Propriety of the reference posterior distribution in Gaussian Process regression.

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May 24, 2018

Abstract
In a seminal article, Berger et al. [2001] compare several objective prior distributions for the parameters of Gaussian Process regression models with isotropic correlation kernel. The reference prior distribution stands out among them insofar as it always leads to a proper posterior. They prove this result for rough correlation kernels - Spherical, Exponential with power \( q < 2 \), Matérn with smoothness \( \nu < 1 \). This paper provides a proof for smooth correlation kernels - Exponential with power \( q = 2 \), Matérn with smoothness \( \nu \geq 1 \), Rational Quadratic.

1 Introduction
In a very influential paper, Berger et al. [2001] pioneered the field of Objective Bayesian analysis of spatial models. Previous works [De Oliveira et al., 1997, Stein, 1999] had noted that commonly used noninformative priors sometimes failed to yield proper posteriors, but Berger et al. [2001] were the first to thoroughly investigate the issue. Among several prior distributions – truncated priors, vague priors, Jeffreys-rule and independence Jeffreys prior – they showed that the reference prior [Bernardo, 2005] is the most satisfying choice for a default prior distribution. This is due in no small part to the fact that, in the wide variety of cases studied by Berger et al. [2001], it systematically yields a proper posterior distribution. In this article, we complete their proof of this property.

Section 2 describes the Gaussian Process models studied by Berger et al. [2001]. Section 3 shows that the proof of reference posterior propriety provided by Berger et al. [2001] only applies to those with rough correlation kernels – Spherical, Exponential with power \( q < 2 \), Matérn with smoothness \( \nu < 1 \). Section 4 contains the core of this paper: a proof of Theorem 9 which asserts that the reference prior leads to a proper posterior for models with smoother correlation kernels – Exponential with power \( q = 2 \), Matérn with smoothness \( \nu \geq 1 \), Rational Quadratic.

The rest of the introduction illustrates the significance of the reference prior yielding a proper posterior.

For smooth one-dimensional parametric families, the reference prior coincides with the Jeffreys-rule prior [Clarke and Barron, 1994]. For finite-dimensional smooth parametric families, the reference prior algorithm requires the user to define groups of dimensions of the parameter and rank them. The reference prior is then defined iteratively:
1. Compute the Jeffreys-rule prior on the lowest-ranking group of dimensions conditionally to all others.

2. Average the likelihood function over this prior.

3. Compute the Jeffreys-rule prior (based on the integrated likelihood function) on the second-lowest-ranking group of dimensions conditionally to all higher-ranking dimensions.

4. Average the integrated likelihood function over this second prior.

5. Continue the process until the Jeffreys-rule prior on the highest-ranking group of dimensions has been computed.

6. The reference prior is defined as the product of all successively computed priors.

In the cases studied by Berger et al. [2001], the dimensions of the parameter can be put in two natural categories: “location” and “covariance”, the latter being higher-ranking because if they were known, the model would be trivialized.

The process entails however a significant difficulty, which arises because the successively computed Jeffreys-rule priors are often improper. We do not consider this difficulty here, but it is touched upon in Berger et al. [2001] and more thoroughly discussed in Ren et al. [2012]. It can be avoided by using “asymptotic marginalization” [Berger and Bernardo, 1992] instead of “exact marginalization”, but Berger et al. [2001] found that the resulting “approximate” reference prior, unlike the “true” reference prior, does not always yield a proper posterior in the studied cases.

Because it is so difficult to obtain a satisfying default prior distribution which consistently yields a proper posterior, it is important to ascertain that the reference prior actually does. Indeed, a vast literature [Paulo, 2005; Ren et al., 2012; Kazianka and Pilz, 2012; Ren et al., 2013] builds upon Berger et al. [2001]’s result and depends on it.

2 Setting

Berger et al. [2001] consider models of Gaussian Process regression, also known as Universal Kriging, with isotropic autocorrelation kernels. Because isotropy is key, define \( \| \cdot \| \) as the usual Euclidean norm if applied to a vector and as the Frobenius norm if applied to a matrix. In Universal Kriging, an unknown mapping from a spatial domain \( \mathcal{D} \subset \mathbb{R}^r \) (\( r \in \mathbb{Z}_+ \)) to \( \mathbb{R} \) is assumed to be a realization of a Gaussian process \( Y \). The mean function \( f \) of the Gaussian process is assumed to belong to some known vector space \( \mathcal{F}_p \) of dimension \( p \in \mathbb{N} \).

If \( p \) is non-zero, once a basis \( \{ f_j \}_{j \in [1, p]} \) of \( \mathcal{F}_p \) has been set, \( f \) can be parametrized by \( \beta = (\beta_1, ..., \beta_p)^\top \in \mathbb{R}^p \) such that \( f = \sum_{j=1}^{p} \beta_j f_j \).

\( Y - f \) is assumed in the model to be an isotropic Gaussian process based on an autocorrelation kernel \( K \). \( K \) is a mapping \( [0, +\infty) \rightarrow \mathbb{R} \) such that for any positive integer \( n \) and any collection of \( n \) distinct points \( \{ x^{(i)} \}_{i \in [1, n]} \) within \( \mathcal{D} \), the symmetric \( n \times n \) matrix \( \Sigma \) with \((i, i')\)-th element \( K(\| x^{(i)} - x^{(i')} \|) \) is a positive definite correlation matrix. Necessarily, \( K(0) = 1 \).
The autocovariance function of the Gaussian process $Y$ is $\sigma^2 K_\theta$, where $K_\theta$ is the autocorrelation kernel parametrized by $\theta \in (0, +\infty)$ and defined by $K_\theta(d) = K(d/\theta)$, making $\sigma^2 \in (0, +\infty)$ the variance of $Y(x)$ for all $x \in D$.

Fix $n \in \mathbb{Z}_+$ and a collection of $n$ distinct points $(x^{(i)})_{i \in [1,n]}$. Let this collection be the design set, i.e. the set of points where $Y$ is observed. $(Y(x^{(1)}), ..., Y(x^{(n)}))^\top$ is a Gaussian vector with mean vector $(f(x^{(1)}), ..., f(x^{(n)}))^\top$ and covariance matrix $\sigma^2 \Sigma_\theta$, where $\Sigma_\theta$ denotes the $n \times n$ matrix with $(i,i')$-th element $K_\theta(||x^{(i)} - x^{(i')}||)$. Table 1 provides the definition of several correlation kernels.

| Kernel                  | $K_\theta(|x|)$                                                                 | parameter range |
|-------------------------|--------------------------------------------------------------------------------|-----------------|
| Spherical ($r = 1, 2, 3$) | $(1 - \frac{3}{2} \left(\frac{|x|}{\theta}\right) + \frac{1}{2} \left(\frac{|x|}{\theta}\right)^3) \mathbf{1}_{\{|x| \leq \theta\}}$ | $\emptyset$     |
| Power Exponential       | $\exp \left\{ - \left(\frac{|x|}{\theta}\right) \right\}$                      | $q \in (0, 2]$  |
| Rational Quadratic      | $\left(1 + \left(\frac{|x|}{\theta}\right)^q \right)^{-q}$                    | $q \in (0, +\infty)$ |
| Matérn                  | $\Gamma(\nu)^{-1} 2^{1-\nu} \left(2 \sqrt{v |x|/\theta}\right)^\nu K_\nu \left(2 \sqrt{v |x|/\theta}\right)$ | $\nu \in (0, +\infty)$ |

Table 1: Formulas for several correlation kernel families. The Squared Exponential kernel is the Power Exponential kernel with $q = 2$. $K_\nu$ is the modified Bessel function of second kind with parameter $\nu$ [Abramowitz and Stegun 1964, 9.6.]. This parametrization of the Matérn family is recommended by [Handcock and Wallis 1994]. To recover the one used by [Berger et al. 2001], simply replace $2\sqrt{v |x|/\theta}$ by $|x|$.

If $p$ is non-zero, let $H$ denote the $n \times p$ matrix with $(i, j)$-th element $f_j(x^{(i)})$. [Note: if $p = 0$, then we adopt the convention that any term involving $H$ can be ignored.] Then $(f(x^{(1)}), ..., f(x^{(n)}))^\top = H \beta$. Denote by $y = (y_1, ..., y_n)^\top$ the observed value of the random vector $(Y(x^{(1)}), ..., Y(x^{(n)}))^\top$. The likelihood function of the parameter triplet $(\beta, \sigma^2, \theta)$ has the following expression:

$$L(y \mid \beta, \sigma^2, \theta) = \left(\frac{1}{2\pi \sigma^2}\right)^{\frac{n}{2}} |\Sigma_\theta|^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2\sigma^2} (y - H \beta)^\top \Sigma_\theta^{-1} (y - H \beta) \right\}. \quad (1)$$

In order for the model to be identifiable, assume that $p < n$ and that $H$ has rank $p$. [Berger et al. 2001] derive the reference prior corresponding to the parameter ordering $\beta \prec (\sigma^2, \theta)$ [if $p = 0$, $\beta$ is meaningless, so the ordering is $(\sigma^2, \theta)$]. One can see [Ren et al. 2012] that the reference prior corresponding with the ordering $\beta \prec \sigma^2 \prec \theta$ [if $p = 0$, $\sigma^2 \prec \theta$] is the same.

To express it conveniently, denote by $Q_\theta$ the matrix $I_n - H (H^\top \Sigma_\theta^{-1} H)^{-1} H^\top \Sigma_\theta^{-1}$ [if $p = 0$, $Q_\theta = I_n$]. Also fix $W$, an $n \times (n-p)$ matrix such that $W^\top W = I_{n-p}$ and $H^\top W$ is the $p \times (n-p)$ null matrix. $W$’s columns form an orthonormal basis of the orthogonal complement of the subspace of $\mathbb{R}^n$ spanned by the columns of $H$ [if $p = 0$, fix $W$ as an orthogonal matrix, for instance $I_n$].

**Proposition 1.** The reference prior with ordering $\beta \prec \sigma^2 \prec \theta$ is $\pi(\beta, \sigma^2, \theta) \propto (\sigma^2)^{-1} \pi(\theta)$, where

$$\pi(\theta) \propto \sqrt{\text{Tr} \left\{ \left(\frac{d}{d\theta} \Sigma_\theta \right) \Sigma_\theta^{-1} Q_\theta \right\}^2} - \frac{1}{n-p} \left[ \text{Tr} \left\{ \left(\frac{d}{d\theta} \Sigma_\theta \right) \Sigma_\theta^{-1} Q_\theta \right\} \right]^2. \quad (2)$$
Denoting \( W^T \Sigma_\theta W \) by \( \Sigma_\theta^W \), \( \pi(\theta) \) can also be written as:

\[
\pi(\theta) \propto \sqrt{\text{Tr} \left\{ \left( \frac{d}{d\theta} \Sigma_\theta^W \right) \left( \Sigma_\theta^W \right)^{-1} \right\}^2} - \frac{1}{n-p} \text{Tr} \left\{ \left( \frac{d}{d\theta} \Sigma_\theta^W \right) \left( \Sigma_\theta^W \right)^{-1} \right\}^2. \tag{3}
\]

Proof. The first assertion is from Ren et al. [2012]. The second is a consequence of Lemma 10.

Proposition 2. If \( p \geq 1 \), after marginalizing \( \beta \) and \( \sigma^2 \) out, we have

\[
L(y|\theta) = \int L(y|\beta, \sigma^2, \theta)/\sigma^2 \, d\sigma^2 = \left( \frac{2\pi^{n-p}}{\Gamma \left( \frac{n+p}{2} \right)} \right)^{-1} \left| \Sigma_\theta^{-1} \right|^\frac{1}{2} \left| H^T \Sigma_\theta^{-1} H \right|^\frac{1}{2} \left( y^T \left( \Sigma_\theta^{-1} W^T y \right)^{\frac{n-p}{2}}. \tag{4}
\]

Alternatively, the integrated likelihood with \( p \geq 1 \) can also be written

\[
L(y|\theta) = \int L(y|\sigma^2, \theta)/\sigma^2 \, d\sigma^2 = \left( \frac{2\pi^{n-p}}{\Gamma \left( \frac{p}{2} \right)} \right)^{-1} \left| \Sigma_\theta^{-1} \right|^\frac{1}{2} \left( y^T \left( W^T \Sigma_\theta^{-1} W \right)^{-1} W^T y \right)^{\frac{n-p}{2}}. \tag{5}
\]

If \( p = 0 \), the integrated likelihood is simply

\[
L(y|\theta) = \int L(y|\sigma^2, \theta)/\sigma^2 \, d\sigma^2 = \left( \frac{2\pi^{n-p}}{\Gamma \left( \frac{p}{2} \right)} \right)^{-1} \left| \Sigma_\theta^{-1} \right|^\frac{1}{2} \left( y^T \left( \Sigma_\theta^{-1} y \right)^{\frac{n}{2}}. \tag{6}
\]

Proof. The result for \( p = 0 \) and the first result for \( p \geq 1 \) are from Berger et al. [2001]. Lemma 10 yields that

\[
W \left( W^T \Sigma_\theta W \right)^{-1} W^T = \Sigma_\theta^{-1} Q_\theta. \tag{7}
\]

So all that remains to be proved is that \( |\Sigma_\theta| = \left| W^T \Sigma_\theta W \right| \left| H^T H \right|^{-1} \left| H^T \Sigma_\theta^{-1} H \right|^{-1} \). Choose an \( n \times p \) matrix \( P \) with columns forming an orthonormal basis of the subspace of \( \mathbb{R}^n \) spanned by the columns of \( H \). \( (WP) \) is therefore an \( n \times n \) orthogonal matrix, so \( |\Sigma_\theta| = |(WP)^T \Sigma_\theta (WP)|. \) Using Schur’s complement, we have

\[
|\Sigma_\theta| = \left| W^T \Sigma_\theta W \right| P^T \Sigma_\theta \left( I_n - W \left( W^T \Sigma_\theta W \right)^{-1} W^T \Sigma_\theta \right) P. \tag{8}
\]

Lemma 10 again yields the result.

3 Smoothness of the correlation kernel

Lemma 2 of Berger et al. [2001] requires that correlation kernel and design set should be such that \( \Sigma_\theta = 11^T + g_0(\theta)D + R_0(\theta) \), where \( 1 \) is the vector with \( n \) entries all equal to 1, \( g_0(\theta) \) is a real-valued function such that \( \lim_{\theta \to +\infty} g_0(\theta) = 0 \), \( D \) is a fixed nonsingular matrix and \( R_0 \) is a mapping from \( (0, +\infty) \) to the set of \( n \times n \) real matrices \( M_n \) such that \( \lim_{\theta \to +\infty} ||\frac{1}{g_0(\theta)} R_0(\theta)|| = 0 \).

What makes this assumption restrictive is the condition that \( D \) should be nonsingular, because it holds for rough correlation kernels only. For instance, as was noted by Paula [2005], it does not hold for the Squared Exponential correlation kernel.
For a given correlation kernel $K$, $D$ is typically a matrix proportional to the matrix with entries $\|x^{(i)} - x^{(j)}\|^q$, where $q$ depends on the smoothness of the correlation kernel but should in any case belong to the interval $(0, 2]$. This is because $K(s) - K(0)$ is equivalent to a constant times $s^q$ when $s \to 0^+$. 

Schoenberg [1937] gives the following result (Theorem 4 in the original paper): 

**Theorem 3.** If $q \in (0, 2)$, the quadratic form $\sum_{i,j=0}^n \|x^{(i)} - x^{(j)}\|^q \xi_i \xi_j$ is nonsingular and its canonical representation contains one positive and $n$ negative squares. 

This means that if the correlation kernel is rough enough to have $q \in (0, 2)$, the assumption that $D$ is nonsingular is reasonable. 

**Corollary 4.** The $n \times n$ matrix with entries $\|x^{(i)} - x^{(j)}\|^q$ with $q \in (0, 2)$ is nonsingular and has one positive eigenvalue and $n$ negative eigenvalues. 

The picture is dramatically different when the correlation kernel $K$ is smooth enough to have $q = 2$. This happens as soon as $K$ is twice continuously differentiable. Gower [1985]’s Theorem 6 implies the following results: 

**Theorem 5.** If $d$ is the dimension of $E_d$, the smallest Euclidean subspace containing all points in the design set, then the $n \times n$ matrix with entries $\|x^{(i)} - x^{(j)}\|^2$ has rank: 

- (a) $d + 1$ (one positive eigenvalue, $d$ negative eigenvalues, any other eigenvalue null) if all points in the design set lie on the surface of a hypersphere of $E_d$; 
- (b) $d + 2$ (one positive eigenvalue, $d + 1$ negative eigenvalues, any other eigenvalue null) otherwise. 

**Corollary 6.** The $n \times n$ matrix with entries $\|x^{(i)} - x^{(j)}\|^2$ has rank lower or equal to $r + 2$. 

For all practical purposes, $n$ is much greater than $r$, so the matrix $D$ is singular when $q = 2$. 

Let us review the values of $q$ for correlation kernels listed in Table 1. Matérn correlation kernels [Matérn, 1986] [Handcock and Stein, 1993] with smoothness parameter $\nu$ have $q = 2 \min(1, \nu)$, thus for $0 < \nu < 1$, $0 < q < 2$ but for $\nu \geq 1$, $q = 2$. Spherical correlation kernels [Wackernagel, 1995] have $q = 1$. Power Exponential kernels [De Oliveira et al., 1997] have $q$ equal to their power. This means that all Power Exponential kernels except the Squared Exponential correlation kernel have $0 < q < 2$. In particular, the Exponential kernel (which is also the Matérn kernel with smoothness $\nu = 1/2$) has $q = 1$, but the Squared Exponential kernel has $q = 2$. Rational Quadratic kernels [Yaglom, 1987] have $q = 2$. For easy reference, the review is summarized in Table 2. 

The above review justifies the claim in the abstract that the Squared Exponential kernel, Matérn kernels with smoothness $\nu \geq 1$ and Rational Quadratic kernels require a proof of the reference posterior’s propriety. 

### 4 Propriety of the reference posterior distribution 

Berger et al. [2001] show that the reference posterior distribution on $\beta$ and $\sigma^2$ conditionally to $\theta$ is proper. In this section, we prove that the joint reference posterior distribution is proper for Matérn kernels with smoothness $\nu \geq 1$, Rational Quadratic kernels and the Squared Exponential kernel.
Table 2: Summary of the results of Section 3. *Answer given assuming \( n > r + 2 \).

**Proposition 7.** For Matérn kernels with smoothness \( \nu \geq 1 \), for Rational Quadratic kernels with parameter \( \nu > 0 \) and for the Squared Exponential kernel, the “marginal” reference prior distribution \( \pi(\theta) \) defined by Proposition 1 has the following behavior.

1. When \( \theta \to 0 \),
   \[
   \pi(\theta) = \begin{cases} 
   o(1) & \text{for Matérn kernels and the Squared Exponential kernel;} \\
   O(\theta^{\nu-1}) & \text{for Rational Quadratic kernels.} 
   \end{cases} 
   \tag{9}
   \]

2. When \( \theta \to +\infty \),
   \[
   \pi(\theta) = \begin{cases} 
   O(\theta^{-1}) & \text{for Matérn kernels;} \\
   o(1) & \text{for Rational Quadratic kernels; } \\
   O(\theta) & \text{for the Squared Exponential kernel.} 
   \end{cases} 
   \tag{10}
   \]

**Proof.** Denoting any of these kernels by \( K \), \( K \) is continuously differentiable.

If \( K \) is Squared Exponential, \( \lim_{\theta \to 0} \frac{d}{d\theta} K(1/\theta) = 0 \). This also holds if \( K \) is Matérn with smoothness \( \nu \geq 1 \) (see Abramowitz and Stegun 1964 9.6.28. and 9.7.2.). If \( K \) is Rational Quadratic with parameter \( \nu > 0 \), \( \frac{d}{d\theta} K(1/\theta) \sim 2\nu \theta^{2\nu-1} \).

Moreover, \( \Sigma_\theta \) converges to \( I_n \) when \( \theta \to 0 \), so its inverse does too. The first assertion follows from these facts.

The second assertion is proved by combining Lemma 22 with Lemma 20, 21, 22 for Matérn, Rational Quadratic and Squared Exponential kernels respectively.

Let \( v_1(\theta) \geq \ldots \geq v_{n-p}(\theta) > 0 \) be the ordered eigenvalues of \( W^\top \Sigma_\theta W \).

**Lemma 8.** For Rational Quadratic and Squared Exponential kernels and for Matérn kernels with smoothness \( \nu \geq 1 \), there exists a hyperplane \( \mathcal{H} \) of \( \mathbb{R}^n \) such that for every \( y \in \mathbb{R}^n \setminus \mathcal{H} \), when \( \theta \to +\infty \):

\[
(y^\top W (W^\top \Sigma_\theta W)^{-1} W^\top y)^{-1} = O(v_{n-p}(\theta)). 
\tag{11}
\]
The proof of this lemma can be found in Appendix D. Combined with Equation (5), it implies that if the observation vector $y$ belongs to $\mathbb{R}^n \setminus \mathcal{H}$, then

$$L(y|\theta)^2 = \prod_{i=1}^{n-p} \frac{O(v_{n-p}(\theta))}{v_i(\theta)} = O(1) \quad \text{when } \theta \to +\infty. \quad (12)$$

In the following, when $y$ belongs to $\mathbb{R}^n \setminus \mathcal{H}$, we write that “$y$ looks nondegenerate”. This terminology relies on the intuition that if the observation were to take some values within $\mathcal{H}$, it would be better explained by a degenerate Gaussian model. The most compelling example is that of a constant observation vector, for which the Kriging model would be grossly inappropriate.

**Theorem 9.** For Matérn kernels with noninteger smoothness $\nu > 1$, for Rational Quadratic kernels and for the Squared Exponential kernel, regardless of the design set and of the mean function space, if $y$ looks nondegenerate, then the reference posterior distribution $\pi(\theta|y)$ is proper.

**Proof.** The first assertion of Proposition 7 implies the reference prior $\pi(\theta)$ is integrable in the neighborhood of 0. Furthermore, when $\theta \to 0$, $\Sigma_\theta \to I_n$ so the reference posterior $\pi(\theta|y)$ is integrable in the neighborhood of 0 as well.

All that remains to be proved is therefore that the reference posterior is integrable in the neighborhood of $+\infty$. In the following $\theta \to +\infty$, so we rely on the asymptotic expansion of $\Sigma_\theta$, which is detailed in Appendix D.

The proof is somewhat trickier for Matérn kernels with integer smoothness, so we tackle this case at the end. Until further notice, assume the kernel is Rational Quadratic, Squared Exponential or Matérn with noninteger smoothness $\nu > 1$.

For Rational Quadratic and Squared Exponential (resp. Matérn with noninteger smoothness parameter $\nu > 1$) kernels, Appendix D.1 (resp. Appendix D.2) shows how $W^\top \Sigma_\theta W$ can be decomposed as

$$W^\top \Sigma_\theta W = g(\theta) \left( W^\top DW + g^*(\theta)W^\top D^*W + R_g(\theta) \right), \quad (13)$$

where

- $g$ is a differentiable function;
- $g^*(\theta) = \theta^{-2l}$ with $l \in (0, +\infty)$ (actually, if the kernel is Rational Quadratic or Squared Exponential, $l \in \mathbb{Z}_+$);
- $R_g$ is a differentiable mapping from $(0, +\infty)$ to $\mathcal{M}_n$ such that $\|R_g(\theta)\| = o(\theta^{-2l})$;
- $D$ and $D^*$ are both fixed symmetric matrices;
- $W^\top DW$ is non-null;
- either $W^\top D^*W$ is non-null or $W^\top DW$ is nonsingular.

Lemma 15 implies that one of the following is true:
1. When $\theta$ is large enough, $W^T DW + g^*(\theta)W^T D' W$ is nonsingular. This case can be further decomposed in the following subcases:

   (a) $W^T DW$ is nonsingular;

   (b) $W^T DW$ is singular, but $W^T DW + g^*(\theta)W^T D' W$ is nonsingular when $\theta$ is large enough.

2. The vector space $\text{Ker} \left( W^T D' W \right) \cap \text{Ker} \left( W^T DW \right)$ is non-trivial.

Let us differentiate $W^T \Sigma_\theta W$:

$$
\frac{d}{d\theta} W^T \Sigma_\theta W = \frac{g'(\theta)}{g(\theta)} W^T \Sigma_\theta W + g(\theta) \left( g^*(\theta)W^T D' W + \frac{d}{d\theta} R_g(\theta) \right).
$$

(14)

We can show that $\| \frac{d}{d\theta} R_g(\theta) \| = o(g^*(\theta))$. This is due to Equation (72) for Rational Quadratic and Squared Exponential kernels, and to Equation (75) for Matérn kernels with noninteger smoothness.

Lemma 11 shows that $\frac{d}{d\theta} W^T \Sigma_\theta W$ can be replaced by $g(\theta) \left( g^*(\theta)W^T D' W + \frac{d}{d\theta} R_g(\theta) \right)$ in Equation (3): $\pi(\theta) \propto w(\theta)$, where

$$
w(\theta)^2 := \text{Tr} \left\{ \left( g(\theta) \left( g^*(\theta)W^T D' W + \frac{d}{d\theta} R_g(\theta) \right) \right) \left( W^T \Sigma_\theta W \right)^{-1} \right\}^2
$$

$$
- \frac{1}{n-p} \text{Tr} \left\{ \left( g(\theta) \left( g^*(\theta)W^T D' W + \frac{d}{d\theta} R_g(\theta) \right) \right) \left( W^T \Sigma_\theta W \right)^{-1} \right\}^2.
$$

(15)

We have $w(\theta) \leq \hat{w}(\theta)$, where

$$
\hat{w}(\theta) := \sqrt{\text{Tr} \left\{ \left( g(\theta) \left( g^*(\theta)W^T D' W + \frac{d}{d\theta} R_g(\theta) \right) \right) \left( W^T \Sigma_\theta W \right)^{-1} \right\}^2}.
$$

(16)

A specific asymptotic analysis is required in each case. This study is conducted in Appendix E. We summarize the results in Table 3.

| Case | Kernels | $\pi(\theta)$ | $L(y|\theta)$ |
|------|---------|---------------|----------------|
| 1.(a) | Matérn ($\nu \in [1, +\infty) \setminus \mathbb{Z}_+$), RQ, SE | $O(\theta^{-2l-1})$ | $O(1)$ |
| 1.(b) | Matérn ($\nu \in [1, +\infty) \setminus \mathbb{Z}_+$), RQ, SE | $O(\theta^{-l})$ | $O(\theta^{-l})$ |
| 2. | Matérn ($\nu \in [1, +\infty) \setminus \mathbb{Z}_+$) | $O(\theta^{-l})$ | $O(\theta^{-l})$ |
| 2. | RQ, SE (usual case) | $O(\theta)$ | $O(\theta^{-1})$ |
| 2. | RQ, SE (special case) | $O(\theta^{-1})$ | $O(\theta^{-1})$ |

Table 3: Asymptotic upper bounds for reference prior $\pi(\theta)$ and likelihood $L(y|\theta)$ for Rational Quadratic (RQ) and Squared Exponential (SE) kernels and Matérn kernels with noninteger smoothness $\nu > 1$ in all three cases. The proof in Appendix E shows that for Rational Quadratic and Squared Exponential kernels, case 2. can be split in two subcases ("usual" and "special").

The posterior distribution resulting from the reference prior is proper in all cases. Matérn kernels with integer smoothness are dealt with in Appendix E.2.
5 Conclusion

The main result of this work is Theorem 9 which ensures that the reference prior leads to a proper posterior distribution for a large class of smooth kernels. This class contains the Squared Exponential correlation kernel as well as the important Matérn family [Stein, 1999] with smoothness parameter $\nu \geq 1$. Rational Quadratic kernels, whose usage is less widespread are also included within this class.

Berger et al. [2001] proved this result for a class of rough correlation kernels. This class includes the complementary set of the Matérn family – kernels with smoothness parameter $\nu < 1$ – as well as all other Power Exponential kernels. Spherical kernels, which are mostly used in the field of geostatistics also belong to this class.

Combining Theorem 9 with the results from Berger et al. [2001], one can appreciate how polyvalent the reference prior is, insofar as it is able to adapt to very different correlation kernels and always leads to a proper posterior. No ad-hoc technique is required to derive useable inference, so this approach seems to be flawless from a Bayesian point of view when no explicit prior information is available. Even when explicit prior information is available, following Druilhet and Marin [2007], it can be used to derive Maximum A Posteriori (MAP) estimates or High Probability Density (HPD) sets that are invariant under reparametrization.

Acknowledgements

The author would like to thank his PhD advisor Professor Josselin Garnier (École Polytechnique, Centre de Mathématiques Appliquées) for his guidance, Loic Le Gratiet (EDF R&D, Chatou) and Anne Dutfoy (EDF R&D, Saclay) for their advice and helpful suggestions. The author acknowledges the support of the French Agence Nationale de la Recherche (ANR), under grant ANR-13-MONU-0005 (project CHORUS).
Appendices

A Algebraic facts

Lemma 10. Let \( a \) and \( b \) be positive integers and let \( \Sigma \) be a nonsingular symmetric \( (a + b) \times (a + b) \) matrix. Then, for any \((a + b) \times a\) matrix \( A \) with rank \( a \) and any \((a + b) \times b\) matrix \( B \) with rank \( b \) such that \( A^\top B \) is the null \( a \times b \) matrix,

\[
B \left( B^\top \Sigma B \right)^{-1} B^\top = \Sigma^{-1} \left( I_{a+b} - A \left( A^\top \Sigma^{-1} A \right)^{-1} A^\top \Sigma^{-1} \right). \tag{17}
\]

Proof. Notice that both matrices have the same kernel, namely the subspace of \( \mathbb{R}^{a+b} \) spanned by \( A \). Indeed, because \( B \) has full column rank and \( \left( B^\top \Sigma B \right)^{-1} \) is nonsingular, the left matrix has the same kernel as \( B^\top \). Besides, the \( a \)-dimensional subspace of \( \mathbb{R}^{a+b} \) spanned by \( A \) in included in this kernel. So because the rank of \( B^\top \) is \( b \), its kernel has dimension \( a \) and the inclusion is an equality.

Similarly, because \( \Sigma^{-1} \) is nonsingular, the right matrix has the same kernel as \( I_{a+b} - A \left( A^\top \Sigma^{-1} A \right)^{-1} A^\top \Sigma^{-1} \). Moreover, because the image of \( A \left( A^\top \Sigma^{-1} A \right)^{-1} A^\top \Sigma^{-1} \) is included within the image of \( A \), its dimension is lower or equal to \( a \). The image of \( I_{a+b} \) on the other hand has dimension \( a + b \), so the image of \( I_{a+b} - A \left( A^\top \Sigma^{-1} A \right)^{-1} A^\top \Sigma^{-1} \) has dimension greater or equal to \( b \) and therefore its kernel has dimension lower or equal to \( a \). Now, a simple computation shows that the \( a \)-dimensional subspace of \( \mathbb{R}^{a+b} \) spanned by \( A \) in included in the kernel, so it is in fact equal to the kernel.

Besides, for any \( z \in \mathbb{R}^b \),

\[
B \left( B^\top \Sigma B \right)^{-1} B^\top (\Sigma Bz) = Bz; \tag{18}
\]

\[
\Sigma^{-1} \left( I_{a+b} - A \left( A^\top \Sigma^{-1} A \right)^{-1} A^\top \Sigma^{-1} \right) (\Sigma Bz) = Bz. \tag{19}
\]

So both matrices act the same way on the subspace spanned by \( \Sigma B \), which is supplementary to their common kernel, hence the equality. \( \Box \)

Lemma 11. Let \( m \) be a positive integer, \( \Sigma \) be a nonsingular \( m \times m \) matrix, and \( A \) and \( B \) be \( m \times m \) matrices. If there exists a real number \( t \) such that

\[
A = t\Sigma + B, \tag{20}
\]

then

\[
\text{Tr} \left[ \{ A\Sigma^{-1} \}^2 \right] - \frac{1}{m} \left[ \text{Tr} \{ A\Sigma^{-1} \} \right]^2 = \text{Tr} \left[ \{ B\Sigma^{-1} \}^2 \right] - \frac{1}{m} \left[ \text{Tr} \{ B\Sigma^{-1} \} \right]^2. \tag{21}
\]

Proof. The lemma follows from a direct calculation:

\[
\text{Tr} [A\Sigma^{-1}] = \text{Tr} [B\Sigma^{-1}] + tm \tag{22}
\]

\[
\text{Tr} \left[ \{ A\Sigma^{-1} \}^2 \right] = \text{Tr} \left[ \{ B\Sigma^{-1} \}^2 \right] + 2t \text{Tr} [B\Sigma^{-1}] + t^2 m \tag{23}
\]
Lemma 12. Let \( m > a \) be positive integers, \( \Sigma \) be an \( m \times m \) symmetric positive definite matrix, \( \Sigma' \) be an \( m \times m \) symmetric matrix and \( A \) be an \( m \times a \) matrix with rank \( a \). Denote by \( Q \) the matrix \( I_m - A (A^\top \Sigma^{-1} A)^{-1} A^\top \Sigma^{-1} \). Then, if there exist \( t_1 \in \mathbb{R} \) and \( t_2 \in [0, +\infty) \) such that the matrix \( F := t_1 \Sigma - \Sigma' \) is positive semi-definite and verifies \( \forall \xi \in \mathbb{R}^m \), \( \xi^\top F \xi \leq t_2 \xi^\top \Sigma \xi \), then

\[
\sqrt{\text{Tr} \left[ (\Sigma' \Sigma^{-1} Q)^2 \right]} - \frac{1}{m-a} \text{Tr} \left[ \Sigma' \Sigma^{-1} Q \right]^2 \leq (m-a)t_2
\]

(24)

Proof. Let \( B \) be an \( m \times (m-a) \) matrix with rank \( m-a \) such that \( A^\top B \) is the null \( a \times (m-a) \) matrix. Such a matrix \( B \) can for instance be constructed by computing a Singular Value Decomposition (SVD) of \( A \): \( A = USV^\top \). In this decomposition, \( U \) and \( V \) are matrices of size \( m \times m \) and \( a \times a \) respectively, and \( S \) is an \( m \times a \) matrix whose only non-null entries are on the main diagonal. Therefore the last \( m-a \) rows of \( S \) are filled with zeros. So define \( B \) as the \( m \times (m-a) \) matrix formed by the last \( m-a \) columns of \( U \).

By applying Lemma [10] we obtain that \( \Sigma^{-1} Q = B (B^\top \Sigma B)^{-1} B^\top \).

Because of the properties of the trace, this implies

\[
\text{Tr} \left[ \Sigma' \Sigma^{-1} Q \right] = \text{Tr} \left[ B^\top \Sigma' B \left( B^\top \Sigma B \right)^{-1} \right] \quad (25)
\]

\[
\text{Tr} \left[ (\Sigma' \Sigma^{-1} Q)^2 \right] = \text{Tr} \left[ \left\{ B^\top \Sigma' B \left( B^\top \Sigma B \right)^{-1} \right\}^2 \right]. \quad (26)
\]

Similarly, we have

\[
\text{Tr} \left[ F \Sigma^{-1} Q \right] = \text{Tr} \left[ B^\top FB \left( B^\top \Sigma B \right)^{-1} \right] \quad (27)
\]

\[
\text{Tr} \left[ (F \Sigma^{-1} Q)^2 \right] = \text{Tr} \left[ \left\{ B^\top FB \left( B^\top \Sigma B \right)^{-1} \right\}^2 \right]. \quad (28)
\]

Because \( B^\top F B = t_1 B^\top \Sigma B - B^\top \Sigma' B \), Lemma [11] implies

\[
\text{Tr} \left[ \left\{ B^\top \Sigma' B \left( B^\top \Sigma B \right)^{-1} \right\}^2 \right] - \frac{1}{m-a} \text{Tr} \left[ B^\top \Sigma' B \left( B^\top \Sigma B \right)^{-1} \right]^2
\]

\[
= \text{Tr} \left[ \left\{ B^\top F B \left( B^\top \Sigma B \right)^{-1} \right\}^2 \right] - \frac{1}{m-a} \text{Tr} \left[ B^\top F B \left( B^\top \Sigma B \right)^{-1} \right]^2 \quad (29)
\]

Combining the 5 equations above yields

\[
\text{Tr} \left[ (\Sigma' \Sigma^{-1} Q)^2 \right] - \frac{1}{m-a} \text{Tr} \left[ \Sigma' \Sigma^{-1} Q \right]^2 = \text{Tr} \left[ (F \Sigma^{-1} Q)^2 \right] - \frac{1}{m-a} \text{Tr} \left[ F \Sigma^{-1} Q \right]^2. \quad (30)
\]

An elementary computation shows that \( \Sigma^{-1} Q = Q^\top \Sigma^{-1} Q \).

Consider the Cholesky decomposition \( \Sigma = LL^\top \). Then \( \Sigma^{-1} Q = Q^\top \Sigma^{-1} Q = Q^\top (L^{-1})^\top L^{-1} Q \).
\[
\text{Tr} \left[ (F \Sigma^{-1}Q)^2 \right] = \text{Tr} \left[ (FQ^T (L^{-1})^T L^{-1}Q)^2 \right] = \text{Tr} \left[ (L^{-1}QFQ^T (L^{-1})^T)^2 \right] \\
\leq \text{Tr} \left[ L^{-1}QFQ^T (L^{-1})^T \right]^2 = \text{Tr} \left[ F \Sigma^{-1}Q \right]^2.
\] 
(31)

The inequality holds because \(L^{-1}QFQ^T (L^{-1})^T\) is a symmetric positive semi-definite matrix.

Let \((\xi^i)_{1 \leq i \leq m}\) be a basis of unit eigenvectors of \(\Sigma^{-1}Q\) such that for every integer \(i \in [1, m] \setminus [1, m - a]\), \(\xi^i\) belongs to the kernel of \(\Sigma^{-1}Q\). Indeed, because \(\Sigma^{-1}Q = B \left( B^\top \Sigma B \right)^{-1} B^\top\), this kernel has the same dimension as the kernel of \(B^\top\): \(a\).

Denoting by \((s_i)_{1 \leq i \leq m}\) the family of the eigenvalues corresponding to the family of eigenvectors \((\xi^i)_{1 \leq i \leq m}\), we have for every integer \(i \in [1, m - a] \) \(s_i \neq 0\) and

\[
(\xi^i)^\top \Sigma \xi^i = s_i^{-2} \left\{ (\xi^i)^\top Q^\top \Sigma^{-1} \right\} \Sigma \left\{ \Sigma^{-1}Q \xi^i \right\} = s_i^{-2} (\xi^i)^\top \Sigma^{-1}Q \xi^i = s_i^{-2} (\xi^i)^\top \Sigma^{-1}Q \xi^i = s_i^{-1}. \quad (32)
\]

This implies the third equality below:

\[
\text{Tr} \left[ F \Sigma^{-1}Q \right] = \sum_{i=1}^{m} (\xi^i)^\top F \Sigma^{-1}Q \xi^i = \sum_{i=1}^{m-a} s_i (\xi^i)^\top F \xi^i = \sum_{i=1}^{m-a} \frac{(\xi^i)^\top F \xi^i}{\Sigma \xi^i} \leq (m - a)t_2. \quad (33)
\]

Equations (30) and (31) yield the result.

\[\square\]

A.1 Entire series

**Lemma 13.** Let \((D_k)_{k \in \mathbb{N}}\) be a sequence of matrices of the same size. If \(\sum_{k \in \mathbb{N}} D_k\) exists and its kernel is the trivial vector space, then there exists a nonnegative integer \(N\) such that \(\cap_{k=0}^{N} \ker D_k\) is the trivial vector space.

**Proof.** Assume the sum \(\sum_{k \in \mathbb{N}} D_k\) exists and its kernel is the trivial vector space. Consider the sequence \((d(n))_{n \in \mathbb{N}}\) where for every nonnegative integer \(n\), \(d(n)\) is the dimension of \(\cap_{k=0}^{n} \ker D_k\). \((d(n))_{n \in \mathbb{N}}\) is a nonincreasing sequence of nonnegative integers, so it is convergent. If its limit is strictly greater than 0, then for every nonnegative integer \(n\), there exists a unit vector \(v_n\) that belongs to \(\cap_{k=0}^{n} \ker D_k\). Because the unit sphere is compact, there exists an increasing mapping \(\phi : \mathbb{N} \to \mathbb{N}\) such that the subsequence \((v_{\phi(n)})_{n \in \mathbb{N}}\) converges to a limit \(v\) such that \(\|v\| = 1\). Besides, for every pair of nonnegative integers \(a \leq n', v_{\phi(n')} \in \cap_{k=0}^{\phi(n')} \ker D_k\). Given this set is closed, the limit \(v\) also belongs to \(\cap_{k=0}^{\phi(n')} \ker D_k\). So for every nonnegative integer \(k\), \(v \in \ker D_k\) and therefore \(v \in \cap_{k=0}^{\phi(n')} \ker D_k\). So \(v\) can only be the null vector, which is absurd since \(\|v\| = 1\). We deduce from this contradiction that the limit of the sequence of integers \((d(n))_{n \in \mathbb{N}}\) is 0. Therefore there exists a nonnegative integer \(N\) such that \(d(N) = 0\). \(\square\)

B Maclaurin series

The lemmas in this subsection deal with the following setting.
Let \( m \) be a positive integer and let \( M \) be a continuous mapping from \( \mathbb{R} \) to \( \mathcal{M}_m \), the set of \( m \times m \) matrices. Assume \( M \) admits the following Maclaurin series:
\[
M(t) = \sum_{k=0}^{N} a_k(t) A_k + B(t). \tag{34}
\]
In the above expression, \( N \) is a nonnegative integer and for every \( k \in [0, N] \):
(a) \( a_k \) is a continuous mapping \( \mathbb{R} \to \mathbb{R} \) such that for all \( t \neq 0 \), \( a_k(t) \neq 0 \);
(b) for every nonnegative integer \( l < k \), \( a_k(t) = o(|a_l(t)|) \) when \( t \to 0 \);
(c) \( A_k \) is a non-null symmetric \( m \times m \) matrix.

\( B \) is a continuous mapping \( \mathbb{R} \to \mathcal{M}_m \) such that for every \( t \in \mathbb{R} \), \( B(t) \) is a symmetric matrix and when \( t \to 0 \), \( \|B(t)\| = o(|a_N(t)|) \).

**Lemma 14.** Consider \( A_k \). If \( \cap_{k=0}^{N} \ker A_k = \text{the trivial vector space} \) and if there exists \( T > 0 \) such that for all \( t \in (-T, T) \), \( M(t) \) is nonsingular, then when \( t \to 0 \), \( \|M(t)^{-1}\| = O(|a_N(t)|^{-1}) \).

**Proof.** Assume that \( \cap_{k=0}^{N} \ker A_k = \text{the trivial vector space} \) and that there exists \( T > 0 \) such that for all \( t \in (-T, T) \), \( M(t) \) is a nonsingular matrix.

If \( N = 0 \), then \( A_0 \) is nonsingular and the conclusion is trivial.

If \( N \geq 1 \), we may assume without loss of generality that \( \cap_{k=0}^{N-1} \ker A_k \) is a nontrivial vector space, otherwise we could replace \( N \) by \( N - 1 \) and \( B(t) \) by \( \{a_N(t) A_N + B(t)\} \) for all \( t \in \mathbb{R} \).

Let \( d_N \) be the codimension of \( \cap_{k=0}^{N-1} \ker A_k \). Let \( W_N \) be an \( m \times (m - d_N) \) matrix whose columns form an orthonormal basis of \( \cap_{k=0}^{N-1} \ker A_k \), and let \( P_N \) be an \( m \times d_N \) matrix whose columns form an orthonormal basis of its orthogonal complement. Then \( (P_N W_N) \) is an orthogonal matrix. For all \( t \in \mathbb{R} \), let us replace \( M(t) \) by \( (P_N W_N)^\top M(t)(P_N W_N) \). Because \( (P_N W_N) \) is an orthogonal matrix, the Frobenius norm of \( M(t)^{-1} \) is unchanged. Naturally, for all \( k \in [0, N] \), \( A_k \) is replaced by \( (P_N W_N)^\top A_k (P_N W_N) \) and for every \( t \in \mathbb{R} \), \( B(t) \) is replaced by \( (P_N W_N)^\top B(t)(P_N W_N) \).

Now, for every \( k \in [1, N] \), \( A_k \) can be decomposed into blocks - a \( d_N \times d_N \) block \( A_k' \), an \( (m - d_N) \times (m - d_N) \) block \( A_k'' \) and a \( d_N \times (m - d_N) \) block \( A_k''' \):
\[
A_k = \begin{pmatrix} A_k' & A_k'' \\ (A_k'')^\top & A_k''' \end{pmatrix} \tag{35}
\]
For all \( t \in \mathbb{R} \), \( B(t) \) can be decomposed in a similar manner (here the ' notation is used to distinguish the blocks, not to express some derivative with respect to \( t \)):
\[
B(t) = \begin{pmatrix} B(t)' & B(t)'' \\ (B(t)'')^\top & B(t)''' \end{pmatrix} \tag{36}
\]
Now, for any symmetric nonsingular matrix
\[
C = \begin{pmatrix} C' & C'' \\ (C'')^\top & C''' \end{pmatrix}. \tag{37}
\]
denoting by $S := \{C' - C'''(C'')^{-1}(C''')^\top\}$ the Schur complement of $C''$, the inverse of $C$ is

$$C^{-1} = \begin{pmatrix} I & 0 \\ -(C'')^{-1}(C''')^\top & I \end{pmatrix} \begin{pmatrix} S^{-1} & 0 \\ 0 & (C'')^{-1} \end{pmatrix} \begin{pmatrix} I & -C'''(C'')^{-1} \\ 0 & I \end{pmatrix}. \quad (38)$$

For every $k \in [0, N - 1]$, $A''_k$ and $A'''_k$ are null. For all $t \in (-T, T)$, $M(t)$ is nonsingular. Its lower $(m - d_N) \times (m - d_N)$ block is $\{a_N(t)A''_N + B(t)''\}$ and its Schur complement $S_N(t)$ is

$$S_N(t) := \sum_{k=0}^N a_k(t)A'_k + B(t)' - \{a_N(t)A''_N + B(t)''\} \{a_N(t)A''_N + B(t)''\}^{-1} \{a_N(t)A''_N + B(t)''\}^\top. \quad (39)$$

Because we are dealing with the finite dimensional vector space of matrices of size $m \times m$, all norms are equivalent. In particular, the Frobenius norm is equivalent to the algebra norm

$$A \mapsto \sup \left\{ \sqrt{\xi^\top A \xi/\xi^\top \xi} : \xi \in \mathbb{R}^m \setminus \{0_m\} \right\}.$$

So there exists a constant $C_m \in (0, +\infty)$ such that for every $t \in (-T, T)$,

$$\|M(t)^{-1}\| \leq C_m \left( \|I_m\| + \left\| \{a_N(t)A''_N + B(t)''\} \{a_N(t)A''_N + B(t)''\}^{-1} \right\|^{2} \left( \|S_N(t)^{-1}\| + \left\| \{a_N(t)A''_N + B(t)''\}^{-1} \right\| \right). \quad (40)$$

$A''_N$ is nonsingular, otherwise $\cap_{k=0}^N \text{Ker} A_k$ would be nontrivial. This means that the norm of the matrix $\{a_N(t)A''_N + B(t)''\} \{a_N(t)A''_N + B(t)''\}^{-1}$ is bounded when $t \to 0$. Because of Equation (38), this implies that there exists $T_N > 0$ and $\lambda_N > 0$ such that for all $t \in (-T_N, T_N)$,

$$\lambda_N \|M(t)^{-1}\| \leq |a_N(t)|^{-1} + \|S_N(t)^{-1}\|. \quad (41)$$

Our goal is to use Equation (41) recursively, by having $S_N(t)$ take the place of $M(t)$. To achieve this, a new expression of $S_N(t)$ is required.

$$S_N(t) = \sum_{k=0}^{N-1} a_k(t)A'_k + B_N(t), \quad (42)$$

where

$$B_N(t) := a_n(t)A''_N + B(t)' - \{a_N(t)A''_N + B(t)''\} \{a_N(t)A''_N + B(t)''\}^{-1} \{a_N(t)A''_N + B(t)''\}^\top. \quad (43)$$

It turns out that when $t \to 0$, the norm of $B_N(t)$ is $O(|a_N(t)|)$. This is due to the fact mentioned above that $\{a_N(t)A''_N + B(t)''\} \{a_N(t)A''_N + B(t)''\}^{-1}$ is bounded when $t \to 0$.

Furthermore, $\cap_{k=0}^{N-1} \text{Ker} A_k'$ is the trivial vector space. Indeed, let $v_1 \in \cap_{k=0}^{N-1} \text{Ker} A_k'$. Then for any vector $v_2 \in \mathbb{R}^{m-d_N}$, $(v_1, v_2)^\top \cap_{k=0}^{N-1} \text{Ker} A_k$. Independently from this, for any vector $v_3 \in \mathbb{R}^{d_N}$, $(v_3, 0_{m-d_N})^\top$ belongs to the orthogonal complement of $\cap_{k=0}^{N-1} \text{Ker} A_k$. So $(v_1, 0_{m-d_N})^\top$ belongs both to $\cap_{k=0}^{N-1} \text{Ker} A_k$ and its orthogonal complement: it is the null vector. Therefore $v_1 = 0_{d_N}$.
The two paragraphs above show that Equation (42) is formally similar to Equation (34): the role of $M(t)$ is held by $S_N(t)$, the role of $N$ by $N-1$, the role of the $A_k$s by the $A_k'$s and the role of $B(t)$ by $B_N(t)$.

Therefore an equation similar to (11) can be derived: there exist $T_{N-1} > 0$ and $\lambda_{N-1} > 0$ such that for all $t \in (-T_{N-1}, T_{N-1}),$

$$\lambda_{N-1} \|S_N(t)^{-1}\| \leq |a_{N-1}(t)|^{-1} + \|S_{N-1}(t)^{-1}\|. \tag{44}$$

Here, $S_{N-1}(t)$ is defined with respect to $S_N(t)$ the same way $S_N(t)$ was defined with respect to $M(t)$.

Recursive application of this reasoning until 0 is reached yields the result.

\textbf{Lemma 15.} Consider (34) with $N = 1$. If $\text{Ker} A_0 \cap \text{Ker} A_1$ is the trivial vector space, then there exists $T > 0$ such that for all $t \in (-T, T)$, $M(t)$ is nonsingular.

\textbf{Proof.} We use the same notations as in the proof of Lemma 14 and redefine matrices the same way: $M(t) := (P_1W_1)^\top M(t)(P_1W_1)$, $B(t) := (P_1W_1)^\top B(t)(P_1W_1)$, $A_0 := (P_1W_1)^\top A_0(P_1W_1)$, $A_1 := (P_1W_1)^\top A_1(P_1W_1)$. For all $t \in \mathbb{R}$, the determinant of $M(t)$ is the product of the determinants of $S_1(t)$ and of $\{a_1(t)A_1'' + B(t)''\}$. Because $\text{Ker} A_0 \cap \text{Ker} A_1$ is the trivial vector space, $A_1''$ is nonsingular. When $|t|$ is small enough therefore, $\{a_1(t)A_1'' + B(t)''\}$ is nonsingular too. Moreover, $\lim_{t \to 0} a_0^{-1}(t)S_1(t) = A_0''$ is also nonsingular. These two facts imply that when $|t|$ is small enough, the determinant of $M(t)$ is non-null and $M(t)$ is nonsingular.

\textbf{Lemma 16.} Consider (34). If $\cap_{k=0}^N \text{Ker} A_k$ is the trivial vector space, if the vector space $\cap_{k=0}^{N-1} \text{Ker} A_k$ is non-trivial, and if there exists $T > 0$ such that for all $t \in (-T, T)$, $M(t)$ is positive definite, then there exists a hyperplane $\mathcal{H}$ of $\mathbb{R}^m$ such that for all $v \in \mathbb{R}^m \setminus \mathcal{H},$

$$\liminf_{t \to 0} \frac{vM(t)^{-1}v}{\|M(t)^{-1}\|} > 0. \tag{45}$$

\textbf{Proof.} This result is trivial if $N = 0$. If $N \geq 1$, it follows from the proof of Lemma 14. Indeed, the requirements of this lemma are stronger than those of Lemma 14, so all intermediate results of its proof are valid. Consider Equation (38) while assuming $C$ is positive definite. In the right member, the matrices on the left and on the right are the transpose of one another, so the middle matrix is necessarily positive definite. In particular, both $S^{-1}$ and $(C'')^{-1}$ are positive definite. Any vector $v \in \mathbb{R}^m$ can be decomposed as $v = (v', v'')^\top$ with $v' \in \mathbb{R}^{d_N}$ and $v'' \in \mathbb{R}^{m-d_N}$. This decomposition yields a lower bound: $v^\top C^{-1}v \geq (v'')^\top (C'')^{-1}v''$. Here, $C$ is $M(t)$, $S$ is $S_N(t)$ and $C''$ is $a_N(t)A_N'' + B''(t)$. Let us recall that $A_N''$ is nonsingular and $\|B''(t)\| = o(|a_N(t)|)$ when $t \to 0$. So as long as $v$ is not orthogonal to $\cap_{k=0}^{N-1} \text{Ker} A_k$, $v''$ is non-zero and there exists $\bar{\lambda}_N(v) > 0$ such that when $|t|$ is small enough, $v^\top M(t)^{-1}v \geq \bar{\lambda}_N(v)|a_N(t)||^{-1}$. Then Lemma 14 yields the result for any hyperplane $\mathcal{H}$ of $\mathbb{R}^m$ that contains the orthogonal complement of $\cap_{k=0}^{N-1} \text{Ker} A_k$.

\textbf{Lemma 17.} If $\cap_{k=0}^N \text{Ker} A_k \neq \text{Ker} A_0$, if $\cap_{k=0}^{N-1} \text{Ker} A_k = \text{Ker} A_0$, and if there exists $T > 0$ such that for all $t \in (-T, T)$, $M(t)$ is positive definite, then the largest eigenvalue $v_1(t)$ and the second largest eigenvalue $v_2(t)$ of $M(t)$ have the following behavior when $t \to 0$:

(a) $v_1(t)^{-1} = O(|a_0(t)|^{-1});$
(b) \( v_2(t)^{-1} = O(|a_N(t)|^{-1}) \).

Proof. It is equivalent to prove that in this situation, there exists \( \lambda > 0 \) such that when \( |t| \) is sufficiently small \( v_1(t) \geq \lambda |a_0(t)| \) and \( v_2(t) \geq \lambda |a_N(t)| \).

When \( t \to 0 \), we have \( a_0(t)^{-1}M(t) \to A_0 \), so \( A_0 \) is either positive or negative semi-definite. Since \( a_0 \) is continuous and non-null everywhere except possibly at 0, its sign is therefore constant: nonnegative if \( A_0 \) is positive semi-definite and nonpositive if \( A_0 \) is negative semi-definite. Without loss of generality, let us assume that \( A_0 \) is positive semi-definite and that \( a_0 \) is nonnegative. \( a_0(t)^{-1}M(t) \to A_0 \) implies that \( a_0(t)^{-1}v_1(t) \) converges to \( A_0 \)'s greatest eigenvalue, which is strictly greater than 0 because \( A_0 \) is non-null. This implies the first result.

Now, since \( A_0 \) is non-null, its rank is greater or equal to 1. If it is greater or equal to 2, then \( a_0(t)^{-1}v_2(t) \) converges to the second greatest eigenvalue of \( A_0 \), so \( v_2^{-1}(t) = O(a_0(t)^{-1}) \) and the second result holds a fortiori.

Assume from now on that \( A_0 \) has rank 1. For every nonnegative integer \( k < N \), \( A_k \) shares \( A_0 \)'s kernel, so \( A_k \) is proportional to \( A_0 \). We may therefore assume without loss of generality that \( N = 1 \). Since \( A_0 \) is a symmetric positive semi-definite matrix with rank 1, there exists a vector \( a_0 \) such that \( A_0 = a_0a_0^\top \).

Choose for all \( t \in (-T, T) \) a unit eigenvector \( V_1(t) \) corresponding to the eigenvalue \( v_1(t) \) of \( M(t) \) and a unit eigenvector \( V_2(t) \) corresponding to the eigenvalue \( v_2(t) \) such that \( V_1(t)^\top V_2(t) = 0 \) (it is always possible to choose \( V_2(t) \) that way because \( M(t) \) is symmetric). When \( t \to 0 \), \( V_1(t) \to a_0/\|a_0\| \). Since \( V_1(t)^\top V_2(t) = 0 \) for all \( t \in (-T, T) \), we have \( \lim_{t \to 0} a_0^\top V_2(t) = 0 \).

\[
v_2(t) = a_0(t) \left( a_0^\top V_2(t) \right)^2 + a_1(t)V_2(t)^\top A_1V_2(t) + V_2(t)^\top B(t)V_2(t) \geq a_1(t) \left\{ V_2(t)^\top A_1V_2(t) + o(1) \right\}
\]

(46)

Because \( M(t) \) is positive definite for all \( t \in (-T, T) \), the restriction of \( A_1 \) to \( \text{Ker} A_0 \) is either positive semi-definite (making \( a_1 \) nonnegative) or negative semi-definite (making \( a_1 \) nonpositive). Moreover, it is non-null.

Since \( v_2(t) = \max\{\xi M(t)\xi \mid \xi \in \mathbb{R}^m \text{ and } \|\xi\| = 1 \text{ and } \xi^\top v_1(t) = 0\} \), the above implies the following: \( \lim_{t \to 0} |a_1(t)|^{-1}v_2(t) > 0 \). So the second result also holds when the rank of \( A_0 \) is 1.

\[\square\]

C  Spectral decomposition

For the following lemmas, we need to set up a few notations. First, denote by \( \tilde{K}_r \) the \( r \)-dimensional Fourier transform of the isotropic correlation kernel \( K \):

\[
\tilde{K}_r(\omega) = (2\pi)^{-r} \int_{\mathbb{R}^r} K(\|x\|) e^{-i\langle \omega, x \rangle} \, dx \quad \text{and} \quad K(\|x\|) = \int_{\mathbb{R}^r} \tilde{K}_r(\omega) e^{i\langle \omega, x \rangle} \, d\omega.
\]

(47)
For all \( \theta \in (0, +\infty) \), using the correlation kernel \( K_\theta(\cdot) = K(\cdot/\theta) \), the correlation matrix \( \Sigma_\theta \) is such that:

\[
\forall \xi \in \mathbb{R}^n, \quad \xi^T \Sigma_\theta \xi = \sum_{j,k=1}^n \xi_j \xi_k K \left( \left\| \frac{x^{(j)} - x^{(k)}}{\theta} \right\| \right) = \int_{\mathbb{R}^r} \tilde{K}_\theta(\omega) \left| \sum_{j=1}^n \xi_j e^{i\langle \omega | x^{(j)} \rangle} \right|^2 d\omega = M_\theta \theta^r I_\theta(\xi). \tag{48}
\]

The factors in the last equality depend on the kernel and are given in Table 4.

| Kernel                | \( M_\theta \)                                                                 | \( I_\theta(\xi) \)                                                                 |
|-----------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| Matérn \((\nu + \frac{1}{2})\pi \Gamma(\nu) \) \((\frac{1}{2} \pi)^{-\nu} \) | \( \int_{\mathbb{R}^r} (4\nu + \theta^2 \|s\|^2)^{-\frac{\nu}{2} - \nu} \left| \sum_{j=1}^n \xi_j e^{i\langle s | x^{(j)} \rangle} \right|^2 ds \) | \( \int_{\mathbb{R}^r} \exp \left( -\frac{\theta^2 \|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i\langle s | x^{(j)} \rangle} \right|^2 ds \) |
| Rational Quadratic \((\frac{1}{2} \pi)^{-\nu} \pi \Gamma(\nu) \) | \( \int_{\mathbb{R}^r} \theta^r \|s\|^r \frac{\nu}{\pi} \int_{\mathbb{R}^r} e^{i\langle \omega | s \rangle} d\omega \) | \( \int_{\mathbb{R}^r} \exp \left( -\frac{\theta^2 \|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i\langle s | x^{(j)} \rangle} \right|^2 ds \) |
| Squared Exponential \((\frac{1}{2} \pi)^{-\nu} \) | \( \int_{\mathbb{R}^r} \exp \left( -\frac{\theta^2 \|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i\langle s | x^{(j)} \rangle} \right|^2 ds \) | \( \int_{\mathbb{R}^r} \exp \left( -\frac{\theta^2 \|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i\langle s | x^{(j)} \rangle} \right|^2 ds \) |

Table 4: \( M_\theta \) and \( I_\theta(\xi) \) for the three considered correlation kernel families. \( \mathcal{K}_\nu \) is the modified Bessel function of second kind with parameter \( \nu \). \cite{AbramowitzStegun} (9.6.)

The spectral decomposition of correlation kernels is a powerful tool.

To use it, we need this Bochner-type result:

**Lemma 18.** Let \( \mu \) be a positive measure on \( \mathbb{R}^r \) with finite non-null total mass that is absolutely continuous with respect to the Lebesgue measure. Then the mapping \( K : \mathbb{R}^r \rightarrow \mathbb{R} \) defined by

\[
K(x) = \int_{\mathbb{R}^r} e^{i\langle \omega | x \rangle} d\mu(\omega)
\]

is positive definite. Moreover, for any \( \xi \in \mathbb{R}^n \setminus \{0_n\} \),

\[
\sum_{k,l \in [1,n]} \xi_k \xi_l K(x^{(k)} - x^{(l)}) > 0. \tag{50}
\]

**Proof.** The first part results from Bochner’s theorem. Let us show the second.

\[
\sum_{k,l \in [1,n]} \xi_k \xi_l K(x^{(k)} - x^{(l)}) = \sum_{k,l \in [1,n]} \xi_k \xi_l \int_{\mathbb{R}^r} e^{i\langle \omega | x^{(k)} - x^{(l)} \rangle} d\mu(\omega) = \int_{\mathbb{R}^r} \left| \sum_{k=1}^n \xi_k e^{i\langle \omega | x^{(k)} \rangle} \right|^2 d\mu(\omega). \tag{51}
\]

Given \( x^{(1)}, \ldots, x^{(n)} \) are all distinct, the mapping \( \mathbb{R}^r \rightarrow \mathbb{C}; \omega \rightarrow \sum_{k=1}^n \xi_k e^{i\langle \omega | x^{(k)} \rangle} \) takes null values on a Borel set that is negligible with respect to the Lebesgue measure. This set is therefore also negligible with respect to \( \mu \), which yields the conclusion.

Let us use spectral decomposition to show this useful fact about Matérn kernels:

**Lemma 19.** For Matérn kernels, when \( \theta \rightarrow +\infty \), \( \| \Sigma_\theta^{-1} \| = O(\theta^{2r}) \).
Proof. When \( \theta \geq 2\sqrt{\nu} \), for any \( \xi \in \mathbb{R}^n \), \( I_\theta(\xi) \geq 2^{-\frac{\nu}{2}}\theta^{-r-2\nu} \int_{\|s\| \geq 1} \|s\|^{-r-2\nu} \left| \sum_{j=1}^n \xi_j e^{i(s^j(x^{(j)}) - x^{(i'))}} \right|^2 ds \).

Define the mapping \( K^{aux} : \mathbb{R}^r \to \mathbb{R} \) by

\[
K^{aux}(x) = \int_{\mathbb{R}^r} e^{i(\omega|x|)} \|s\|^{-r-2\nu} 1_{\|s\| \geq 1} ds.
\]

By Lemma (58), the \( n \times n \) matrix \( M \) with \((i,i')\)-th element \( K^{aux,\xi}(x(x(i)) - x(x(i'))) \) is positive definite. For any \( \xi \in \mathbb{R}^n \),

\[
\int_{\|s\| \geq 1} \|s\|^{-r-2\nu} \left| \sum_{j=1}^n \xi_j e^{i(s^j(x^{(j)}) - x^{(i'))}} \right|^2 ds = \xi^\top M \xi.\]

Denote by \( M \) the smallest eigenvalue of \( M \). For any \( \xi \in \mathbb{R}^n \), when \( \theta \geq 2\sqrt{\nu} \), \( I_\theta(\xi) \geq 2^{-\frac{\nu}{2}}\theta^{-r-2\nu} \|\xi\|^2 \).

Equation (48) implies the result.

More generally, it can be used to study the behavior of the reference prior. From Equation (48), we obtain that \( \forall \theta \in (0, +\infty), \forall \xi \in \mathbb{R}^n \):

\[
\xi^\top \left( \frac{d}{d\theta} \Sigma_\theta \right) \xi = M_r \theta^{-r-1} I_\theta(\xi) + M_r \theta^{-r} \frac{d}{d\theta} I_\theta(\xi). \tag{53}
\]

The next three lemmas are used to prove the second assertion of Proposition (7). Since the proof varies for each of the three different kernel families considered, \( I_\theta \) is written \( I_\theta^M \) for Matérn kernels, \( I_\theta^{RQ} \) for Rational Quadratic kernels and \( I_\theta^{SE} \) for the Squared Exponential kernel.

Lemma 20. For Matérn kernels, the matrix \( F_\theta := r\theta^{-1} \Sigma_\theta - \frac{d}{d\theta} \Sigma_\theta \) is symmetric positive definite. Furthermore, for any \( \xi \in \mathbb{R}^n \), \( \xi^\top F_\theta \xi \leq (2\nu + r)\theta^{-1} \xi^\top \Sigma_\theta \xi \).

Proof. For any \( \theta \in (0, +\infty) \) and any \( \xi = (\xi_1, ..., \xi_n)^\top \in \mathbb{R}^n \),

\[
\frac{d}{d\theta} I_\theta^M(\xi) = (-2) \left( \frac{r}{2} + \nu \right) \theta \int_{\mathbb{R}^r} \|s\|^2 \left( 4\nu + \theta^2 \|s\|^2 \right)^{\frac{r}{2} - \nu - 1} \left| \sum_{j=1}^n \xi_j e^{i(s^j(x^{(j)}) - x^{(i'))}} \right|^2 ds
\]

\[
= -(2\nu + r)\theta^{-1} \int_{\mathbb{R}^r} \frac{\theta^2}{4\nu + \theta^2 \|s\|^2} \left( 4\nu + \theta^2 \|s\|^2 \right)^{\frac{r}{2} - \nu - 1} \left| \sum_{j=1}^n \xi_j e^{i(s^j(x^{(j)}) - x^{(i'))}} \right|^2 ds.
\]

Since the ratio in the integrand is smaller than 1, for any \( \theta \in (0, +\infty) \) and any non-null vector \( \xi \in \mathbb{R}^n \),

\[
0 < -\frac{d}{d\theta} I_\theta^M(\xi) \leq (2\nu + r)\theta^{-1} I_\theta^M(\xi). \tag{55}
\]

Combining Equations (48), (53) and (55) yields the result.

Lemma 21. For Rational Quadratic isotropic correlation kernels, the matrix \( F_\theta := r\theta^{-1} \Sigma_\theta - \frac{d}{d\theta} \Sigma_\theta \) is symmetric positive definite. If \( \theta \) is large enough, it verifies \( \forall \xi \in \mathbb{R}^n \), \( \xi^\top F_\theta \xi \leq (r + 2)\xi^\top \Sigma_\theta \xi \).

Proof. In the following, denote by \( K_\nu \) the modified Bessel function of second kind with parameter \( \nu \).

[Abramowitz and Stegun, 1964] (9.6.)
For any \( \theta \in (0, +\infty) \) and any \( \xi \in \mathbb{R}^n \),

\[
\frac{d}{d\theta} I_{\theta}^{RQ}(\xi) = \int_{\mathbb{R}^n} \|s\| \frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\}_{z = \theta\|s\|} \left[ \sum_{j=1}^{n} \xi_j e^{i(s|\xi|^{j})} \right]^2 ds.
\]  

We now compute \( \frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\} \). Following [Abramowitz and Stegun 1964] (9.6.28.),

\[
\frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\} = \begin{cases} 
-z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \nu \log(z) & \text{if } \nu - \frac{1}{2} > 0, \\
-z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \nu - 1 (\nu - 1) z^{2\nu - r - 1} K_{\nu - \frac{d}{d\theta}} \left( z \right) & \text{if } 0 < \nu - \frac{1}{2} < 1, \\
\frac{1}{z^{\log(z)}} K_{\nu - \frac{d}{d\theta}} \left( z \right) & \text{if } \nu - \frac{1}{2} < 0.
\end{cases}
\]  

Combining this with Equations (48) and (53) proves that \( F_\theta \) is positive definite.

We now have to deal with the behavior of \( K_{\nu - \frac{d}{d\theta}} \left( z \right) \) when \( z \to 0 \) and when \( z \to +\infty \).

Let us start with \( z \to 0 \). Using [Abramowitz and Stegun 1964] (9.6.9.), we obtain:

\[
K_{\nu - \frac{d}{d\theta}} \left( z \right) \sim \begin{cases} 
\frac{2(\nu - \frac{1}{2})!}{z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)}} & \text{if } \frac{1}{2} < \nu > 1, \\
-z \log(z) K_{\nu - \frac{d}{d\theta}} \left( z \right) & \text{if } \nu - \frac{1}{2} = 1, \\
\frac{1}{z^{\log(z)}} K_{\nu - \frac{d}{d\theta}} \left( z \right) & \text{if } \nu - \frac{1}{2} < 1.
\end{cases}
\]  

So, for any \( \nu > 0 \), there exists \( a_{r, \nu} > 0 \) such that, as long as \( z \) is small enough, \( K_{\nu - \frac{d}{d\theta}} \left( z \right) \leq a_{r, \nu} z K_{\nu - \frac{d}{d\theta}} \left( z \right) \).

Moreover, [Abramowitz and Stegun 1964] (9.7.2.) states that when \( z \to +\infty \), \( K_{\nu - \frac{d}{d\theta}} \left( z \right) \sim \exp(-z) \sqrt{\pi} / \sqrt{2z} \).

Because \( K_{\nu - \frac{d}{d\theta}} \left( z \right) \) is a continuous function on \((0, +\infty)\), the two results above imply that

\[
\forall \lambda > 1 \quad \exists a_{r, \nu} > 0 \quad \forall z > 0 \quad z K_{\nu - \frac{d}{d\theta}} \left( z \right) \leq \max(a_{r, \nu}, \lambda z) K_{\nu - \frac{d}{d\theta}} \left( z \right).
\]  

Now, \( \frac{d}{d\theta} I_{\theta}^{RQ}(\xi) = J_0^1(\xi) + J_0^2(\xi), \) with

\[
J_0^1(\xi) := \int_{\|s\| \leq 1} \|s\| \frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\}_{z = \theta\|s\|} \left[ \sum_{j=1}^{n} \xi_j e^{i(s|\xi|^{j})} \right]^2 ds;
\]

\[
J_0^2(\xi) := \int_{\|s\| > 1} \|s\| \frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\}_{z = \theta\|s\|} \left[ \sum_{j=1}^{n} \xi_j e^{i(s|\xi|^{j})} \right]^2 ds.
\]  

Set \( 0 < \epsilon < 1 \). When \( z \in [\epsilon, 1] \), \( \frac{d}{dz} \left\{ z^{\nu - \frac{d}{d\theta} K_{\nu - \frac{d}{d\theta}} \left( z \right)} \right\} \) is bounded away from 0, so there exists \( m_\epsilon \) such that

\[
\theta |J_0^1(\xi)| \geq m_\epsilon \int_{\frac{1}{2} < \|\xi\| < 1} \left[ \sum_{j=1}^{n} \xi_j e^{i(s|\xi|^{j})} \right]^2 ds = m_\epsilon \theta^{-r} \int_{\epsilon < \|\omega\| < 1} \left[ \sum_{j=1}^{n} \xi_j e^{i(\omega|\xi|^{j})} \right]^2 d\omega.
\]  

The Lebesgue measure on \( \{\omega \in \mathbb{R}^n : \epsilon < \|\omega\| < 1\} \) is a finite positive measure. Lemma 18 asserts that the mapping \( K^\epsilon : \mathbb{R}^n \to \mathbb{R} \) defined by

\[
K^\epsilon(x) = \int_{\epsilon < \|\omega\| < 1} e^{i(\omega|x|)} d\omega
\]  

(62)
is positive definite. It is an isotropic covariance kernel: \( K^\theta \) only depends on \( x \) through its norm \( \|x\| \). Let \( \Sigma^\theta_0 \) be the correlation matrix corresponding with \( K^\theta \): its \((i, i')\)-th element is \( K^\theta \left( (x^{(i)} - x^{(i')})/\theta \right) \). The Lebesgue measure on \( \{ \omega \in \mathbb{R}^r : \epsilon < \|\omega\| < 1 \} \) is absolutely continuous with respect to the Lebesgue measure on \( \mathbb{R}^r \), so Lemma 18 also asserts that \( \Sigma^\theta_0 \) is positive definite.

Moreover, for every nonnegative integer \( k \), \( \int \|\omega\|^k \mathbf{1}_{\epsilon < \|\omega\| < 1} d\omega \) is smaller than the mass of the Lebesgue measure on \( \{ \omega \in \mathbb{R}^r : \epsilon < \|\omega\| < 1 \} \). The Maclaurin series of \( K^\theta \) has therefore infinite radius of convergence. For any nonnegative integer \( k \), denote by \( D^{(k)} \) the \( n \times n \) matrix with \((i, i')\)-th element \( \|x^{(i)} - x^{(i')}\|^{2k} \). Because the Maclaurin series has infinite radius of convergence, \( \Sigma^\theta_0 \) is equal to its asymptotic expansion regardless of the value of \( \theta \). There exist real numbers \( a_k \) \((k \in \mathbb{N})\) such that for all \( \theta \in (0, +\infty) \), \( \Sigma^\theta_0 = \sum_{k=0}^{\infty} a_k \theta^{-2k} D^{(k)} \).

Because \( \Sigma^\theta_0 \) is positive definite, Lemma 13 ensures there exists a nonnegative integer \( N \) such that the vector space \( \cap_{k=0}^{N} \ker a_k D^{(k)} \) is positive definite. It is an isotropic covariance kernel:

Applying Lemma 13 then yields that when \( \theta \to +\infty \), \( \|\Sigma^\theta_0^{-1}\| = O(\theta^{2N}) \). Because the greatest eigenvalue of a positive definite matrix is the smallest eigenvalue of its inverse, this implies the existence of a constant \( c_\epsilon > 0 \) such that when \( \theta \) is large enough

\[
\min_{\xi \in \mathbb{R}^n, \|\xi\| = 1} \xi^T \Sigma^\theta_0 \xi \geq c_\epsilon \theta^{-2N}.
\]  

(63)

So when \( \theta \) is large enough, for every \( \xi \in \mathbb{R}^n \),

\[
\int \mathbf{1}_{\epsilon < \|\omega\| < 1} \left| \sum_{j=1}^{n} \xi_j e^{i \langle \omega, x^{(j)} \rangle} \right|^2 d\omega \geq c_\epsilon \|\xi\|^2 \theta^{-2N}.
\]  

(64)

This provides a lower bound for \( |J^\theta_0(\xi)| \):

\[
\theta |J^\theta_0(\xi)| \geq \tilde{m}_\epsilon c_\epsilon \|\xi\|^2 \theta^{-r-2N}.
\]  

(65)

Besides, we have

\[
\theta |J^\theta_0(\xi)| \leq n^2 \|\xi\|^2 \int_{\|s\| > 1} (\|s\|)^{\nu - \frac{r}{2} - \frac{1}{2}} \exp(-\theta \|s\|) ds
\]

\[
= n^2 \|\xi\|^2 \frac{2\pi^{\frac{r-1}{2}}}{\Gamma \left( \frac{r-1}{2} \right)} \int_{1}^{+\infty} (\theta t)^{\nu - \frac{r}{2} - \frac{1}{2}} \exp(-\theta t)t^{r-1} dt
\]

\[
\leq n^2 \|\xi\|^2 \frac{2\pi^{\frac{r-1}{2}}}{\Gamma \left( \frac{r-1}{2} \right)} \Gamma \left( \nu + \frac{r-1}{2} \right) \theta^{\nu - \frac{r}{2} - \frac{1}{2}} \exp(-\theta - 1)).
\]  

(66)

From Equations (63) and (66), we gather that when \( \theta \to +\infty \), \( \sup_{\|\xi\| = 1} |J^\theta_0(\xi)| = o \left( \inf_{\|\xi\| = 1} |J^\theta_0(\xi)| \right) \), so for any \( \lambda > 1 \), when \( \theta \) is large enough, \( -\frac{d}{d\theta} f^\theta_Q(\xi) \leq -\lambda |J^\theta_0(\xi)| \). Denote by \( (r-2\nu)_+ \) the quantity \( \max(0, r-2\nu) \).
Then, combining Equations (67) and (69), there exists $a'_{r, \nu} > 0$ such that

$$-\theta \frac{d}{d\theta} I^\text{RQ}_\theta (\xi) \leq \lambda \int_{|s| \leq 1} \max \left( a'_{r, \nu}, (\lambda + (r - 2\nu)_+) \theta \|s\| \right) \left( \theta \|s\|^\nu - \frac{\pi}{\|s\|} \right) d\theta \|s\| d\theta \|s\| ds$$

$$\leq \lambda \max \left( a'_{r, \nu}, (\lambda + (r - 2\nu)_+) \theta \right) \int_{|s| \leq 1} \left( \theta \|s\|^\nu - \frac{\pi}{\|s\|} \right) d\theta \|s\| ds \left| \sum_{j=1}^n \xi_j e^{i(s|w^{(j)})} \right|^2 ds.$$  \hspace{1cm} (67)

When $\theta$ is large enough, $a'_{r, \nu} \leq \lambda \theta$ so

$$-\theta \frac{d}{d\theta} I^\text{RQ}_\theta (\xi) \leq \lambda (\lambda + (r - 2\nu)_+) \theta I^\text{RQ}_\theta (\xi).$$  \hspace{1cm} (68)

From this, we obtain that for any non-null vector $\xi \in \mathbb{R}^n$, for any $\lambda > 1$, provided $\theta$ is large enough,

$$0 < -\theta \frac{d}{d\theta} I^\text{RQ}_\theta (\xi) \leq \lambda (\lambda + (r - 2\nu)_+) \theta I^\text{RQ}_\theta (\xi).$$  \hspace{1cm} (69)

Combining Equations (68), (69) and (69) yields the result.

\[\] 

**Lemma 22.** For the Squared Exponential kernel, the matrix $F_\theta := \theta^{-1} \Sigma_\theta - \frac{d}{d\theta} \Sigma_\theta$ is symmetric positive definite. If $\theta$ is large enough, it verifies $\forall \xi \in \mathbb{R}^n$, $\xi^\top F_\theta \xi \leq \theta \xi^\top \Sigma_\theta \xi$.

**Proof.** For any $\theta \in (0, +\infty)$ and any $\xi \in \mathbb{R}^n$,

$$\frac{d}{d\theta} I^\text{SE}_\theta (\xi) = \int_{\mathbb{R}^r} \frac{\theta\|s\|^2}{2} \exp \left( -\frac{\theta^2\|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i(s|w^{(j)})} \right|^2 ds.$$  \hspace{1cm} (70)

So $F_\theta$ is positive definite.

Similarly to the Rational Quadratic case (cf. proof of Lemma 21), one can show that for any $\lambda > 1$, for large enough $\theta$ and for any non-null vector $\xi \in \mathbb{R}^n$,

$$0 < -\frac{d}{d\theta} I^\text{SE}_\theta (\xi) \leq \lambda \int_{|s| \leq 1} \frac{\theta\|s\|^2}{2} \exp \left( -\frac{\theta^2\|s\|^2}{4} \right) \left| \sum_{j=1}^n \xi_j e^{i(s|w^{(j)})} \right|^2 ds \leq \frac{\lambda}{2} \theta I^\text{SE}_\theta (\xi).$$  \hspace{1cm} (71)

Combining Equations (68), (69) and (71) yields the result.

\[\] 

**D** Asymptotic study of the correlation matrix $\Sigma_\theta$

**D.1** Rational Quadratic and Squared Exponential kernels

For all $\nu > 0$, the series expansion of the mapping $x \mapsto (1 + x)^{-\nu}$ at $x = 0$ has radius of convergence 1. Moreover, the series expansion of the exponential function has infinite radius of convergence. From these
facts follows that when $\theta$ is large enough, if a Rational Quadratic kernel or a Squared Exponential kernel is used,

$$
\Sigma_\theta = \sum_{k=0}^{\infty} \frac{a_k}{\theta^{2k}} D^{(k)}.
$$

(72)

In the above expression, for every $k$, $D^{(k)}$ is the $n \times n$ matrix with $(i, i')$-th element $\|x^{(i)} - x^{(i')}\|^{2k}$ and $a_k$ is a non-null real number. To be precise, $a_k = (-1)^k \left( \prod_{l=0}^{k} (\nu + l) \right)/k!$ for Rational Quadratic kernels and $a_k = (-1)^k/k!$ for the Squared Exponential kernel.

Equation (72) implies

$$
W^\top \Sigma_\theta W = \sum_{k=0}^{\infty} \frac{a_k}{\theta^{2k}} W^\top D^{(k)} W.
$$

(73)

$\Sigma_\theta$ is positive definite and the kernel of $W$ is trivial so $W^\top \Sigma_\theta W$ is positive definite. Let $k_1$ be the smallest nonnegative integer such that $W^\top D^{(k_1)} W$ is non-null. Define $D := a_{k_1} D^{(k_1)}$. If $W^\top D^{(k_1)} W$ is nonsingular, then define $k_2 := k_1 + 1$ and $D^* := a_{k_2} D^{(k_2)}$. If $W^\top D^{(k_1)} W$ is singular, then because $W^\top \Sigma_\theta W$ is nonsingular, there must exist an integer $k > k_1$ such that $W^\top D^{(k)} W$ is non-null. Then let $k_2$ be the smallest of them and define $D^* := a_{k_2} D^{(k_2)}$. Now, define the mappings $g(\theta) = \theta^{-2k_1}$ and $g^*(\theta) = \theta^{-2(k_2-k_1)}$.

Finally, define

$$
R_g(\theta) = g(\theta)^{-1} \sum_{k=k_2+1}^{\infty} \frac{a_k}{\theta^{2k}} W^\top D^{(k)} W.
$$

(74)

Notice that $\|R_g(\theta)\| = o(g^*(\theta))$ and that $\|\frac{d}{d\theta} R_g(\theta)\| = o(g^*(\theta))$.

D.2 Matérn kernels with noninteger smoothness $\nu$

If a Matérn kernel with noninteger smoothness $\nu > 0$ (whether greater or smaller than 1) is used, we can write $\Sigma_\theta$ as [Abramowitz and Stegun, 1964] (9.6.2. and 9.6.10.):

$$
\Sigma_\theta = \sum_{k=0}^{[\nu]} \frac{a_k}{\theta^{2k}} D^{(k)} + \frac{a_{\nu}}{\theta^{2\nu}} D^{(\nu)} + R(\theta).
$$

(75)

Like in the case of Rational Quadratic and Squared Exponential kernels, for every $k$, $D^{(k)}$ is the $n \times n$ matrix with $(i, i')$-th element $\|x^{(i)} - x^{(i')}\|^{2k}$.

The $a_k$’s, of course, are different: $a_k = (-1)^k \Gamma(\nu - k) \nu^k / (k! \Gamma(\nu))$. Moreover, $D^{(\nu)}$ is the $n \times n$ matrix with $(i, i')$-th element $\|x^{(i)} - x^{(i')}\|^{2\nu}$, $a_\nu = \Gamma(-\nu) \nu^\nu / \Gamma(\nu)$ and $R$ is a differentiable mapping from $(0, +\infty)$ to the set of real $n \times n$ matrices $\mathcal{M}_n$ such that $\|R(\theta)\| = O(\theta^{-2([\nu]+1)})$ and $\|\frac{d}{d\theta} R(\theta)\| = O(\theta^{-2([\nu]+1)-1})$. Lemma (19) implies that when $\theta$ is large enough $\Sigma_\theta - R(\theta)$ is positive definite.

Equation (75) implies

$$
W^\top \Sigma_\theta W = \sum_{k=0}^{[\nu]} \frac{a_k}{\theta^{2k}} W^\top D^{(k)} W + \frac{a_{\nu}}{\theta^{2\nu}} W^\top D^{(\nu)} W + W^\top R(\theta) W.
$$

(76)
Finally, if a Matérn kernel with integer smoothness \( \nu \) is used, we can write \( \Sigma_\theta \) as [Abramowitz and Stegun 1964 (9.6.11.):

\[
\Sigma_\theta = \sum_{k=0}^{\nu-1} \frac{a_k}{\theta^{2k}} D^{(k)} + \hat{a}_\nu \left( \frac{\log(\theta)}{\theta^{2\nu}} D^{(\nu)} + \frac{1}{\theta^{2\nu}} \hat{D}^{(\nu)} \right) + R(\theta).
\]

Equation (78) implies

\[
W^\top \Sigma_\theta W = \sum_{k=0}^{\nu-1} \frac{a_k}{\theta^{2k}} W^\top D^{(k)} W + \frac{\log(\theta)}{\theta^{2\nu}} \tilde{a}_\nu W^\top D^{(\nu)} W + \frac{1}{\theta^{2\nu}} \tilde{D}^{(\nu)} W + W^\top R(\theta) W.
\]

When \( \theta \) is large enough, \( \Sigma_\theta - R(\theta) \) is positive definite. Since the kernel of \( W \) is trivial, when \( \theta \) is large enough, \( W^\top \Sigma_\theta W - W^\top R(\theta) W \) is positive definite. If it exists, let \( k_1 \) be the smallest nonnegative integer smaller than \( \nu \) such that \( W^\top D^{(k_1)} W \) is non-null and define \( D := a_{k_1} D^{(k_1)} \) and \( g(\theta) := \theta^{-2k_1} \). If not, then define \( D := a_\nu D^{(\nu)} \) and \( g(\theta) := \theta^{-2\nu} \). Either way \( W^\top D W \) is non-null.

If \( W^\top D W \) is nonsingular, then
• either \( k_1 \) exists and is strictly smaller than \( \nu - 1 \), in which case define \( D^* := a_{k_1+1}D^{(k_1+1)} \) and \( g^*(\theta) := \theta^{-2} \);

• or \( k_1 \) exists and is equal to \( \nu - 1 \), in which case define \( D^* := a_{\nu}D^{(\nu)} \) and \( g^*(\theta) := \log(\theta)\theta^{-2} \);

• or \( k_1 \) exists and is equal to \( \nu \), in which case define \( D^* := \tilde{a}_\nu\tilde{D}^{(\nu)} \) and \( g^*(\theta) := \log(\theta)^{-1} \);

• or \( k_1 \) does not exist, in which case define \( D^* \) as the null \( n \times n \) matrix and \( g^*(\theta) := \theta^{-1} \).

If \( W^\top DW \) is singular, then \( k_1 \) necessarily exists:

• either \( k_1 \) is strictly smaller than \( \nu \). Then there are two possibilities. The first is that there exists a smallest integer \( k_2 \in [k_1+1, \nu] \) such that \( W^\top D^{(k_2)}W \) is non-null, in which case define \( D^* := a_{k_2}D^{(k_2)} \) and \( g^*(\theta) := \theta^{-(2k_2-k_1)} \) \((k_2 < \nu)\) or \( D^* := a_{\nu}D^{(\nu)} \) and \( g^*(\theta) := \log(\theta)\theta^{-(2(\nu-k_1))} \) \((k_2 = \nu)\). The second is that no such \( k_2 \) exists, but then \( W^\top \tilde{D}^{(\nu)}W \) is necessarily non-null, so define \( D^* := \tilde{a}_\nu\tilde{D}^{(\nu)} \) and \( g^*(\theta) := \theta^{-2(\nu-k_1)} \).

• or \( k_1 \) is equal to \( \nu \). Then \( W^\top \tilde{D}^{(\nu)}W \) is necessarily non-null, so define \( D^* := \tilde{a}_\nu\tilde{D}^{(\nu)} \) and \( g^*(\theta) := \log(\theta)^{-1} \).

Finally, define
\[
R_y(\theta) := g(\theta)^{-1}g^*(\theta)^{-1}\left(W^\top \Sigma_0 W - g(\theta)W^\top DW - g(\theta)g^*(\theta)W^\top D^*W\right).
\] (80)

In all situations, \( \|R_y(\theta)\| = o(g^*(\theta)) \) and \( \|\frac{\partial}{\partial \theta} R_y(\theta)\| = o(g^*(\theta)) \).

### D.4 Proof of Lemma 8

For Rational Quadratic and Squared Exponential kernels, Equation (72) implies thanks to Lemma 13 that there exists \( k' \in \mathbb{N} \) such that \( \cap_{k=0}^{k'} \text{Ker} \left(W^\top D^{(k)}W\right) \) is the trivial vector space and \( \cap_{0 \leq k < k'} \text{Ker} \left(W^\top D^{(k)}W\right) \) is a non-trivial vector space (if \( k' = 0 \), the intersection is done over an empty index set, so we take it to be \( \mathbb{R}^{n-p} \) by convention).

Lemma 14 implies that there exists a constant \( c_{k'} > 0 \) such that for large enough \( \theta \), \( v_{n-p}(\theta) \geq c_{k'}\theta^{-2k'} \). Thanks to Lemma 16, there exists a hyperplane \( \mathcal{H}_{n-p} \) of \( \mathbb{R}^{n-p} \) such that for every \( y' \in \mathbb{R}^{n-p} \setminus \mathcal{H}_{n-p} \), there exists \( c_{y'} > 0 \) such that for large enough \( \theta \),
\[
(y')^\top \left(W^\top \Sigma_0 W\right)^{-1} y' \geq c_{y'} \left\| \left(W^\top \Sigma_0 W\right)^{-1} \right\|.
\] (81)

So for every \( y \in \mathbb{R}^n \) such that \( W^\top y \in \mathbb{R}^{n-p} \setminus \mathcal{H}_{n-p} \), there exists \( c_y > 0 \) such that for large enough \( \theta \)
\[
y^\top W \left(W^\top \Sigma_0 W\right)^{-1} W^\top y \geq c_y \left\| \left(W^\top \Sigma_0 W\right)^{-1} \right\|.
\] (82)

Because the matrix \( W^\top \) has full row rank, the vector space of all \( v \in \mathbb{R}^n \) such that \( W^\top v \in \mathcal{H}_{n-p} \) is included within a hyperplane \( \mathcal{H}_n \) of \( \mathbb{R}^n \), so for every \( y \in \mathbb{R}^n \setminus \mathcal{H}_n \), there exists \( c_y > 0 \) such that for large \( \theta \) the above equation holds.
For Matérn kernels with noninteger smoothness $\nu > 0$ (resp. with integer smoothness $\nu > 0$), Equation (75) (resp. Equation (73)) allows a similar argument. Indeed, Lemma 19 asserts that $\| \Sigma_\nu^{-1} \| = O(\theta^{2\nu})$, so $\cap_{k=0}^{\nu} \text{Ker}(W^T D^{(k)} W) \cap \text{Ker}(W^T D^{(\nu)} W)$ (resp. $\cap_{k=0}^{\nu} \text{Ker}(W^T D^{(k)} W) \cap \text{Ker}(W^T D^{(\nu)} W)$) is necessarily the trivial vector space.

E Details of the proof of Theorem 9

In this the last part of the proof of Theorem 9 is given in detail.

E.1 Rational Quadratic, Squared Exponential and Matérn ($\nu \in [1, +\infty) \setminus \mathbb{Z}_+$) kernels

Let us first tackle the case of Rational Quadratic and Squared Exponential kernels and of Matérn kernels with noninteger smoothness $\nu > 1$.

In case 1. (a), Lemma 14 yields $\hat{w}(\theta) = O(g^{*}(\theta))$.

This implies $\pi(\theta) = O(g^{*}(\theta)) = O(\theta^{-2l-1})$, so the reference prior is proper. Given the likelihood function is bounded (cf. Equation (12), the reference posterior is proper as well.

In case 1. (b), Lemma 14 yields $\hat{w}(\theta) = O(g^{*}(\theta)g^{*}(\theta)^{-1})$.

This implies $\pi(\theta) = O(g^{*}(\theta)g^{*}(\theta)^{-1}) = O(\theta^{-1})$. Moreover, $v_{n-p}(\theta) = O(g(\theta)g^{*}(\theta))$. As the rank of $W^T DW$ is at least one, $v_1(\theta)^{-1} = O(\theta^{-1})$. Gathering all this, $v_{n-p}(\theta)/v_1(\theta) = O(g^{*}(\theta))$, so Equation (12) implies $L(y|\theta) = O(g^{*}(\theta)^{1/2}) = O(\theta^{-1})$. The reference posterior is then proportional to $L(y|\theta)\pi(\theta) = O(\theta^{-1})$ and is proper.

In case 2., we must distinguish between Matérn kernels and the others. For Matérn kernels with noninteger smoothness $\nu > 1$, Proposition 7 asserts that the reference prior is $O(\theta^{-1})$ so the argument used in case 1. (b) still holds. For Rational Quadratic and Squared Exponential kernels, Equation (72) implies

$$W^T \Sigma_\theta W = \sum_{k=0}^{\infty} \frac{a_k}{\theta^{2k}} W^T D^{(k)} W. \quad (83)$$

Let $k_1$ be the smallest nonnegative integer such that $W^T D^{(k)} W$ is not the null matrix. Then

$$g(\theta)W^T DW = a_{k_1} \theta^{-2k_1} W^T D^{(k_1)} W. \quad (84)$$

and for some integer $k_2 > k_1$,

$$g(\theta)g^{*}(\theta)W^T D^* W = a_{k_2} \theta^{-2k_2} W^T D^{(k_2)} W. \quad (85)$$

Things are easiest if $W^T D^{(k_1+1)} W$ is null, because then $k_2 > k_1 + 1$. Since we are dealing with case 2., $\text{Ker}(W^T D^* W) \cap \text{Ker}(W^T D^{(k_1)} W)$ is not the trivial vector space so Equation (83) yields $v_{n-p}(\theta) = O(\theta^{-2(k_2+1)}) = O(\theta^{-2(k_1+3)})$. Besides, the smallest eigenvalue of $(W^T \Sigma_\theta W)^{-1}$ verifies $v_1(\theta)^{-1} = O(\theta^{-2k_1})$ so $v_{n-p}(\theta)/v_1(\theta) = O(\theta^{-6})$. Recall Proposition 7 asserts that $\pi(\theta) = O(\theta)$. The reference posterior is proportional to $L(y|\theta)\pi(\theta) = O(\theta^{-2})$ and thus proper.
In the following, assume $W^T D^{(k_1+1)} W$ is not null. Then $k_2 = k_1 + 1$.

If we assume that $W^T D^{(k_1)} W$ has rank greater or equal to 2, then a similar reasoning can be applied. The two smallest eigenvalues of $W^T \Sigma_v W$ verify $v_1(\theta)^{-1} = O(\theta^{-2k_1})$ and $v_2(\theta)^{-1} = O(\theta^{-2k_1})$. Then $v_{n-p}(\theta) = O(\theta^{-2(k_1+1)}) = O(\theta^{-2(k_1+2)})$. From this we obtain $v_{n-p}(\theta)/v_1(\theta) = O(\theta^{-4})$ and $v_{n-p}(\theta)/v_2(\theta) = O(\theta^{-4})$. Equation (12) then implies $L(y|\theta) = O(\theta^{-2})$. The reference posterior is proportional to $L(y|\theta) \pi(\theta) = O(\theta^{-3})$ and thus proper.

Now, assume that $W^T D^{(k_1)} W$ has rank 1. We need to distinguish between two possibilities: either $\text{Ker}(W^T D^{(k_1+2)} W) \cap \text{Ker}(W^T D^{(k_1+1)} W) \cap \text{Ker}(W^T D^{(k_1)} W)$ is the trivial vector space, or it is not.

If it is not, Equation (83) yields $v_{n-p}(\theta) = O(\theta^{-2(k_1+3)})$ and the conclusion is the same as in the case where $W^T D^{(k_1)} W$ is null.

Let us now deal with the situation where $\text{Ker}(W^T D^{(k_1+2)} W) \cap \text{Ker}(W^T D^{(k_1+1)} W) \cap \text{Ker}(W^T D^{(k_1)} W)$ is the trivial vector space. Two further subcases must be distinguished here: either $\text{Ker}(W^T D^{(k_1+1)} W) \cap \text{Ker}(W^T D^{(k_1)} W)$ is equal to $\text{Ker}(W^T D^{(k_1)} W)$, or it is strictly included within $\text{Ker}(W^T D^{(k_1)} W)$.

If it is strictly included, then Lemma 17 is applicable and $v_1(\theta)^{-1} = O(\theta^{-2k_1})$ and $v_2(\theta)^{-1} = O(\theta^{-2k_1+1})$. Because this is case 2., $\text{Ker}(W^T D^{(k_1+1)} W) \cap \text{Ker}(W^T D^{(k_1)} W)$ is not the trivial vector space, so Equation (83) yields $v_{n-p}(\theta) = O(\theta^{-2(k_1+2)})$. From there we obtain $v_{n-p}(\theta)/v_1(\theta) = O(\theta^{-4})$ and $v_{n-p}(\theta)/v_2(\theta) = O(\theta^{-2})$. Equation (12) then implies $L(y|\theta) = O(\theta^{-3})$, so the reference posterior is proper.

In the second subcase, $\text{Ker}(W^T D^{(k_1+1)} W) \cap \text{Ker}(W^T D^{(k_1)} W) = \text{Ker}(W^T D^{(k_1)} W)$. Since $\text{Ker}(W^T D^{(k_1)} W)$ is a hyperplane of $\mathbb{R}^{n-p}$, this implies that $\text{Ker}(W^T D^{(k_1+1)} W)$ is the same hyperplane. So $W^T D^{(k_1+1)} W$ and $W^T D^{(k_1)} W$ are symmetric matrices of rank 1 with the same kernel. This means there exists $b \in \mathbb{R} \setminus \{0\}$ such that $W^T D^{(k_1+1)} W = b W^T D^{(k_1)} W$. So, if we redefine $g(\theta) := a_{k_1} \theta^{-2k_1} + a_{k_1+1} b \theta^{-2(k_1+1)}$, $g^*(\theta) := a_{k_1+2} \theta^{-2(k_1+2)} g(\theta)^{-1}$, $D^* := D^{(k_1+2)}$ and $R_g(\theta) := g(\theta)^{-1} \sum_{k=k_1+3}^{\infty} a_k \theta^{-2k}$, the situation is similar to case 1.(b), except that $g^*(\theta)$ is not necessarily of the form $\theta^{-2l}$.

However, $g^*(\theta) = g^*(\theta) (-2(k_1 + 2) \theta^{-1} - g'(\theta) g(\theta)^{-1}) = O(\theta^{-1})$ so $g^*(\theta) g'(\theta)^{-1} = O(\theta^{-1})$. In addition, $g^*(\theta) = O(\theta^{-2})$. Therefore the arguments of the study of case 1.(b) apply: $\pi(\theta) = O(\theta^{-1})$ and $L(y|\theta) = O(g^*(\theta)^{1/2}) = O(\theta^{-1})$. The reference posterior is proportional to $L(y|\theta) \pi(\theta) = O(\theta^{-2})$: it is proper. This particular subcase, because it is analogous to case 1.(b) is called “special”. All other subcases of case 2. collectively form the “usual” case.

E.2 Matérn ($\nu \in \mathbb{Z}_+$) kernels

We now address the case where the correlation kernel is Matérn with integer smoothness $\nu$. The proof strategy remains the same as for the other kernels, but the execution is a little trickier.

It still relies on the asymptotic expansion of $\Sigma_\theta$. For Matérn kernels with integer smoothness $\nu$, the decomposition is detailed in Appendix D.3.

First, assume either $D$ is not proportional to $D^{(\nu)}$ or $D^*$ is not proportional to $D^{(\nu)}$. In Equation (13), $g^*(\theta)$ may be $\theta^{-2l} \log(\theta)$ instead of $\theta^{-2l}$. Then its derivative is $g''(\theta) = \theta^{-2l-1}(1 - 2l \log(\theta))$. 

In case 1.(a), the reference prior (and posterior) is $O(g^*(\theta)) = O(\theta^{-2l-1} \log(\theta))$ and thus proper. It is useless to distinguish cases 1.(b) and 2. because thanks to Proposition 7, the reference prior is $O(\theta^{-1})$. In either case, the rank of $W^T DW$ is at least one, so $v_{n-p}(\theta)/v_1(\theta) = O(g^*(\theta))$. Equation (12) implies $L(y|\theta) = O(g^*(\theta)^{1/2}) = O(\theta^{-1} \log(\theta)^{1/2})$, so the reference posterior is proportional to $L(y|\theta)\pi(\theta) = O(\theta^{-1-1} \log(\theta)^{1/2})$ and thus proper.

Now, assume $D$ is proportional to $D^{(v)}$ and $D^*$ is proportional to $\hat{D}^{(v)}$. In Equation (13), $g^*(\theta) = \log(\theta)^{-1}$. Its derivative is $g^*'(\theta) = -\theta^{-1} \log(\theta)^{-2}$.

In case 1.(a), the reference prior (resp. posterior) is $O(g^*(\theta)) = O(\theta^{-1} \log(\theta)^{-2})$ and is thus proper. In case 1.(b), the reference prior is $O(g^*(\theta)g^*(\theta)^{-1}) = O(\theta^{-1} \log(\theta)^{-1})$. Besides, as the rank of $W^T DW$ is at least one, Lemma 17 yields $v_{n-p}(\theta)/v_1(\theta) = O(g^*(\theta))$, so Equation (12) implies $L(y|\theta) = O(g^*(\theta)^{1/2}) = O(\log(\theta)^{-1/2})$. The reference posterior is then proportional to $L(y|\theta)\pi(\theta) = O(\theta^{-1} \log(\theta)^{-3/2})$: it is proper. Case 2. cannot occur because Lemma 19 asserts that $\|\Sigma_\theta^{-1}\| = O(\theta^{2v})$. 

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