Gaussian Processes with Derivative Observations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\frac{\partial s}{\partial x_i} = \frac{3(x_i - z_i)}{l^2 s}, \quad \frac{\partial s}{\partial z_j} = -\frac{3(x_j - z_j)}{l^2 s}, \text{(what if } s = 0\text{?)} \lim_{\mathbf{x} \to \mathbf{z}} \frac{\partial s}{\partial x_i} = -\frac{\sqrt{3}}{l\sqrt{d}}, \quad \lim_{\mathbf{x} \to \mathbf{z}} \frac{\partial s}{\partial z_j} = \frac{\sqrt{3}}{l\sqrt{d}}$$

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

$$\Rightarrow \frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{3\delta(i,j)}{l^2 s} - \frac{1}{s} \frac{\partial s}{\partial x_i} \frac{\partial s}{\partial z_j}, \text{(what if } s = 0\text{?)} \lim_{\mathbf{x} \to \mathbf{z}} \frac{\partial^2 s}{\partial x_i \partial z_j} = 0$$

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

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

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

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

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

$$2s\frac{\partial s}{\partial x_i} = \frac{2(x_i - z_i)}{l^2} \Rightarrow \frac{\partial s}{\partial x_i} = \frac{x_i - z_i}{l^2 s}, \frac{\partial s}{\partial z_j} = -\frac{x_j - z_j}{l^2 s}, (s=0?) \lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial s}{\partial x_i} = \frac{1}{l\sqrt{d}}, \lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial s}{\partial z_j} = -\frac{1}{l\sqrt{d}}$$

$$\Rightarrow \frac{\partial s}{\partial z_j}\frac{\partial s}{\partial x_i} + s\frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{\delta(i,j)}{l^2} \Rightarrow \frac{\partial^2 s}{\partial x_i \partial z_j} = -\frac{\delta(i,j)}{l^2 s} - \frac{1}{s}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j}, (s=0?) \lim_{\mathbf{x}\to\mathbf{z}} \frac{\partial^2 s}{\partial x_i \partial z_j} = 0$$

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