E}\zeta(ds)\bar{\zeta}(dt) = \delta_s(dt)\, G(ds)$$

Set

$$Z_s = \int_\Omega e^{i\omega s}\zeta(d\omega) = \int_{\Omega_+} \cos(\omega s)\zeta_0(d\omega) - \int_{\Omega_+} \sin(\omega s)\zeta_1(d\omega) \tag{7}$$

I'm not sure how to think of this in Polar coordinates, or how to extend it to ≥ 2 dimensions, but I expect that's possible useful interesting and, probably, old. The Free Euclidean Field should be an example.

3 Compact Ranges

Fourier transforms and harmonic analysis are most commonly studied on Euclidean space $\mathbb{R}^d$, but many of the ideas extend to bounded spaces like the closed unit ball $B^d \subset \mathbb{R}^d$ or its boundary the unit sphere S^{d-1} (the disc and circle, for $d = 2$), or even to locally compact groups.

In this section we'll consider functions on the unit ball B^d. Because it is compact, functions in $L_2(B^d)$ will have Fourier *series* with a discrete index set, rather than the Fourier *transforms* of Section (1).

3.1 Fourier-Bessel Expansions in $d = 2$ Dimensions

The key for $d = 2$ is the orthogonality relationship for Bessel functions of the first kind (Abramowitz and Stegun, 1964, §9.1):

$$\int_0^1 J_\alpha(rj_{\alpha,n})\, J_\alpha(rj_{\alpha,n'})\, r\, dr = \tfrac{1}{2}\delta_{nn'}[J_{\alpha+1}(j_{\alpha,n})]^2,$$

where $j_{\alpha,n}$ is the nth positive zero of $J_\alpha(x)$, for any $n, n' \in \mathbb{Z}$ and any $\alpha \in \mathbb{R}$. For integers α, $J_\alpha(-x) = (-1)^\alpha J_\alpha(x)$, so $[J_{\alpha+1}(j_{\alpha,n})]^2 = [J_{|\alpha|+1}(j_{\alpha,n})]^2$ and $j_{\alpha,n} = j_{-\alpha,n}$. It follows that for $m \in \mathbb{Z}$ and $n \in \mathbb{N}$ the functions

$$\phi_{mn}(r,\theta) \equiv \frac{1}{\sqrt{\pi}\, J_{|m|+1}(j_{m,n})} J_m(rj_{m,n})\, e^{im\theta} \tag{8}$$

are orthonormal in $L_2(B^2)$. In fact they form a CONS, so any function $f \in L_2(B^2)$ has a convergent expansion

$$f(r,\theta) = \sum_{\substack{m\in\mathbb{Z}\\ n\in\mathbb{N}}} a_{mn}\, \phi_{mn}(r,\theta) = \sum_{\substack{m\in\mathbb{Z}\\ n\in\mathbb{N}}} \frac{a_{mn}}{c_{mn}}\, J_m(rj_{m,n})e^{im\theta}$$

where

$$c_{mn} = \sqrt{\pi}\, J_{|m|+1}(j_{m,n}), \qquad a_{mn} = \int_{B^2} f(r,\theta)\overline{\phi_{mn}(r,\theta)}\, r\, dr\, d\theta. \tag{9}$$

Note a_{mn} from (9) can also be evaluated in *Cartesian* coordinates if, for example, f is known on a rectangular grid containing B^2— just multiply the integrand by $\mathbf{1}_{B^2}$ and replace $r\, dr\, d\theta$ with $dx\, dy$. Both the Bessel functions J_m and the zeros $j_{m,n}$ are available in `R`. From Bessel's differential equation

$$z^2 \frac{\partial^2}{\partial z^2} J_m(z) + z \frac{\partial}{\partial z} J_m(z) + (z^2 - m^2) J_m(z) = 0$$

(Abramowitz and Stegun, 1964, §9.1.1), ϕ_{mn} is an eigenfunction of the Laplacian with eigenvalue $-j_{m,n}^2$ satisfying Dirichlet boundary conditions $\phi_{mn}(1,\theta) \equiv 0$ on $S^1 = \partial B^2$, so the negative Laplacian of f is given in polar coordinates by

$$\begin{aligned} -\Delta f(r,\theta) &\equiv -\left\{ \frac{1}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} \right\} \\ &= \sum (j_{m,n})^2 (a_{mn}/c_{mn}) J_m(r j_{m,n}) e^{im\theta}. \end{aligned}$$

The squared L_2 and Sobolev H_1 norms of f are

$$\langle f, f\rangle = \sum |a_{mn}|^2, \qquad \|f\|_1^2 = \langle (-\Delta + I) f, f\rangle = \sum (1 + j_{m,n}^2)\, |a_{mn}|^2,$$

so one reasonable scale-invariant measure of roughness would be

$$\frac{\langle \nabla f, \nabla f\rangle}{\langle f, f\rangle} = \frac{\langle -\Delta f, f\rangle}{\langle f, f\rangle} = \frac{\sum j_{m,n}^2\, |a_{mn}|^2}{\sum |a_{mn}|^2}$$

or, similarly but more generally, the ratio of squared Sobolev norms

$$\frac{\|f\|_s^2}{\|f\|_0^2} = \frac{\langle (-\Delta + I)^s f, f\rangle}{\langle f, f\rangle} = \frac{\sum (1 + j_{m,n}^2)^s\, |a_{mn}|^2}{\sum |a_{mn}|^2}$$

for any $s > 0$. Another measure depending only on angular roughness would be

$$\frac{\sum |m|^{2s}\, |a_{mn}|^2}{\sum |a_{mn}|^2}$$

for any $s > 0$. Similar results hold for $d = 3$ (using the spherical Bessel function j_α) or for other boundary conditions. Each of these measures is the moment of some "roughness" aspect, for the discrete probability distribution with masses proportional to the squared Fourier coefficients $|a_{mn}|^2$.

3.2 Fourier Expansions in $d = 1$ Dimension

This section has a brief review of one-dimensional Sobolev spaces on an interval, for context and intuition.

Let $\mathcal{T} = [0, T]$ be a closed interval in $\mathbb{R}^1$. The functions

$$\phi_n(x) = \sin(n\pi x/T)\sqrt{2/T}$$

are a CONS in $L_2(\mathcal{T}, dx)$ of eigenfunctions of $-\Delta$ (with eigenvalues $n^2\pi^2/T^2$), with Dirichlet boundary conditions at $\partial\mathcal{T}$, so every function $f \in L_2(\mathcal{T}, dx)$ has a convergent expansion of the form

$$f(x) = \sum_{n\in\mathbb{N}} a_n \phi_n(x), \tag{10}$$

with coefficients

$$a_n := \int_{\mathcal{T}} f(x)\, \phi_n(x)\, dx.$$

For $s \in \mathbb{R}$ the closed linear span H_s of $\{\phi_n\}$ in the norm

$$\begin{aligned} \|f\|_s &:= \left\{ \sum |a_n|^2 \left(1 + n^2\pi^2/T^2\right)^s \right\}^{\frac{1}{2}} \\ &= \langle (-\Delta + I)^s f, f \rangle^{\frac{1}{2}} \end{aligned} \tag{11}$$

is a Banach space (complete separable normed metric space) whose dual space is H_{-s}. The self-dual Hilbert space H_0 is just $L_2(\mathcal{T}, dx)$.

Differentiating (10) gives

$$\begin{aligned} \|f'\|_0^2 &= \Big\| \sum_{n\in\mathbb{N}} a_n \frac{n\pi}{T} \cos(n\pi \cdot /T) \sqrt{2/T} \Big\|_0^2 \\ &= \sum_{n,m\in\mathbb{N}} a_n a_m \frac{nm\pi^2}{T^2} \frac{2}{T} \int_0^T \cos(n\pi x/T) \cos(m\pi x/T)\, dx \\ &= \sum_{n\in\mathbb{N}} a_n^2 \frac{n^2\,\pi^2}{T^2} = \sum_{n\in\mathbb{N}} |a_n|^2\, n^2\pi^2/T^2 \\ &= \|f\|_1^2 - \|f\|_0^2, \end{aligned}$$

so $f \in H_1$ if and only if $f \in H_0$ and $f' \in H_0$. Similarly one can show that $f \in H_s \Rightarrow f' \in H_{s-1}$ for any $s \in \mathbb{R}$. For $s > 0$, H_s consists of those

functions with s derivatives in L_2, while H_{-s} consists of sth derivatives of L_2 functions.

In particular, for $t \in \mathcal{T}$ the Dirac delta function $\delta_t \in H_{-1}$ but $\delta_t \notin H_0$. For example, for $T = \pi$ and $t = \pi/2$, $f \equiv \delta_t$ has coefficients

$$a_n \equiv \int_0^\pi f(x) \sin(nx) \sqrt{2/\pi}\, dx = \begin{cases} \sqrt{2/\pi} & n \equiv 1 \pmod 4 \\ -\sqrt{2/\pi} & n \equiv 3 \pmod 4 \end{cases},$$

otherwise zero, with eigenvalues n^2, so

$$\|\delta_t\|_s^2 = \frac{2}{\pi} \sum_{k=1}^{\infty} \left(1 + (2k+1)^2\right)^s .$$

This is only finite for $s < -\frac{1}{2}$, so $\delta_t \in H_s$ only for $s < -\frac{1}{2}$.

The boundary $\partial\mathcal{T}$ and boundary conditions play a subtle rôle in $H_s(\mathcal{T})$. For example, in the interior of $\mathcal{T} = [0, T]$ for $T > 0$ the function

$$f(x) = x(T - x)$$

satisfies $f''(x) \equiv -2$ and hence

$$(-\Delta + I) f(x) = x(T - x) + 2$$

and so, at least for non-negative integers s,

$$(-\Delta + I)^s f(x) = x(T - x) + 2s.$$

One might expect $f \in H_s$ for all $s > 0$, with

$$\begin{aligned} \|f\|_s^2 &\equiv \langle (-\Delta + I)^s f,\, f \rangle \\ &\stackrel{?}{=} \int_0^T [x(T - x) + 2s][x(T - x)]\, dx \\ &= T^5/30 + sT^3/3, \end{aligned}$$

suggesting (wrongly) that $f \in H_s$ for all $s > 0$. In fact the coefficients are

$$a_n := \int_{\mathcal{T}} f(x)\, \phi_n(x)\, dx = 4\sqrt{2} T^{5/2}/(n\pi)^3$$

for odd n, and zero for even n, so

$$\begin{aligned}\|f\|_s^2 \equiv & \sum_{n=1}^{\infty} |a_n|^2 \left(n^2\pi^2/T^2+1\right)^s \\ = & \frac{32T^5}{\pi^6} \sum_{k=1}^{\infty} \frac{\left((2k+1)^2\pi^2/T^2+1\right)^s}{(2k+1)^6}\end{aligned}$$

which is only finite for $s < 5/2$. The problem is that even the first derivative f' fails to satisfy Dirichlet boundary conditions $f(\partial\mathcal{T}) = 0$. Integrating by parts,

$$\begin{aligned}\int_{\mathcal{T}} f'(x)\, f'(x)\, dx &= f'(x) f(x)\big|_0^T - \int_{\mathcal{T}} f''(x)\, f(x)\, dx \\ &= -\int_{\mathcal{T}} f''(x)\, f(x)\, dx = \langle(-\Delta)f, f\rangle \\ \int_{\mathcal{T}} f''(x)\, f''(x)\, dx &= f''(x) f'(x)\big|_0^T - \int_{\mathcal{T}} f'''(x)\, f'(x)\, dx \\ &= 4T - f'''(x)\, f(x)\big|_0^T + \int_{\mathcal{T}} f''''(x)\, f(x)\, dx \\ &= \langle(-\Delta)^2 f, f\rangle + 4T\end{aligned}$$

so for $s \geq 2$ a non-zero boundary term enters the integration by parts and the naive calculation fails. Intuitively, what happens is that $f(x)$ takes the constant value of zero outside $\mathcal{T}$ and so derivatives beyond the first pick up something like a Dirac delta function *at the boundary.*

Something similar happens in $d = 2$ dimensions for functions f that satisfy Dirichlet boundary conditions at ∂B^2 but whose derivatives do not, such as

$$f(x, y) = (1 - x^2 - y^2) \vee 0$$

for which $-\Delta f \equiv 4$ and hence $(-\Delta + I)^s f = f + 4s$ in the interior. Still, $f \in H_s$ only for $s < 5/2$ because by circular symmetry its Fourier-Bessel coefficients are $a_{mn} = 0$ for $m \neq 0$, while

$$\begin{aligned}a_{0n} &= \frac{2\pi}{\sqrt{\pi} J_1(j_{0,n})} \int_0^1 (r - r^3) J_0(r j_{0,n})\, dr = \frac{8\sqrt{\pi}}{j_{0,n}^3}, \quad \text{so} \\ \|f\|_n^2 &= 64\pi \sum_{n=1}^{\infty} (1 + \lambda_{0n}^2)^s j_{0,n}^{-6},\end{aligned}$$

which is only finite for $s < 5/2$ since $j_{0,n} \asymp n\pi$.

4 Stochastic Expansions

4.1 Brownian Bridge on One Dimensional Interval

As in Sec. 3.2, let

$$\phi_n(x) = \sin(n\pi x/T)\sqrt{2/T}$$

be a CONS in $L_2(\mathcal{T}, dx)$ for $\mathcal{T} = [0,T] \subset \mathbb{R}^1$, and consider the *Brownian Bridge* Gaussian stochastic process X_t with mean and covariance

$$\mathsf{E}X_t \equiv 0 \qquad \mathsf{Cov}(X_s, X_t) = \mathsf{E}X_s\, X_t = (s \wedge t)\big(1 - (s \vee t)/T\big),$$

identical to unit-rate Brownian motion conditioned to reach $X_T = 0$. The Fourier coefficients for a random path $\{X_t\}$ are Gaussian random variables

$$A_n := \int_{\mathcal{T}} Z_t \phi_n(s)\, dt$$

with mean zero and covariance

$$\begin{aligned}\mathsf{E}A_m\, A_n =& \frac{2}{T^2}\int_{\mathcal{T}^2} (s \wedge t)\big(T - (s \vee t)\big)\sin(m\pi s/T)\, \sin(n\pi t/T)\, ds\, dt \\ =& \begin{cases} 0 & m \neq n \\ \frac{T^2}{n^2\pi^2} & m = n \end{cases}\end{aligned}$$

so the $\{A_n\} \overset{\text{ind}}{\sim} \mathsf{No}\big(0, \big(\frac{T}{n\pi}\big)^2\big)$ are independent and the expected squared H_s norm of the sample path $s \rightsquigarrow Z_s$ is

$$\begin{aligned}\mathsf{E}\|Z_\bullet\|_s^2 =& \sum_{n\in\mathbb{N}} \frac{T^2(1 + n^2\pi^2/T^2)^s}{n^2\pi^2} \\ <& \infty \text{ if and only if } s < \tfrac{1}{2},\end{aligned}$$

with $\mathsf{E}\|Z_\bullet\|_0^2 = T^2/6$. Roughly speaking, Brownian motion paths have just under one-half of a derivative.

Beginning with iid $\zeta_n \overset{\text{iid}}{\sim} \mathsf{No}(0,1)$ one can *construct* a Brownian Bridge process as the sum

$$Z_t := \sum_{n=1}^{\infty} \frac{T}{n\pi}\zeta_n \phi_n(t)$$

or fractional derivatives of it by

$$Z_t^\sigma := \sum_{n=1}^{\infty} \left[\frac{T}{n\pi}\right]^{1-\sigma} \zeta_n \phi_n(t),$$

which will be centered Gaussian processes with about $\frac{1}{2} - \sigma$ derivatives—smooth paths, for $\sigma \ll 0$ or, for $\sigma > 0$, generalized stochastic processes that only make sense as convolutions $Z[\psi] = \int Z_t \psi(t)\, dt$ for $\psi \in H_s$ with $s > \sigma - \frac{1}{2}$.

4.2 Stochastic Expansions in Two Dimensions

As in Section (3.1) let

$$\phi_{mn}(r,\theta) \equiv \frac{1}{\sqrt{\pi}\, J_{|m|+1}(j_{m,n})} J_m(r j_{m,n})\, e^{im\theta} \tag{8}$$

be a CONS in $L_2(B^2)$, and let $\zeta_{mn} \overset{\text{iid}}{\sim} \mathsf{No}(0,1)$ for $m \in \mathbb{Z}$, $n \in \mathbb{N}$. Fix $\sigma \in \mathbb{R}$ and set

$$Z^\sigma(r,\theta) := \sum [j_{m,n}]^\sigma\, \zeta_{mn}\, \phi_{mn}(r,\theta)$$

for $(r,\theta) \in B^2$. The expected squared H_s norm of Z^σ is

$$\begin{aligned} \mathsf{E}\langle Z^\sigma, Z^\sigma\rangle_s &= \mathsf{E}\langle (-\Delta + I)^s\, Z^\sigma, Z^\sigma\rangle \\ &= \sum (j_{m,n}^2 + 1)^s\, j_{m,n}^\sigma \end{aligned}$$

Since $j_{m,n} \asymp \pi(n + |m|/2 - 1/4)$ (Abramowitz and Stegun, 1964, §9.5.12), this is finite by the integral test if and only if

$$\infty > \int_1^\infty (r^2+1)^s r^\sigma\, r\, dr,$$

so $Z^\sigma \in H_s$ almost-surely for $\sigma < -2(s+1)$— or $\sigma < -2$ for $s = 0$.

4.3 Reproducing Kernel Hilbert Space (RKHS)

Now let X_s be an arbitrary mean-zero Gaussian process with (positive definite) covariance kernel

$$k(s,t) = \mathsf{E} X_s X_t$$

for $s, t \in \mathcal{T}$, and consider the Hilbert space $\mathcal{H}$ consisting of limits of linear combinations of the $\{X_{s_j}\}$ for $\{s_j\} \subset \mathcal{T}$. For tame enough functions $f, g : \mathcal{T} \to \mathbb{R}$ this space will include elements $X_f \equiv \int_{\mathcal{T}} f(s) Z_s\, ds$ and $X_g \equiv \int_{\mathcal{T}} g(t) Z_t\, dt$, each Gaussian with mean zero and covariance

$$< X_f, X_g > \equiv \int_{\mathcal{T}^2} f(s) k(s,t) g(t)\, ds\, dt,$$

the inner-product in $L_2(\mathcal{T})$ of f and Kg for the operator $K: \; L_2(\mathcal{T}) \to L_2(\mathcal{T})$ with kernel k,

$$Kg(s) \equiv \int_{\mathcal{T}} k(s,t)\, g(t)\, dt.$$

If $k \in L_2(\mathcal{T}^2)$ that operator is Hilbert-Schmidt, with a complete orthornormal set $\{\phi_n\}$ of eigenfunctions

$$K\phi_n(s) \equiv \int_{\mathcal{T}} k(s,t)\, \phi_n(t)\, dt = \lambda_n \phi_n(s)$$

whose eigenvalues are square-summable, with

$$\int_{\mathcal{T}^2} k(s,t)^2\, ds\, dt = \sum \lambda_n^2 < \infty.$$

In this case for iid $\{\zeta_n\} \overset{\text{iid}}{\sim} \mathsf{No}(0,1)$ the series

$$Z_s \equiv \sum \lambda_n\, \zeta_n\, \phi_n(s)$$

converges almost-surely in L_2 to a Gaussian process with mean zero and covariance k, the so-called *Karhunen-Loève* expansion. The example of Sec. 4.1 was an example of this. As in that example, often k is the Greens function for a differential operator (here $-\partial^2/\partial x^2$ with Dirichlet boundary conditions), and the eigenfunctions may be found as solutions to differential equations.

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