Gaussian Processes with Derivative Observations

$$\mathrm{cov}\left(f, f'\right) = k(\mathbf{x}, \mathbf{z}) = k(s), \; s = s(r, l), \; r = r(\mathbf{x}, \mathbf{z})$$

$$\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial k(\mathbf{x}, \mathbf{z})}{\partial z_j} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial z_j}$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, f'\right) = \frac{\partial k(\mathbf{x}, \mathbf{z})}{\partial x_i} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial x_i} = \mathrm{cov}\left(f, \frac{\partial f'}{\partial z_i}\right) \text{ (symmetry)}$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial^2 k(\mathbf{x}, \mathbf{z})}{\partial x_i \partial z_j} = \frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j} + \frac{\partial k}{\partial s}\frac{\partial^2 s}{\partial x_i \partial z_j}$$

$$\frac{\partial k}{\partial \log l} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial l}\frac{\partial \log l}{\partial l} = l\frac{\partial k}{\partial s}\frac{\partial s}{\partial l}$$

$$\frac{\partial^2 k}{\partial z_j \partial \log l} = l\left(\frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial z_j}\frac{\partial s}{\partial l} + \frac{\partial k}{\partial s}\frac{\partial^2 s}{\partial z_j \partial l}\right)$$

$$\frac{\partial^2 k}{\partial x_i \partial \log l} = l\left(\frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial l} + \frac{\partial k}{\partial s}\frac{\partial^2 s}{\partial x_i \partial l}\right)$$

$$\frac{\partial^3 k}{\partial x_i \partial z_j \partial \log l} = l\left(\frac{\partial^3 k}{\partial s^3}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j}\frac{\partial s}{\partial l} + \frac{\partial^2 k}{\partial s^2}\left(\frac{\partial^2 s}{\partial x_i \partial z_j}\frac{\partial s}{\partial l} + \frac{\partial s}{\partial x_i}\frac{\partial^2 s}{\partial z_j \partial l} + \frac{\partial s}{\partial x'_k}\frac{\partial^2 s}{\partial x_i \partial l}\right) + \frac{\partial k}{\partial s}\frac{\partial^3 s}{\partial x_i \partial z_j \partial l}\right)$$

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp(s), \quad s(r, l) = -\frac{r^2}{2l^2}, \quad r(\mathbf{x}, \mathbf{z}) = \sqrt{\sum_{i=1}^{d} (x_i - z_i)^2}$$

$$\frac{\partial k}{\partial s} = k, \quad \frac{\partial^2 k}{\partial s^2} = k, \quad \frac{\partial^3 k}{\partial s^3} = k$$

$$\frac{\partial s}{\partial x_i} = -\frac{x_i - z_i}{l^2}, \quad \frac{\partial s}{\partial z_j} = \frac{x_j - z_j}{l^2}, \quad \frac{\partial^2 s}{\partial x_i \partial z_j} = \frac{\delta(i, j)}{l^2}$$

$$\frac{\partial s}{\partial l} = -\frac{2}{l} s, \quad \frac{\partial^2 s}{\partial x_i \partial l} = -\frac{2}{l} \frac{\partial s}{\partial x_i}, \quad \frac{\partial^2 s}{\partial z_j \partial l} = -\frac{2}{l} \frac{\partial s}{\partial z_j}, \quad \frac{\partial^3 s}{\partial x_i \partial z_j \partial l} = -\frac{2}{l} \frac{\partial^2 s}{\partial x_i \partial z_j}$$

$$k_{\nu=3/2} = \sigma_f^2\,(1-s)\exp(s), \quad s(r,l) = -\frac{\sqrt{3}r}{l}, \quad r(\mathbf{x},\mathbf{z}) = \sqrt{\sum_{i=1}^{d}(x_i - z_i)^2}, \;\Rightarrow\; s^2 = \frac{3r^2}{l^2}$$

$$\frac{\partial k}{\partial s} = \sigma_f^2\,(-1 + (1-s))\exp(s) = \sigma_f^2\,(-s)\exp(s)$$

$$\frac{\partial^2 k}{\partial s^2} = \sigma_f^2\,(-1-s)\exp(s)$$

$$\frac{\partial^3 k}{\partial s^3} = \sigma_f^2\,(-1 + (-1-s))\exp(s) = \sigma_f^2\,(-2-s)\exp(s)$$

$$\frac{\partial s}{\partial x_i} = \frac{3(x_i - z_i)}{l^2 s}, \quad \frac{\partial s}{\partial z_j} = -\frac{3(x_j - z_j)}{l^2 s}$$

$$\Rightarrow s\frac{\partial s}{\partial x_i} = \frac{3(x_i - z_i)}{l^2} \Rightarrow \frac{\partial s}{\partial z_j}\frac{\partial s}{\partial x_i} + s\frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{3\delta(i,j)}{l^2}$$

$$\Rightarrow \frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{3\delta(i,j)}{l^2 s} - \frac{1}{s}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j}$$

$$\frac{\partial s}{\partial l} = -\frac{1}{l}s, \quad \frac{\partial^2 s}{\partial x_i \partial l} = -\frac{1}{l}\frac{\partial s}{\partial x_i}, \quad \frac{\partial^2 s}{\partial z_j \partial l} = -\frac{1}{l}\frac{\partial s}{\partial z_j}, \quad \frac{\partial^3 s}{\partial x_i \partial z_j \partial l} = -\frac{1}{l}\frac{\partial^2 s}{\partial x_i \partial z_j}$$

$$k_{s<1}(s) = \sigma_f^2 \left(\frac{2+\cos(2\pi s)}{3}(1-s) + \frac{1}{2\pi}\sin(2\pi s) \right), \quad s(r,l) = \frac{r}{l}, r(\mathbf{x},\mathbf{z}) = \sqrt{\sum_{i=1}^{d}(x_i - z_i)^2}, \Rightarrow s^2 = \frac{r^2}{l^2}$$

$$\frac{\partial k}{\partial s} = \sigma_f^2 \left(\frac{-2\pi\sin(2\pi s)}{3}(1-s) - \frac{2+\cos(2\pi s)}{3} + \cos(2\pi s) \right) = \frac{2\sigma_f^2}{3}\left(\cos(2\pi s) - \pi\sin(2\pi s)(1-s) - 1\right)$$

$$\frac{\partial^2 k}{\partial s^2} = \frac{2\sigma_f^2}{3}\left(-2\pi\sin(2\pi s) - 2\pi^2\cos(2\pi s)(1-s) + \pi\sin(2\pi s)\right) = \frac{-2\pi\sigma_f^2}{3}\left(\sin(2\pi s) + 2\pi\cos(2\pi s)(1-s)\right)$$

$$\frac{\partial^3 k}{\partial s^3} = \frac{-2\pi\sigma_f^2}{3}\left(2\pi\cos(2\pi s) - 4\pi^2\sin(2\pi s)(1-s) - 2\pi\cos(2\pi s)\right) = \frac{8\pi^3\sigma_f^2}{3}\sin(2\pi s)(1-s)$$

$$2s\frac{\partial s}{\partial x_i} = \frac{2(x_i - z_i)}{l^2} \Rightarrow \frac{\partial s}{\partial x_i} = \frac{x_i - z_i}{l^2 s}, \frac{\partial s}{\partial z_j} = -\frac{x_j - z_j}{l^2 s}$$

$$\Rightarrow \frac{\partial s}{\partial z_j}\frac{\partial s}{\partial x_i} + s\frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{\delta(i,j)}{l^2} \Rightarrow \frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{\delta(i,j)}{l^2 s} - \frac{1}{s}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j}$$

$$\frac{\partial s}{\partial l} = -\frac{1}{l}s, \quad \frac{\partial^2 s}{\partial x_i \partial l} = -\frac{1}{l}\frac{\partial s}{\partial x_i}, \quad \frac{\partial^2 s}{\partial z_j \partial l} = -\frac{1}{l}\frac{\partial s}{\partial z_j}, \quad \frac{\partial^3 s}{\partial x_i \partial z_j \partial l} = -\frac{1}{l}\frac{\partial^2 s}{\partial x_i \partial z_j}$$

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp(s), \quad s(r, l) = -\frac{r^2}{2l^2}, \quad r(\mathbf{x}, \mathbf{z}) = \sqrt{\sum_{i=1}^{d} (x_i - z_i)^2}$$

$$\frac{\partial k}{\partial z_j} = \sigma_f^2 \exp(s) \frac{x_j - z_j}{l^2} = k \frac{x_j - z_j}{l^2}$$

$$\frac{\partial^2 k}{\partial \log l \partial z_j} = l \sigma_f^2 \exp(s) \frac{x_j - z_j}{l^2} \left(\frac{-2}{l} + \frac{-2}{l} s \right) = \frac{\partial k}{\partial z_j} (-2s - 2)$$

$$\frac{\partial^2 k}{\partial x_i \partial z_j} = \sigma_f^2 \exp(s) \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) = k \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right)$$

$$\frac{\partial^3 k}{\partial \log l \partial x_i \partial z_j} = \frac{\partial k}{\partial \log l} \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) + k \left(\frac{-2\delta(i,j)}{l^3} + 4 \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right)$$

$$k_{\nu=3/2} = \sigma_f^2 \,(1-s)\exp(s), \quad s(r,l) = -\frac{\sqrt{3}r}{l}, \quad r(\mathbf{x},\mathbf{z}) = \sqrt{\sum_{i=1}^{d}(x_i - z_i)^2}, \;\Rightarrow\; s^2 = \frac{3r^2}{l^2}$$

$$\frac{\partial k}{\partial z_j} = \sigma_f^2 \exp(s)\left(-\frac{3(x_j - z_j)}{l^2 s}\right)(-1 + (1-s)) = 3\sigma_f^2 \exp(s)\frac{(x_j - z_j)}{l^2}$$

$$\frac{\partial^2 k}{\partial \log l \,\partial z_j} = l\sigma_f^2 \exp(s)\frac{3(x_j - z_j)}{l^2}\left(\frac{-2}{l} + \frac{\sqrt{3}r}{l^2}\right) = \frac{\partial k}{\partial z_j}(-s-2)$$

$$\frac{\partial^2 k}{\partial x_i \partial z_j} = 3\sigma_f^2 \exp(s)\left(\frac{\delta(i,j)}{l^2} + \frac{3}{s}\frac{(x_i - z_i)}{l^2}\frac{(x_j - z_j)}{l^2}\right)$$

$$\frac{\partial^3 k}{\partial \log l \,\partial x_i \partial z_j} = 3\sigma_f^2 \exp(s)\left(\frac{-2\delta(i,j)}{l^2} - \frac{9}{s}\frac{(x_i - z_i)}{l^2}\frac{(x_j - z_j)}{l^2}\right) - \frac{\partial^2 k}{\partial x_i \partial z_j} s$$

what if $s = 0$?

$$\lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial^2 k}{\partial x_i \partial z_j} = 3\sigma_f^2 \frac{\delta(i,j)}{l^2}$$

$$\lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial^3 k}{\partial \log l \,\partial x_i \partial z_j} = -6\sigma_f^2 \frac{\delta(i,j)}{l^2}$$

$$\frac{\partial k}{\partial \log l} = l\,\frac{\partial k}{\partial s}\frac{\partial s}{\partial l} = l\,\frac{\partial k}{\partial s}\left(\frac{-s}{l}\right) = -\frac{\partial k}{\partial s}s$$

$$\frac{\partial k}{\partial z_j} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial z_j} = -\frac{\partial k}{\partial s}\frac{x_j - z_j}{l^2 s} = -\frac{2\sigma_f^2}{3}\left(\cos(2\pi s) - \pi\sin(2\pi s)(1-s) - 1\right)\frac{x_j - z_j}{l^2 s}$$

$$\frac{\partial^2 k}{\partial \log l\,\partial z_j} = l\left(\frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial l}\left(-\frac{x_j - z_j}{l^2 s}\right) - \frac{1}{l}\frac{\partial k}{\partial z_j}\right) = \frac{\partial^2 k}{\partial s^2}\frac{x_j - z_j}{l^2} - \frac{\partial k}{\partial z_j}$$

$$= \frac{-2\pi\sigma_f^2}{3}\left(\sin(2\pi s) + 2\pi\cos(2\pi s)(1-s)\right)\frac{x_j - z_j}{l^2} - \frac{\partial k}{\partial z_j}$$

$$\frac{\partial^2 k}{\partial x_i \partial z_j} = \frac{\partial^2 k}{\partial s^2}\left(\frac{x_i - z_i}{l^2 s}\right)\left(-\frac{x_j - z_j}{l^2 s}\right) + \frac{\partial k}{\partial s}\left(-\frac{\delta(i,j)}{l^2 s} - \frac{x_j - z_j}{l^2}\left(\frac{-1}{s^2}\right)\frac{x_i - z_i}{l^2 s}\right)$$

$$= -\frac{\partial^2 k}{\partial s^2}\frac{x_i - z_i}{l^2 s}\frac{x_j - z_j}{l^2 s} + \frac{\partial k}{\partial s}\left(-\frac{\delta(i,j)}{l^2 s} + \frac{1}{s^3}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)$$

$$= \frac{2\pi\sigma_f^2}{3}\left(\sin(2\pi s) + 2\pi\cos(2\pi s)(1-s)\right)\frac{x_i - z_i}{l^2 s}\frac{x_j - z_j}{l^2 s}$$

$$+ \frac{2\sigma_f^2}{3}\left(\cos(2\pi s) - \pi\sin(2\pi s)(1-s) - 1\right)\left(-\frac{\delta(i,j)}{l^2 s} + \frac{1}{s^3}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)$$

what if $s = 0$?, $\lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial k}{\partial z_j} = 0$, $\lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial^2 k}{\partial x_i \partial z_j} = \frac{4\pi^2\sigma_f^2}{3}\frac{\delta(i,j)}{l^2}$

$$k_{s<1}(s) = \sigma_f^2 \left(\frac{2+\cos(2\pi s)}{3}(1-s) + \frac{1}{2\pi}\sin(2\pi s) \right), \quad s(r,l) = \frac{r}{l}, r(\mathbf{x},\mathbf{z}) = \sqrt{\sum_{i=1}^{d}(x_i - z_i)^2}, \Rightarrow s^2 = \frac{r^2}{l^2}$$

$$\begin{aligned}
\frac{\partial^3 k}{\partial \log l \partial x_i \partial z_j} &= -l \frac{\partial^3 k}{\partial s^3} \frac{x_i - z_i}{l^2 s} \frac{x_j - z_j}{l^2 s} \left(\frac{-s}{l}\right) - l \frac{\partial^2 k}{\partial s^2} \frac{x_i - z_i}{l^2 s} \frac{x_j - z_j}{l^2 s} \left(\frac{-2}{l}\right) \\
&+ l \frac{\partial^2 k}{\partial s^2} \left(-\frac{\delta(i,j)}{l^2 s} + \frac{1}{s^3} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) \left(\frac{-s}{l}\right) + l \frac{\partial k}{\partial s} \left(\frac{-\delta(i,j)}{l^2 s} + \frac{1}{s^3} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) \left(\frac{-1}{l}\right) \\
&= \frac{\partial^3 k}{\partial s^3} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \frac{1}{s} + \frac{\partial^2 k}{\partial s^2} \left(\frac{\delta(i,j)}{l^2 s} + \frac{1}{s^2} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) + \frac{\partial k}{\partial s} \left(\frac{\delta(i,j)}{l^2 s} - \frac{1}{s^3} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right) \\
&= \frac{8\pi^3 \sigma_f^2}{3} \sin(2\pi s)(1-s) \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \frac{1}{s} \\
&+ \frac{-2\pi \sigma_f^2}{3} \left(\sin(2\pi s) + 2\pi \cos(2\pi s)(1-s)\right) \left(\frac{\delta(i,j)}{l^2} + \frac{x_i - z_i}{l^2 s} \frac{x_j - z_j}{l^2 s} \right) \\
&+ \frac{2\sigma_f^2}{3} \left(\cos(2\pi s) - \pi \sin(2\pi s)(1-s) - 1\right) \left(\frac{\delta(i,j)}{l^2 s} - \frac{1}{s^3} \frac{x_i - z_i}{l^2} \frac{x_j - z_j}{l^2} \right)
\end{aligned}$$

what if $s = 0$?, $\lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial^3 k}{\partial \log l \partial x_i \partial z_j} = \frac{-8\pi^2 \sigma_f^2}{3} \frac{\delta(i,j)}{l^2}$