Autocorrelation Function Approximately Corresponding to a Second Derivative
Bill Menke, December 20, 2021

One way to analyze the relationship between a covariance matrix, $\mathbf{C}_m$, and the corresponding weighting matrices, $\mathbf{C}_m^{-½}$, is to take the limit in which the number of rows, $N \to \infty$, and the spacing in distance, $\Delta x \to 0$, so that the identity, $\mathbf{C}_m^{-½}\mathbf{C}_m^{-½}\mathbf{C}_m = \mathbf{I}$, becomes the differential equation [Menke and Eilon, 2015; Menke and Creel, 2021]:

$$\mathcal{D}^{\dagger}\mathcal{D}\, c(x) = \delta(x) \tag{1}$$

with boundary conditions, $c(x) \to 0$ as $|x| \to \infty$. Here, the autocorrelation function, $c(x)$, is analogous to $\mathbf{C}_m$, the differential operator, $\mathcal{D}$, is analogous to $\mathbf{C}_m^{-½}$, the Dirac function, $\delta(x)$, is analogous to $\mathbf{I}$, and x is lag. By specifying a $\mathcal{D}$ and solving for $c(x)$, we have identified the $c(x)$ corresponding to a given $\mathcal{D}$. Unfortunately, when $\mathcal{D} = \mathrm{d}^2/\mathrm{d}x^2$, the solution cannot satisfy the boundary conditions, because it is a polynomial, and no polynomial (except zero) goes to zero at $\pm\infty$. The best that we can do is to consider a differential operator that is only approximately a second derivative. On possible choice is:

$$\mathcal{D} = \frac{1}{a}\left(s^2 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \tag{2}$$

Here, s is a scale parameter, and the constant, a, will be chosen later so that $c(0) = \gamma^2$, where γ^2 is a variance. The condition under which (2) approximates a second derivative can be understood by considering the oscillatory function, $y(x) = A\cos(k_0 x)$. Applying the operator yields:

$$\mathcal{D}y = \frac{1}{a}\left(s^2 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)y = \frac{1}{a}(s^2 + k_0^2)y \tag{3}$$

Increasing the wavenumber, while holding the scale parameter fixed, leads to the limit:

$$\lim_{k_0^2 \to \infty} \mathcal{D}y = \frac{1}{a}k_0^2 y = -\frac{1}{a}\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} \tag{4}$$

In this limit, $\mathcal{D}y \propto -\mathrm{d}^2y/\mathrm{d}x^2$ and the operator, $\mathcal{D}$, approximately acts as a second derivative. Thus, the approximation is most accurate when the scale length, k_0^{-1}, of features that are being determined is smaller than the scale length, s^{-1}, over which the noise correlates.

We now solve for $c(x)$. Combining Equations (1) and (2) and Fourier transforming position, x, to wavenumber, k, yields:

$$(s^2 + k^2)^2 \ \tilde{c}(k) = a^2 \quad \text{or} \quad \tilde{c}(k) = \frac{a^2}{(s^2 + k^2)^2}$$

(13.30)

Taking the inverse Fourier transform yields:

$$c(x) = a^2 \int_{-\infty}^{\infty} \tilde{c}(k) \exp(ikx)\, \mathrm{d}k = 2a^2 \int_{0}^{\infty} \frac{\cos(kx)}{(s^2 + k^2)^2} \mathrm{d}k = \frac{\pi a^2}{2s^3} (1 + s|x|) \exp(-s|x|)$$

(13.31)

Here, we have used integral 3.729.1 of Gradshteyn and Ryzhik (1980). Choosing $a^2 = 2s^3\gamma^2/\pi$ yields:

$$c(x) = \gamma^2 (1 + s|x|) \exp(-s|x|) \quad \text{and}$$

$$\mathcal{D} = \left(\frac{\pi}{2s^3\gamma^2}\right)^{½} \left(s^2 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \approx -\left(\frac{\pi}{2s^3\gamma^2}\right)^{½} \frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

(13.32)

The autocorrelation function, $c(x)$, has a shape similar to that of a Gaussian at small $|x|$, but is much longer tailed (Figure 1).

References

Gradshteyn, I.S. and Ryzhik, I.M., 1980, Table of Integral, Series and Products, Corrected and Enlarged Edition, Academic Press, 1160pp.

Menke, W. and Creel, R.C., 2021, Gaussian Process Regression Reviewed in the Context of Inverse Theory, Surveys in Geophysics 42, 473–503.

Menke, W. and Eilon, Z. Relationship between data smoothing and the regularization of inverse problems, Pure and Applied Geophysics 172, 2711-2726, 2015.

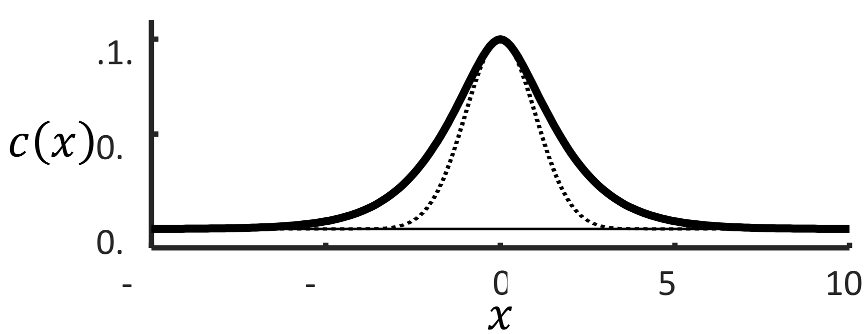

Figure 1. Autocorrelation function, $c(x)$ (bold curve), as defined in Equation (13.32), with amplitude, $\gamma^2 = 1$ and scale parameter, $s = 0.1$, compared to a Gaussian autocorrelation function (dotted curve) with the same amplitude and scale parameter.