

Notes on Kernels for Normalized Functions

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1 Introduction

Suppose that we want a GP model for a function $n(k)$ that satisfies a momentum-space normalization of the type

$$\int_0^\infty \frac{4\pi dk}{(2\pi)^3} k^2 n(k) = N$$

or, in general

$$\int_0^\infty dk k^2 n(k) = A$$

where $A = 2\pi^2 N$. If we have some data on $n(k)$, we could fit a vanilla GP to it, but there would be no guarantee that any function that one sampled from it would satisfy the normalization condition.

Instead, suppose we start from a zero-mean GP with base covariance kernel $\langle n(k_1)n(k_2) \rangle = C(k_1, k_2)$. We can proceed by updating this kernel based on a zero-noise observation of the normalization integral

$$I[n(\cdot)] \equiv \int_0^\infty dk k^2 n(k). \quad (1.1)$$

The required covariance relations are

$$\begin{aligned} \langle I \times n(k_1) \rangle &= \int_0^\infty dk_2 k_2^2 \langle n(k_2)n(k_1) \rangle \\ &= \int_0^\infty dk_2 k_2^2 \times C(k_1, k_2) \\ &\equiv C_1(k_1), \end{aligned} \quad (1.2)$$

$$\begin{aligned} \langle I^2 \rangle &= \int_0^\infty dk_1 k_1^2 \int_0^\infty dk_2 k_2^2 \langle n(k_2)n(k_1) \rangle \\ &= \int_0^\infty dk_1 \int_0^\infty dk_2 k_1^2 k_2^2 C(k_1, k_2) \\ &\equiv C_0. \end{aligned} \quad (1.3)$$

Given a choice of $C(\cdot, \cdot)$ that permits these integrals to be computed, the updated GP conditioned on the observation $I[n(\cdot)] = A$ has a non-zero mean function $\mu(k)$ given by the standard formula

$$\mu(k) = C_1(k) \times C_0^{-1} \times A, \quad (1.4)$$

and a covariance kernel $K(k_1, k_2)$ given by the equally-standard formula

$$K(k_1, k_2) = C(k_1, k_2) - C_1(k_1)C_0^{-1}C_1(k_2). \quad (1.5)$$

Note that $\int_0^\infty dk \mu(k) = C_0 C_0^{-1} A = A$, and functions $n(k)$ sampled from $GP[\mu(\cdot), K(\cdot, \cdot)]$ have normalizations $I[n(\cdot)]$ that satisfy $\langle I^2 \rangle = \int_0^\infty dk_1 \int_0^\infty dk_2 k_1^2 k_2^2 K(k_1, k_2) = C_0 - C_0 = 0$. So I is fixed at its mean value A with zero uncertainty. In effect, Equation (1.5) shows that $K(\cdot, \cdot)$ is just $C(\cdot, \cdot)$ with the function $C_1(k)$ projected out, so that it has a zero eigenvalue corresponding to this eigenfunction.

In order for this to work, the integrals in Equations (1.2) and (1.3) must exist. This is awkward, because it precludes us from choosing a stationary kernel $C(k_1, k_2) = g(k_1 - k_2)$, for which the integral in Equation (1.3) diverges. This divergence is expected, because a stationary kernel choice in effect asserts that the statistical behavior of the function is the same throughout \mathbb{R} , whereas any function possessing a finite normalization integral in Equation (1.1) must necessarily go to zero faster than k^{-1} as $k \rightarrow \infty$.

Fortunately, we can conveniently taper covariance kernels such as $g(k_1 - k_2)$ using a rapidly-decaying function $f(k)$, so that $C(k_1, k_2) = f(k_1)g(k_1 - k_2)f(k_2)$ —such a kernel is obviously non-negative definite if $g(k_1 - k_2)$ is non-negative definite. This gives hope that we can locate some kernel models for which the required integrals are doable.

2 A Proof-of-Concept Kernel

Let us begin with the popular squared-exponential kernel

$$g(k_1 - k_2) = \exp \left[-\frac{(k_1 - k_2)^2}{\sigma^2} \right], \quad (2.1)$$

and taper it using Gaussians, i.e.

$$f(k) = \exp \left[-\frac{k^2}{\gamma^2} \right], \quad (2.2)$$

so that our covariance model will be

$$\begin{aligned} C(k_1, k_2) &= f(k_1)g(k_1 - k_2)f(k_2) \\ &= \exp \left[-k^T P k \right], \end{aligned} \quad (2.3)$$

where we define $k^T \equiv \begin{bmatrix} k_1 & k_2 \end{bmatrix}$ and

$$P \equiv \begin{bmatrix} a & b \\ b & a \end{bmatrix}, \quad (2.4)$$

with

$$a \equiv \sigma^{-2} + \gamma^{-2} \quad (2.5)$$

$$b \equiv -\sigma^{-2}. \quad (2.6)$$

The required integral $C_1(k_1)$ is given by

$$\begin{aligned} C_1(k_1) &= \int_0^\infty dk_2 k_2^2 \exp \left[-k^T P k \right] \\ &= \int_0^\infty dk_2 k_2^2 \exp \left[-\left(a k_1^2 + 2 b k_1 k_2 + a k_2^2 \right) \right] \\ &= \int_0^\infty dk_2 k_2^2 \exp \left[-a \left(k_2 + b k_1 / a \right)^2 - a \left(1 - b^2 / a^2 \right) k_1^2 \right] \\ &= \exp \left[-a \left(1 - b^2 / a^2 \right) k_1^2 \right] a^{-3/2} \int_{a^{-1/2} b k_1}^\infty ds \left(s - a^{-1/2} b k_1 \right)^2 \exp \left[-s^2 \right] \\ &= \exp \left[-a \left(1 - b^2 / a^2 \right) k_1^2 \right] a^{-3/2} \int_{a^{-1/2} b k_1}^\infty ds \left(s^2 - 2 a^{-1/2} b k_1 s + a^{-1} b^2 k_1^2 \right) \exp \left[-s^2 \right]. \end{aligned} \quad (2.7)$$

We may use

$$\begin{aligned}
\int_l^\infty ds s^2 \exp[-s^2] &= \left\{ \left(-\frac{d}{d\lambda} \right) \int_l^\infty ds \exp[-\lambda s^2] \right\}_{\lambda=1} \\
&= \left\{ \left(-\frac{d}{d\lambda} \right) \lambda^{-1/2} \int_{\lambda^{1/2}l}^\infty du \exp[-u^2] \right\}_{\lambda=1} \\
&= \left\{ \frac{1}{2} \lambda^{-3/2} \int_{\lambda^{1/2}l}^\infty du \exp[-u^2] + \frac{1}{2} \lambda^{-1} l \exp[-\lambda l^2] \right\}_{\lambda=1} \\
&= \frac{\pi^{1/2}}{4} \operatorname{erfc}[l] + \frac{l}{2} \exp[-l^2], \tag{2.8}
\end{aligned}$$

$$\begin{aligned}
\int_l^\infty ds s \exp[-s^2] &= \frac{1}{2} \int_{l^2}^\infty du \exp[-u] \\
&= \frac{1}{2} \exp[-l^2], \tag{2.9}
\end{aligned}$$

and

$$\int_l^\infty ds \exp[-s^2] = \frac{\pi^{1/2}}{2} \operatorname{erfc}[l]. \tag{2.10}$$

The result is

$$\begin{aligned}
C_1(k_1) &= \exp \left[-a \left(1 - b^2/a^2 \right) k_1^2 \right] a^{-3/2} \\
&\times \left\{ \frac{\pi^{1/2}}{4} \operatorname{erfc} \left[a^{-1/2} b k_1 \right] + \frac{a^{-1/2} b k_1}{2} \exp \left[-b^2 k_1^2/a \right] \right. \\
&\quad \left. - 2a^{-1/2} b k_1 \times \frac{1}{2} \exp \left[-b^2 k_1^2/a \right] + a^{-1} b^2 k_1^2 \frac{\pi^{1/2}}{2} \operatorname{erfc} \left[a^{-1/2} b k_1 \right] \right\} \\
&= \frac{\pi^{1/2}}{4} a^{-3/2} \left(1 + 2 \frac{b^2 k_1^2}{a} \right) \exp \left[-a \left(1 - b^2/a^2 \right) k_1^2 \right] \operatorname{erfc} \left[a^{-1/2} b k_1 \right] \\
&\quad - \frac{b k_1}{2a^2} \times \exp \left[-a k_1^2 \right]. \tag{2.11}
\end{aligned}$$

To get an expression for C_0 , one could integrate this expression with respect to k_1 , but the algebra would be very tedious, and fortunately there's a (slightly) better way. Define

$$p(k_1, k_2) \equiv k^T P k, \tag{2.12}$$

and the spheroidal coordinates

$$R = p(k_1, k_2)^{1/2} \tag{2.13}$$

$$t = k_2/k_1. \tag{2.14}$$

The inverse transformation is easily obtained by $R = p(k_1, t k_1)^{1/2} = k_1 p(1, t)^{1/2}$, whence

$$k_1 = R p(1, t)^{-1/2}. \tag{2.15}$$

Similarly, $R = p(t^{-1} k_2, k_2)^{1/2} = k_2 p(t^{-1}, 1)^{1/2} = k_2 t^{-1} p(1, t)^{1/2}$, from which

$$k_2 = R t p(1, t)^{-1/2}. \tag{2.16}$$

The determinant of the Jacobian of the transformation is

$$\begin{aligned}
\det J &= \det \begin{bmatrix} p(1, t)^{-1/2} & t p(1, t)^{-1/2} \\ -R p(1, t)^{-3/2} (at + b) & R (p(1, t)^{-1/2} - p(1, t)^{-3/2} t (at + b)) \end{bmatrix} \\
&= R p(1, t)^{-2} \det \begin{bmatrix} 1 & t \\ -(at + b) & (bt + a) \end{bmatrix} \\
&= R p(1, t)^{-1}. \tag{2.17}
\end{aligned}$$

We therefore have

$$\begin{aligned}
C_0 &= \int_0^\infty dk_1 \int_0^\infty dk_2 k_1^2 k_2^2 \exp[-p(k_1, k_2)] \\
&= \int_0^\infty R^5 dR \exp[-R^2] \times \int_0^\infty dt \frac{t^2}{(at^2 + 2bt + a)^3}.
\end{aligned} \tag{2.18}$$

The first integral is

$$\begin{aligned}
\int_0^\infty R^5 dR \exp[-R^2] &= \frac{1}{2} \int_0^\infty ds s^2 \exp[-s] \\
&= 1.
\end{aligned} \tag{2.19}$$

So we're left with

$$\begin{aligned}
C_0 &= \int_0^\infty dt \frac{t^2}{(at^2 + 2bt + a)^3} \\
&= \int_0^\infty dt \frac{t^2}{((a^{1/2}t + a^{-1/2}b)^2 + a^{-1}(a^2 - b^2))^3}.
\end{aligned} \tag{2.20}$$

Now substitute w for t , where

$$a^{-1/2}(a^2 - b^2)^{1/2}w = a^{1/2}t + a^{-1/2}b$$

so that

$$\begin{aligned}
w &= (a^2 - b^2)^{-1/2} (at + b) \\
t &= a^{-1} (a^2 - b^2)^{1/2} \left[w - (a^2 - b^2)^{-1/2} b \right].
\end{aligned}$$

We then have

$$\begin{aligned}
C_0 &= (a^2 - b^2)^{-3/2} \int_{b(a^2 - b^2)^{-1/2}}^\infty dw \frac{\left[w - (a^2 - b^2)^{-1/2} b \right]^2}{(w^2 + 1)^3} \\
&= (a^2 - b^2)^{-3/2} I_2 - 2(a^2 - b^2)^{-2} b I_1 + (a^2 - b^2)^{-5/2} b^2 I_0,
\end{aligned} \tag{2.21}$$

where

$$I_n \equiv \int_{b(a^2 - b^2)^{-1/2}}^\infty dw \frac{w^n}{(w^2 + 1)^3}. \tag{2.22}$$

With the substitution $w = \tan \psi$, and the fact that $\arctan \left[b (a^2 - b^2)^{-1/2} \right] = \arcsin (b/a) = \arccos \left[(1 - b^2/a^2)^{1/2} \right]$ we have

$$\begin{aligned}
\frac{w^2 dw}{(w^2 + 1)^3} &= \sin^2 \psi \cos^2 \psi d\psi \\
&= \frac{1}{4} \sin^2 2\psi d\psi \\
&= \frac{1}{8} (1 - \cos 4\psi) d\psi \\
&= \frac{1}{8} d \left[\psi - \frac{1}{4} \sin 4\psi \right] \\
&= \frac{1}{8} d \left[\psi - \frac{1}{2} \sin 2\psi \cos 2\psi \right] \\
&= \frac{1}{8} d \left[\psi - \sin \psi \cos \psi (1 - 2 \sin^2 \psi) \right]
\end{aligned}$$

so that

$$\begin{aligned}
I_2 &= \frac{1}{8} \int_{\psi=\arctan[b(a^2-b^2)^{-1/2}]}^{\psi=\pi/2} d \left[\psi - \sin \psi \cos \psi \left(1 - 2 \sin^2 \psi \right) \right] \\
&= \frac{1}{8} \left\{ \pi/2 - \arcsin(b/a) + (b/a) \left(1 - b^2/a^2 \right)^{1/2} \left(1 - 2b^2/a^2 \right) \right\} \\
&= \frac{1}{8} \left\{ \pi/2 - \arcsin(b/a) + a^{-4} b \left(a^2 - b^2 \right)^{1/2} \left(a^2 - 2b^2 \right) \right\}.
\end{aligned} \tag{2.23}$$

Similarly,

$$\begin{aligned}
\frac{w \, dw}{(w^2 + 1)^3} &= \sin \psi \cos^3 \psi \, d\psi \\
&= \frac{1}{4} \sin 2\psi (1 + \cos 2\psi) \, d\psi \\
&= \left(\frac{1}{4} \sin 2\psi + \frac{1}{8} \sin 4\psi \right) d\psi \\
&= d \left[-\frac{1}{8} \cos 2\psi - \frac{1}{32} \cos 4\psi \right] \\
&= -d \left[\frac{1}{8} (1 - 2 \sin^2 \psi) + \frac{1}{32} (1 - 2 \sin^2 2\psi) \right] \\
&= -d \left[\frac{1}{8} (1 - 2 \sin^2 \psi) + \frac{1}{32} (1 - 8 \sin^2 \psi \cos^2 \psi) \right],
\end{aligned}$$

so that

$$\begin{aligned}
I_1 &= \frac{1}{32} \int_{\psi=\arctan[b(a^2-b^2)^{-1/2}]}^{\psi=\pi/2} d \left[-4 (1 - 2 \sin^2 \psi) - (1 - 8 \sin^2 \psi \cos^2 \psi) \right] \\
&= \frac{1}{32} \left\{ 3 + 4 (1 - 2b^2/a^2) + (1 - 8 (b^2/a^2) (1 - b^2/a^2)) \right\} \\
&= \frac{1}{32} \{ 8 - 16b^2/a^2 + 8b^4/a^4 \} \\
&= \frac{1}{4a^4} \{ a^4 - 2a^2b^2 + b^4 \} \\
&= \frac{(a^2 - b^2)^2}{4a^4}.
\end{aligned} \tag{2.24}$$

Finally,

$$\begin{aligned}
\frac{dw}{(w^2+1)^3} &= \cos^4 \psi \, d\psi \\
&= \frac{1}{4} (1 + \cos 2\psi)^2 \, d\psi \\
&= \frac{1}{4} \left[1 + 2 \cos 2\psi + \frac{1}{2} (1 + \cos 4\psi) \right] d\psi \\
&= \frac{1}{4} d \left[\frac{3}{2} \psi + \sin 2\psi + \frac{1}{8} \sin 4\psi \right] \\
&= \frac{1}{4} d \left[\frac{3}{2} \psi + 2 \sin \psi \cos \psi + \frac{1}{4} \sin 2\psi \cos 2\psi \right] \\
&= \frac{1}{4} d \left[\frac{3}{2} \psi + 2 \sin \psi \cos \psi + \frac{1}{2} \sin \psi \cos \psi (1 - 2 \sin^2 \psi) \right] \\
&= \frac{1}{4} d \left[\frac{3}{2} \psi + \frac{5}{2} \sin \psi \cos \psi - \sin^3 \psi \cos \psi \right],
\end{aligned}$$

and we find

$$\begin{aligned}
I_0 &= \frac{1}{4} \int_{\psi=\arctan[b(a^2-b^2)^{-1/2}]}^{\psi=\pi/2} d \left[\frac{3}{2} \psi + \frac{5}{2} \sin \psi \cos \psi - \sin^3 \psi \cos \psi \right] \\
&= \frac{1}{4} \left\{ \frac{3\pi}{4} - \frac{3}{2} \arcsin(b/a) - \frac{5}{2} (b/a) (1 - b^2/a^2)^{1/2} + (b/a)^3 (1 - b^2/a^2)^{1/2} \right\} \\
&= \frac{1}{8} \left\{ \frac{3\pi}{2} - 3 \arcsin(b/a) - (b/a) (1 - b^2/a^2)^{1/2} (5 - 2b^2/a^2) \right\} \\
&= \frac{1}{8} \left\{ \frac{3\pi}{2} - 3 \arcsin(b/a) - a^{-4} b (a^2 - b^2)^{1/2} (5a^2 - 2b^2) \right\}. \tag{2.25}
\end{aligned}$$

Final assembly:

$$\begin{aligned}
C_0 &= (a^2 - b^2)^{-3/2} \times \frac{1}{8} \left\{ \pi/2 - \arcsin(b/a) + a^{-4} b (a^2 - b^2)^{1/2} (a^2 - 2b^2) \right\} \\
&\quad - 2 (a^2 - b^2)^{-2} b \times \frac{(a^2 - b^2)^2}{4a^4} \\
&\quad + (a^2 - b^2)^{-5/2} b^2 \times \frac{1}{8} \left\{ \frac{3\pi}{2} - 3 \arcsin(b/a) - a^{-4} b (a^2 - b^2)^{1/2} (5a^2 - 2b^2) \right\} \\
&= \frac{1}{8} (a^2 - b^2)^{-5/2} (a^2 + 2b^2) \left[\frac{\pi}{2} - \arcsin(b/a) \right] - \frac{b}{2a^4} \\
&\quad + \frac{1}{8} (a^2 - b^2)^{-2} a^{-4} b \left[(a^2 - b^2) (a^2 - 2b^2) - b^2 (5a^2 - 2b^2) \right] \\
&= \frac{1}{8} (a^2 - b^2)^{-5/2} (a^2 + 2b^2) \left[\frac{\pi}{2} - \arcsin(b/a) \right] - \frac{b}{2a^4} \\
&\quad + \frac{1}{8} (a^2 - b^2)^{-2} a^{-4} b [a^4 - 8a^2 b^2 + 4b^4] \\
&= \frac{1}{8} (a^2 - b^2)^{-5/2} (a^2 + 2b^2) \left[\frac{\pi}{2} - \arcsin(b/a) \right] \\
&\quad + \frac{1}{8} (a^2 - b^2)^{-2} a^{-4} b \left[a^4 - 8a^2 b^2 + 4b^2 - 4(a^2 - b^2)^2 \right] \\
&= \frac{1}{8} (a^2 - b^2)^{-5/2} (a^2 + 2b^2) \left[\frac{\pi}{2} - \arcsin(b/a) \right] + \frac{1}{8} (a^2 - b^2)^{-2} a^{-4} b [-3a^4] \\
&= \frac{1}{8} (a^2 - b^2)^{-5/2} (a^2 + 2b^2) \left[\frac{\pi}{2} - \arcsin(b/a) \right] - \frac{3}{8} (a^2 - b^2)^{-2} b. \tag{2.26}
\end{aligned}$$