Gaussian Processes with Derivative Observations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
\int_0^R k(r)dr &= \int_0^R \sigma_f^2 \left(\frac{2+\cos(2\pi r)}{3}(1-r) + \frac{1}{2\pi}\sin(2\pi r) \right) dr, \quad r = \frac{1}{l}\sqrt{\sum_{i=1}^{d}(x_i - z_i)^2} \\
&= \left[\sigma_f^2 \left(\frac{2}{3}r + \frac{\sin(2\pi r)}{6\pi} - \frac{1}{3}r^2 - \frac{1}{3}\left(\frac{r\sin(2\pi r)}{2\pi} + \frac{\cos(2\pi r)}{4\pi^2} \right) - \frac{\cos(2\pi r)}{4\pi^2} \right) \right]_0^R \\
&= \frac{\sigma_f^2}{6\pi^2} \left[2\pi^2 r(2-r) + \pi(1-r)\sin(2\pi r) - 2\cos(2\pi r) \right]_0^R \\
&= \frac{\sigma_f^2}{6\pi^2} \left(2\pi^2 R(2-R) + \pi(1-R)\sin(2\pi R) - 2\cos(2\pi R) + 2 \right), \quad R = \min(R, 1)
\end{aligned}
$$

$$\mathrm{cov}\left(f, f'\right) = k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{2l^2}\right) = \sigma_f^2 \exp\left(-\frac{1}{2l^2}\sum_{i=1}^{d}(x_i - z_i)^2\right)$$

$$\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial z_j} = \frac{x_j - z_j}{l^2} k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \frac{x_j - z_j}{l^2} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{2l^2}\right)$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, f'\right) = \frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial x_i} = -\frac{x_i - z_i}{l^2} k(\mathbf{x}, \mathbf{x}') = -\sigma_f^2 \frac{x_i - z_i}{l^2} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{2l^2}\right)$$

$$\begin{aligned}\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial^2 k(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial z_j} &= \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) k(\mathbf{x}, \mathbf{x}') \\ &= \frac{\sigma_f^2}{l^2}\left(\delta(i,j) - \frac{(x_i - z_i)(x_j - z_j)}{l^2}\right) \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{2l^2}\right)\end{aligned}$$

Gaussian Processes with Derivative Observations

Squared Exponential Covariance Function

$$\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} = \frac{\partial l}{\partial \log l}\frac{\partial \mathrm{cov}(f_i, f_j)}{\partial l} = \frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{l^2} k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{l^2} \exp\Bigg(-\frac{(\mathbf{x}-\mathbf{x}'}{2}$$

$$\begin{aligned}
\frac{\partial \mathrm{cov}\left(f, \partial f_j'\right)}{\partial \log l} &= \left(-2\frac{x_j - z_j}{l^2} + \frac{x_j - z_j}{l^2}\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{l^2}\right) k(\mathbf{x}, \mathbf{x}') \\
&= \frac{x_j - z_j}{l^2}\left(\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{l^2} - 2\right) k(\mathbf{x}, \mathbf{x}') \\
&= \frac{x_j - z_j}{l^2}\left(\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} - 2k(\mathbf{x}, \mathbf{x}')\right) = \frac{x_j - z_j}{l^2}\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} - 2\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) \\
\frac{\partial \mathrm{cov}(\partial f_i, f')}{\partial \log l} &= -\frac{\partial \mathrm{cov}(f, \partial f_i')}{\partial \log l} \\
\frac{\partial \mathrm{cov}\left(\partial f_i, \partial f_j'\right)}{\partial \log l} &= \left(-2\frac{\delta(i,j)}{l^2} + 4\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2} + \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{l^2}\right) \\
&= \left(-2\frac{\delta(i,j)}{l^2} + 4\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) k(\mathbf{x}, \mathbf{x}') + \left(\frac{\delta(i,j)}{l^2} - \frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} \\
&= \left(\frac{-2\delta(d,e)}{l^2} + \frac{4}{l^4}(x_{id} - x_{jd})(x_{ie} - x_{je})\right) k(\mathbf{x}, \mathbf{z}) + \mathrm{cov}(\partial f_i, \partial f_j)\frac{(\mathbf{x}-\mathbf{z})^{\mathrm{T}}(\mathbf{x}-\mathbf{z})}{l^2}
\end{aligned}$$

$$\mathrm{cov}\left(f, f'\right) = k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{s}{2l^2}\right), \quad s = \sum_{i=1}^{d} (x_i - z_i)^2$$

$$\frac{\partial k}{\partial s} = \frac{-\sigma_f^2}{2l^2} \exp\left(-\frac{s}{2l^2}\right), \quad \frac{\partial^2 k}{\partial s^2} = \frac{\sigma_f^2}{4l^4} \exp\left(-\frac{s}{2l^2}\right), \quad \frac{\partial^3 k}{\partial s^3} = \frac{-\sigma_f^2}{8l^6} \exp\left(-\frac{s}{2l^2}\right)$$

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

$$\lim_{r \to 0} k \to 0, \quad \frac{\partial k}{\partial z_j} \to 0, \quad \frac{\partial k}{\partial x_i} \to 0, \quad \frac{\partial^2 k}{\partial x_i \partial z_j} \to 0$$

$$\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial k}{\partial z_j} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial z_j} = \frac{\sigma_f^2}{l^2}(x_j - z_j) \exp\left(-\frac{s}{2l^2}\right)$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, f'\right) = \frac{\partial k}{\partial x_i} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial x_i} = -\frac{\sigma_f^2}{l^2}(x_i - z_i) \exp\left(-\frac{s}{2l^2}\right)$$

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

$$\mathrm{cov}\left(f, f'\right) = k_{\nu=3/2}(r) = \sigma_f^2 \left(1 + \frac{\sqrt{3}r}{l}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right), \quad \text{where} \quad r = |\mathbf{x} - \mathbf{x}'| = \sqrt{\sum_{i=1}^{d}(x_i - z_i)^2}$$

$$\frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial s} = \sigma_f^2 \left(\frac{\sqrt{3}}{l} - \left(1 + \frac{\sqrt{3}r}{l}\right)\frac{\sqrt{3}}{l}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) = -\sigma_f^2 \frac{3r}{l^2} \exp\left(-\frac{\sqrt{3}r}{l}\right),$$

$$\frac{\partial s}{\partial x_i} = \frac{x_i - z_i}{s}, \quad \frac{\partial s}{\partial z_j} = -\frac{x_j - z_j}{s}$$

$$\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial x'_j} = \frac{\partial s}{\partial z_j}\frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial s} = 3\sigma_f^2 \frac{x_j - z_j}{l^2} \exp\left(-\frac{\sqrt{3}r}{l}\right)$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, f'\right) = \frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial x_i} = \frac{\partial s}{\partial x_i}\frac{\partial k(\mathbf{x}, \mathbf{x}')}{\partial s} = -3\sigma_f^2 \frac{x_i - z_i}{l^2} \exp\left(-\frac{\sqrt{3}r}{l}\right)$$

$$\begin{aligned}
\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, \frac{\partial f'}{\partial z_j}\right) &= \frac{\partial^2 k(\mathbf{x}, \mathbf{x})}{\partial x_i \partial z_j} = 3\sigma_f^2 \left(\frac{\delta(i,j)}{l^2} + \frac{x_j - z_j}{l^2}\left(-\frac{\sqrt{3}}{l}\right)\frac{x_i - x_i}{s}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) \\
&= 3\sigma_f^2 \left(\frac{\delta(i,j)}{l^2} - 3\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) \overset{r \approxeq 0}{=} \frac{3\sigma_f^2}{l^2}\delta(i,j) \\
&= \frac{3\sigma_f^2}{l^2}\left(\delta(i,j) - \frac{\sqrt{3}(x_i - z_i)(x_j - z_j)}{lr}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right)
\end{aligned}$$

From previous slide,

$$\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} = l\sigma_f^2 \left(-\frac{\sqrt{3}r}{l^2} + \left(1 + \frac{\sqrt{3}r}{l}\right)\frac{\sqrt{3}r}{l^2}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) = \sigma_f^2 \left(\frac{\sqrt{3}r}{l}\right)^2 \exp\left(-\frac{\sqrt{3}r}{l}\right)$$

$$\begin{aligned}
\frac{\partial \mathrm{cov}\left(f, \partial f_j'\right)}{\partial \log l} &= l3\sigma_f^2 \left(\frac{-2}{l}\frac{x_j - z_j}{l^2} + \frac{x_j - z_j}{l^2}\frac{\sqrt{3}r}{l^2}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) \\
&= 3\sigma_f^2 \frac{x_j - z_j}{l^2}\left(\frac{\sqrt{3}r}{l} - 2\right) \exp\left(-\frac{\sqrt{3}r}{l}\right)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathrm{cov}(\partial f_i, \partial f_j)}{\partial \log l} &= l3\sigma_f^2 \Bigg(\left(-2\frac{\delta(i,j)}{l^3} + \frac{9}{l}\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) \\
&\quad + \left(\frac{\delta(i,j)}{l^2} - 3\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)\frac{\sqrt{3}r}{l^2}\Bigg) \exp\left(-\frac{\sqrt{3}r}{l}\right) \\
&= 3\sigma_f^2 \Bigg(\left(-2\frac{\delta(i,j)}{l^2} + 9\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) \\
&\quad + \left(\frac{\delta(i,j)}{l^2} - 3\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right)\frac{\sqrt{3}r}{l}\Bigg) \exp\left(-\frac{\sqrt{3}r}{l}\right) \\
&= 3\sigma_f^2 \left(-2\frac{\delta(i,j)}{l^2} + 9\frac{l}{\sqrt{3}r}\frac{x_i - z_i}{l^2}\frac{x_j - z_j}{l^2}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) + \mathrm{cov}\left(\frac{\partial f}{\partial x_i}, \frac{\partial f'}{\partial z_j}\right)\frac{\sqrt{3}r}{l} \\
&= \frac{3\sigma_f^2}{l^2}\left(\left(\frac{\sqrt{3}r}{l} - 2\right)\delta(i,j) - \frac{\sqrt{3}(x_{id} - x_{jd})(x_{ie} - x_{je})}{lr}\left(\frac{\sqrt{3}r}{l} - 3\right)\right) \exp\left(-\frac{\sqrt{3}r}{l}\right)
\end{aligned}$$

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

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

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

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

$$\lim_{r \to 0} k \to 0, \quad \frac{\partial k}{\partial z_j} \to 0, \quad \frac{\partial k}{\partial x_i} \to 0, \quad \frac{\partial^2 k}{\partial x_i \partial z_j} \to 0$$

$$\mathrm{cov}\left(f, \frac{\partial f'}{\partial z_j}\right) = \frac{\partial k}{\partial z_j} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial z_j} = -\frac{x_j - z_j}{l^2 r}\frac{\partial k}{\partial s}$$

$$\mathrm{cov}\left(\frac{\partial f}{\partial x_i}, f'\right) = \frac{\partial k}{\partial x_i} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial x_i} = \frac{x_i - z_i}{l^2 r}\frac{\partial k}{\partial s}$$

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

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

From previous slide,

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

$$r^2 = \frac{\sum_{i=1}^d (x_i - z_i)^2}{l^2} \Rightarrow 2r\partial r = -2\frac{\sum_{i=1}^d (x_i - z_i)^2}{l^3}\partial l \Rightarrow \frac{\partial s}{\partial l} = -\frac{s}{l}$$

$$\frac{\partial \mathrm{cov}(f, f')}{\partial \log l} = \frac{\partial k}{\partial s}\frac{\partial s}{\partial l}\frac{\partial l}{\partial \log l} = -r\frac{\partial k}{\partial s}$$

$$\frac{\partial \mathrm{cov}\Big(f, \partial f_j'\Big)}{\partial \log l} = -\frac{\partial s}{\partial z_j}\frac{\partial k}{\partial s} - r\frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial z_j} = -\frac{\partial s}{\partial z_j}\left(\frac{\partial k}{\partial s} + r\frac{\partial^2 k}{\partial s^2}\right) = \frac{x_j - z_j}{l^2 r}\left(\frac{\partial k}{\partial s} + r\frac{\partial^2 k}{\partial s^2}\right)$$

$$\begin{aligned}
\frac{\partial \mathrm{cov}(\partial f_i, \partial f_j)}{\partial \log l} &= -\frac{\partial^2 s}{\partial x_i \partial z_j}\left(\frac{\partial k}{\partial s} + r\frac{\partial^2 k}{\partial s^2}\right) - \frac{\partial s}{\partial z_j}\left(\frac{\partial^2 k}{\partial s^2}\frac{\partial s}{\partial x_i} + \frac{\partial s}{\partial x_i}\frac{\partial^2 k}{\partial s^2} + r\frac{\partial^3 k}{\partial s^3}\frac{\partial s}{\partial x_i}\right) \\
&= -\frac{\partial^2 s}{\partial x_i \partial z_j}\left(\frac{\partial k}{\partial s} + r\frac{\partial^2 k}{\partial s^2}\right) - \frac{\partial s}{\partial x_i}\frac{\partial s}{\partial z_j}\left(2\frac{\partial^2 k}{\partial s^2} + r\frac{\partial^3 k}{\partial s^3}\right) \\
&= \left(\frac{\delta(i,j)}{l^2 r} - \frac{1}{s}\frac{x_i - z_i}{l^2 r}\frac{x_j - z_j}{l^2 r}\right)\left(\frac{\partial k}{\partial s} + r\frac{\partial^2 k}{\partial s^2}\right) + \frac{x_i - z_i}{l^2 r}\frac{x_j - z_j}{l^2 r}\left(2\frac{\partial^2 k}{\partial s^2} + r\frac{\partial^3 k}{\partial s^3}\right)
\end{aligned}$$