Bound on distance for NND

If we want cross-covariance to be Matern

For the 4*4 covariance matrix, the determinant first and second principal matrix is always bigger than zero. Now, the determinant of the whole matrix looks like-

$$
\begin{aligned}
f(d) &= 1 + e^{-2(\phi_{11}+\phi_{22})d} + 4\sigma_{12}^2(e^{-(\phi_{12}+\phi_{11})d} + e^{-(\phi_{12}+\phi_{22})d}) + \sigma_{12}^4 + \sigma_{12}^4 e^{-4\phi_{12}d} \\
&\quad - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2(e^{-2\phi_{12}d}+1)\sigma_{12}^2 e^{-(\phi_{11}+\phi_{22})d} - 2\sigma_{12}^2 e^{-2\phi_{12}d} - 2\sigma_{12}^2 - 2\sigma_{12}^4 e^{-2\phi_{12}d} \\
&= (1-\sigma_{12}^2)^2 + 4\sigma_{12}^2(e^{-(\phi_{12}+\phi_{11})d} + e^{-(\phi_{12}+\phi_{22})d}) + (e^{-(\phi_{11}+\phi_{22})d} - \sigma_{12}^2 e^{-2\phi_{12}d})^2 \\
&\quad - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2\sigma_{12}^2 e^{-(\phi_{11}+\phi_{22})d} - 2\sigma_{12}^2 e^{-2\phi_{12}d} - 2\sigma_{12}^4 e^{-2\phi_{12}d}
\end{aligned}
$$

Clearly, you can see, $\lim_{d\to\infty} f(d) = 1 - 2\sigma_{12}^2 + \sigma_{12}^4 = (1-\sigma_{12}^2)^2 > 0$

Now, as, $0 < \sigma_{12}^2 < 1$, $f(d) > (1-\sigma_{12}^2)^2 - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2e^{-(\phi_{11}+\phi_{22})d} - 2e^{-2\phi_{12}d} - 2e^{-2\phi_{12}d} = g(d)$. \ Clearly, $g(d)$ is strictly increasing function of d and $\lim_{d\to\infty} g(d) = (1-\sigma_{12}^2)^2 > 0$.

For fixed $\phi_{11}, \phi_{12}, \phi_{22}, \sigma_{12}$, we can find d_0 such that $g(d) > 0 \forall d > d_0$. And, as $f(d) > g(d)$ always, we get, $f(d) > 0 \forall d > d_0$.

Now for practical purposes, if we can't estimate σ_{12} before, then we can assume $0 < \sigma_{12}^2 < .975$, say, then we can pick our favourite ϕ_{12}, take $g(d) = .025^2 - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2e^{-(\phi_{11}+\phi_{22})d} - 2e^{-2\phi_{12}d} - 2e^{-2\phi_{12}d}$. Observe that $g(d)$ is now a known function of d as we have estimated ϕ_{11},ϕ_{22} before and we can run numerical methods to find d_0 now.

Now, for the third principal minor, the determinant looks like -

$$h(d) = 1 + 2\sigma_{12}^2 e^{-(\phi_{12}+\phi_{11})d} - \sigma_{12}^2 - \sigma_{12}^2 e^{-2\phi_{12}d} - e^{-2\phi_{11}d}$$

Now, as, $0 < \sigma_{12}^2 < 1$, $h(d) > (1-\sigma_{12}^2) - e^{-2\phi_{12}d} - e^{-2\phi_{11}d} = m(d)$, again $m(d)$ is a stricly increasing function convergint to $(1-\sigma_{12}^2) > 0$. Hence, we can find similar way like previous a d_1 such that $h(d) > 0 \forall d > d_1$.

So, we take $\hat{d} = max(d_0, d_1)$ and we get $f(d), h(d) > 0 \forall \hat{d}$. And hence, $\forall d > \hat{d}$, the matrix is NND.

(Ideally, we should pick ϕ_{12} such that d is minimum).

If we don't care about cross-covariance being Matern

Let, u be the cross-covariance term which was $e^{-\phi_{12}d}$ previously.

$f(d) > (1-\sigma_{12}^2)^2 - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2e^{-(\phi_{11}+\phi_{22})d} - 4u^2 = g(d)$

Then, for practical purposes we take $g(d) = .025^2 - e^{-2\phi_{11}d} - e^{-2\phi_{22}d} - 2e^{-(\phi_{11}+\phi_{22})d} - 4u^2$, then take $u < (.025/4)$ and get d_0 by finding root of $g(d)$ i.e. solving $.025^2 - 4u^2 = (e^{-\phi_{11}d} + e^{-\phi_{22}d})^2$.

Similarly, take $m(d) = .025 - u^2 - e^{-2\phi_{11}d}$, we have already taken $u < \sqrt{0.025}$, so, we find d_1 by solving $.025 - u^2 = e^{-2\phi_{11}d}$.

Then, we similarly find $\hat{d}$, observing a little bit closer, you can see that, we should take $u = 0$ for the optimum solution of d here.