Matérn52 Kernel With Derivatives

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1 Matérn 52 Kernel

$$k(r) = (1 + \sqrt{5}r + \frac{5}{3}r^2)\exp\left(-\sqrt{5}r\right) \tag{1}$$

$$r(\mathbf{x}^m, \mathbf{x}^n) = \sqrt{\sum_d \frac{(x_d^m - x_d^n)^2}{l_d^2}} \tag{2}$$

2 First Derivatives

$$\begin{aligned}
\frac{dk}{dr} = \frac{d\left(1 + \sqrt{5}r + \frac{5}{3}r^2\right)}{dr}\exp\left(-\sqrt{5}r\right) + \left(1 + \sqrt{5}r + \frac{5}{3}r^2\right)\frac{d\exp(-\sqrt{5}r)}{dr} = \\
= \left(\sqrt{5} + \frac{10}{3}r\right)\exp\left(-\sqrt{5}r\right) + (-\sqrt{5})\left(1 + \sqrt{5}r + \frac{5}{3}r^2\right)\exp\left(-\sqrt{5}r\right) = \\
= \left(\sqrt{5} + \frac{10}{3}r\right)\exp\left(-\sqrt{5}r\right) - \left(\sqrt{5} + 5r + \frac{5\sqrt{5}}{3}r^2\right)\exp\left(-\sqrt{5}r\right) = \\
= \exp\left(-\sqrt{5}r\right)\left(\sqrt{5} + \frac{10}{3}r - \sqrt{5} - 5r - \frac{5\sqrt{5}}{3}r^2\right) = \\
= \exp\left(-\sqrt{5}r\right)\left(-\frac{5}{3}r - \frac{5\sqrt{5}}{3}r^2\right) = \\
= -\frac{5}{3}r\left(1 + \sqrt{5}r\right)\exp\left(-\sqrt{5}r\right)
\end{aligned} \tag{3}$$

$$
\begin{aligned}
\frac{\partial r}{\partial x_i^n} = \frac{\partial \left(\sum_d \frac{(x_d^m - x_d^n)^2}{l_d^2}\right)^{\frac{1}{2}}}{\partial x_i^n} = \\
= \frac{1}{2}\left(\sum_d \frac{(x_d^m - x_d^n)^2}{l_d^2}\right)^{-\frac{1}{2}} \frac{2}{l_i^2}\left(x_i^m - x_i^n\right)(-1) = \\
= -\frac{x_i^m - x_i^n}{r l_i^2}
\end{aligned}
\tag{4}
$$

$$
\begin{aligned}
\frac{\partial r}{\partial x_j^m} = \frac{\partial \left(\sum_d \frac{(x_d^m - x_d^n)^2}{l_d^2}\right)^{\frac{1}{2}}}{\partial x_j^m} = \\
= \frac{1}{2}\left(\sum_d \frac{(x_d^m - x_d^n)^2}{l_d^2}\right)^{-\frac{1}{2}} \frac{2}{l_j^2}\left(x_j^m - x_j^n\right) = \\
= \frac{x_j^m - x_j^n}{r l_j^2}
\end{aligned}
\tag{5}
$$

$$
\begin{aligned}
\frac{\partial k}{\partial x_i^n} = \frac{dk}{dr}\frac{\partial r}{\partial x_i^n} = \\
= -\frac{5}{3} r\left(1 + \sqrt{5} r\right)\exp\left(-\sqrt{5} r\right)\left(-\frac{x_i^m - x_i^n}{r l_i^2}\right) = \\
= \frac{5}{3}\left(1 + \sqrt{5} r\right)\exp\left(-\sqrt{5} r\right)\left(\frac{x_i^m - x_i^n}{l_i^2}\right)
\end{aligned}
\tag{6}
$$

3 Second Derivatives

$$\frac{d^2k}{dr^2} = \frac{d\left(-\frac{5}{3}r\left(1+\sqrt{5}r\right)\exp(-\sqrt{5}r)\right)}{dr} =$$

$$= \frac{d\left(-\frac{5}{3}r\right)}{dr}\left(1+\sqrt{5}r\right)\exp\left(-\sqrt{5}r\right)+$$

$$\left(-\frac{5}{3}r\right)\frac{d\left(1+\sqrt{5}r\right)}{dr}\exp\left(-\sqrt{5}r\right)+\left(-\frac{5}{3}r\right)\left(1+\sqrt{5}r\right)\frac{d\exp\left(-\sqrt{5}r\right)}{dr} =$$

$$= -\frac{5}{3}\left(1+\sqrt{5}r\right)\exp\left(-\sqrt{5}r\right)+\left(-\frac{5}{3}r\right)\left(\sqrt{5}\right)\exp\left(-\sqrt{5}r\right)+\left(-\frac{5}{3}r\right)\left(1+\sqrt{5}r\right)\left(-\sqrt{5}\right)\exp\left(-\sqrt{5}r\right) =$$

$$= \left(-\frac{5}{3}-\frac{5\sqrt{5}}{3}r\right)\exp\left(-\sqrt{5}r\right)-\frac{5\sqrt{5}}{3}r\exp\left(-\sqrt{5}r\right)+\left(\frac{5\sqrt{5}}{3}r+\frac{25}{3}r^2\right)\exp\left(-\sqrt{5}r\right) =$$

$$= \exp\left(-\sqrt{5}r\right)\left(-\frac{5}{3}-\frac{5\sqrt{5}}{3}r-\frac{5\sqrt{5}}{3}r+\frac{5\sqrt{5}}{3}r+\frac{25}{3}r^2\right) =$$

$$= \exp\left(-\sqrt{5}r\right)\left(-\frac{5}{3}-\frac{5\sqrt{5}}{3}r+\frac{25}{3}r^2\right) =$$

$$= \frac{5}{3}\left(5r^2-\sqrt{5}r-1\right)\exp\left(-\sqrt{5}r\right) \quad (7)$$

$$\frac{\partial}{\partial x_j^m}\frac{\partial r}{\partial x_i^n} = \frac{\partial}{\partial x_j^m}\left(-\frac{x_i^m-x_i^n}{l_i^2}\left(\frac{1}{r}\right)\right) =$$

$$= \frac{\partial}{\partial x_j^m}\left(-\frac{x_i^m-x_i^n}{l_i^2}\right)\frac{1}{r}+\left(-\frac{x_i^m-x_i^n}{l_i^2}\right)\frac{\partial}{\partial x_j^m}\left(\sum_d\frac{(x_d^m-x_d^n)^2}{l_d^2}\right)^{-\frac{1}{2}} =$$

$$= -\frac{1}{rl_i^2}\delta_{ij}+\left(-\frac{x_i^m-x_i^n}{l_i^2}\right)\left(-\frac{1}{2}\right)\left(\sum_d\frac{(x_d^m-x_d^n)^2}{l_d^2}\right)^{-\frac{3}{2}}\frac{2}{l_j^2}\left(x_j^m-x_j^n\right) =$$

$$= \frac{x_j^m-x_j^n}{l_j^2}\frac{x_i^m-x_i^n}{l_i^2}\frac{1}{r^3}-\frac{1}{rl_i^2}\delta_{ij} \quad (8)$$

$$\frac{\partial^2k}{\partial x_j^m\partial x_i^n} = \frac{\partial}{\partial x_j^m}\left(\frac{\partial k}{\partial x_i^n}\right) = \frac{\partial}{\partial x_j^m}\left(\frac{dk}{dr}\frac{\partial r}{\partial x_i^n}\right) =$$

$$\frac{\partial}{\partial x_j^m}\left(\frac{dk}{dr}\right)\frac{\partial r}{\partial x_i^n}+\frac{dk}{dr}\frac{\partial}{\partial x_j^m}\left(\frac{\partial r}{\partial x_i^n}\right) =$$

$$= \frac{d}{dr}\left(\frac{dk}{dr}\right)\frac{\partial r}{\partial x_j^m}\frac{\partial r}{\partial x_i^n}+\frac{dk}{dr}\frac{\partial}{\partial x_j^m}\left(\frac{\partial r}{\partial x_i^n}\right) \quad (9)$$

Substituting in terms in Equation 9 gives

$$\frac{\partial^2 k}{\partial x_j^m \partial x_i^n} =$$

$$= \frac{5}{3}\left(5r^2 - \sqrt{5}r - 1\right)\exp\left(-\sqrt{5}r\right)\left(-\frac{x_i^m - x_i^n}{rl_i^2}\right)\left(\frac{x_j^m - x_j^n}{rl_j^2}\right)$$

$$+ -\frac{5}{3}r\left(1+\sqrt{5}r\right)\exp\left(-\sqrt{5}r\right)\left(\frac{x_j^m - x_j^n}{l_j^2}\frac{x_i^m - x_i^n}{l_i^2}\frac{1}{r^3} - \frac{1}{rl_i^2}\delta_{ij}\right) \quad (10)$$

To simplify, define b

$$b = \left(\frac{x_i^m - x_i^n}{l_i^2}\right)\left(\frac{x_j^m - x_j^n}{l_j^2}\right) \quad (11)$$

Equation 10 becomes

$$-\frac{5}{3r^2}\left(5r^2 - \sqrt{5}r - 1\right)\exp\left(-\sqrt{5}r\right)b - \frac{5}{3}r\left(1+\sqrt{5}r\right)\exp\left(-\sqrt{5}r\right)\left(\frac{b}{r^3} - \frac{\delta_{ij}}{rl_i^2}\right) =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[\frac{b}{r^2}\left(5r^2 - \sqrt{5}r - 1\right) + r\left(1+\sqrt{5}r\right)\left(\frac{b}{r^3} - \frac{\delta_{ij}}{rl_i^2}\right)\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[\frac{5br^2}{r^2} - \frac{\sqrt{5}br}{r^2} - \frac{b}{r^2} + \left(r + \sqrt{5}r^2\right)\left(\frac{b}{r^3} - \frac{\delta_{ij}}{rl_i^2}\right)\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[\frac{5br^2}{r^2} - \frac{\sqrt{5}br}{r^2} - \frac{b}{r^2} + \frac{br}{r^3} - \frac{r\delta_{ij}}{rl_i^2} + \frac{\sqrt{5}br^2}{r^3} - \frac{\sqrt{5}r^2\delta_{ij}}{rl_i^2}\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[5b - \frac{\sqrt{5}b}{r} - \frac{b}{r^2} + \frac{b}{r^2} - \frac{\delta_{ij}}{l_i^2} + \frac{\sqrt{5}b}{r} - \frac{\sqrt{5}r\delta_{ij}}{l_i^2}\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[5b - \frac{\delta_{ij}}{l_i^2} - \frac{\sqrt{5}r\delta_{ij}}{l_i^2}\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[5b - \frac{\delta_{ij}}{l_i^2}\left(1+\sqrt{5}r\right)\right] =$$

$$= -\frac{5}{3}\exp\left(-\sqrt{5}r\right)\left[5\left(\frac{x_i^m - x_i^n}{l_i^2}\right)\left(\frac{x_j^m - x_j^n}{l_j^2}\right) - \frac{\delta_{ij}}{l_i^2}\left(1+\sqrt{5}r\right)\right] \quad (12)$$

4 Diagonal

For t training points with d input dimensions, the first t entries of the diagonal will be $cov(f^t, f^t)$. The next td entries will be $cov(\omega_d^t, \omega_d^t)$. The first t entries will be $k(0) = 1$. When $m = n$ and $i = j$, then $r = 0$, so Equation 12 simplifies to

$$\frac{\partial^2 k}{\partial x_j^m \partial x_j^m} = \frac{5}{3l_j^2} \tag{13}$$