

Supplement to "nimblewomble: An R package for Bayesian Wombling with nimble"

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Theorem 1. On each rectilinear segment, $C_{t^*} = \{s_0 + tu : t \in [0, t^*]\}$, where u is a unit vector and $u^\perp$ is its normal, the terms in the cross-covariance matrix are

$$\begin{aligned} k_{ij}(t^*, t^*) &= (-1)^i \int_0^{t^*} \int_0^{t^*} a_i(t_1)^T \partial^{i+j} K(\Delta(t_1, t_2)) a_j(t_2) \|s'(t_1)\| \|s'(t_2)\| dt_1 dt_2, \\ &= (-1)^i t^* \int_{-t^*}^{t^*} a_i^T \partial^{i+j} K(xu) a_j dx, \quad i, j = 1, 2, \end{aligned}$$

where $a_1(t) = n(s(t))$ is the normal to the segment, $a_2(t) = \mathcal{E}_2 n(s(t)) \otimes n(s(t))$, where $\mathcal{E}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ is an elimination matrix and $\Delta(t_1, t_2) = s_2(t) - s_1(t)$.

Proof. Considering the parametric segment, $C_{t^*} = \{s_0 + tu : t \in [0, t^*]\}$, where $u = (u_1, u_2)^T$ is a unit vector, $\|u\| = 1$, $u^\perp$ is its normal, $u^T u^\perp = 0$, $a_1(t) = a_1 = u^\perp$ and $a_2(t) = a_2 = \mathcal{E}_2(u^\perp \otimes u^\perp)$ are free of t , and $\Delta(t_1, t_2) = (t_2 - t_1)u$. The integrand in $k_{ij}(t^*, t^*) = (-1)^i \int_0^{t^*} \int_0^{t^*} a_i^T \partial^{i+j} K((t_2 - t_1)u) a_j dt_1 dt_2$, depends only on $(t_2 - t_1)$. Making a change of variable—define $x = t_2 - t_1$, $y = t_2 + t_1$, implying $\frac{x+y}{2} = t_2$ and $\frac{y-x}{2} = t_1$. The Jacobian is $\frac{1}{2}$. Hence, $0 \leq y + x \leq 2t^*$ and $0 \leq y - x \leq 2t^*$. This implies $0 \leq y \leq 2t^*$ and $-t^* \leq x \leq t^*$. Making the substitution above reduces, $k_{ij}(t^*, t^*) = \frac{(-1)^i}{2} \int_0^{2t^*} \int_{-t^*}^{t^*} a_i^T \partial^{i+j} K(xu) a_j dx dy = (-1)^i t^* \int_{-t^*}^{t^*} a_i^T \partial^{i+j} K(xu) a_j dx$. Setting $i = j = 1$, produces the scenario in ?. $\square$

Theorem 2. For the Matérn kernel, with $\nu = 3/2$, the variance of the gradient based wombling measure is $k_{11}(t^*, t^*) = 2\sqrt{3}\sigma^2\phi t^* G(1, \sqrt{3}\phi t^*)$. In case $\nu = 5/2$, the cross-covariance matrix for the wombling measures based on spatial gradient and curvature requires $k_{11}(t^*, t^*) = \frac{2\sqrt{5}}{3}\sigma^2\phi t^* \{G(1, \sqrt{5}\phi t^*) + G(2, \sqrt{5}\phi t^*)\}$, $k_{22}(t^*, t^*) = 10\sqrt{5}\sigma^2\phi^3 t^* G(1, \sqrt{5}\phi t^*)$ and $k_{21}(t^*, t^*) = -k_{12}(t^*, t^*) = 0$, where $G(a, \frac{x}{b}) = \int_0^{t^*} x^{a-1} e^{-\frac{x}{b}} dx$ is the lower incomplete Gamma function with shape parameter a and scale parameter b . For the Gaussian kernel,

$$\mathbf{V}_\Gamma(t^*) = 2\sigma^2\sqrt{\pi}\phi t^* \left\{ 2\Phi(\sqrt{2}\phi t^*) - 1 \right\} \begin{pmatrix} 1 & 0 \\ 0 & 6\phi^2 \end{pmatrix},$$

where $\Phi(\cdot)$ is the cdf for the standard Gaussian probability density.

Proof. Using ??, if $\nu = 3/2$, then we obtain $k_{11}(t^*, t^*) = 3\sigma^2\phi^2 t^* \int_{-t^*}^{t^*} e^{-\sqrt{3}\phi|x|} dx = 2\sqrt{3}\sigma^2\phi t^* G(1, \sqrt{3}\phi t^*)$. If $\nu = 5/2$, then $k_{11}(t^*, t^*) = \frac{5}{3}\sigma^2\phi t^* \int_{-t^*}^{t^*} (1 + \sqrt{5}\phi|x|) e^{-\sqrt{5}\phi|x|} dx = \frac{2\sqrt{5}}{3}\sigma^2\phi t^* \{G(1, \sqrt{5}\phi t^*) + G(2, \sqrt{5}\phi t^*)\}$. For terms k_{21} and k_{12} , let us consider $a_1^T \partial^3 K(xu) a_2 = \frac{25}{3}\sigma^2\phi e^{-\sqrt{5}\phi|x|} |x| \{a_1^T \mathbf{A}_1 a_2 - \sqrt{5}\phi|x| a_1^T \mathbf{A}_2 a_2\}$, where

$$\mathbf{A}_1 = \begin{pmatrix} 3u_1 & u_2 & u_1 \\ u_2 & u_1 & 3u_2 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} u_1^3 & u_1^2 u_2 & u_2^2 u_1 \\ u_1^2 u_2 & u_2^2 u_1 & u_2^3 \end{pmatrix}.$$

The first and the second term both reduce to 0. Hence, $k_{21}(t^*, t^*) = -k_{12}(t^*, t^*) = 0$. Next, $a_2^T \partial^4 K(xu) a_2 = \frac{25}{3}\sigma^2\phi^4 e^{-\sqrt{5}\phi|x|} \{a_2^T \mathbf{A}_3 a_2 - \sqrt{5}\phi|x| a_2^T \mathbf{A}_4 (\sqrt{5}\phi|x| + 1) a_2\}$, where

$$\mathbf{A}_3 = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 3 \end{pmatrix}, \quad \mathbf{A}_4(x') = \begin{pmatrix} 6u_1^2 - x' u_1^4 & (3-x' u_1^2) u_1 u_2 & 1-x' u_1^2 u_2^2 \\ (3-x' u_1^2) u_1 u_2 & 1-x' u_1^2 u_2^2 & (3-x' u_2^2) u_1 u_2 \\ 1-x' u_1^2 u_2^2 & (3-x' u_2^2) u_1 u_2 & 6u_2^2 - x' u_2^4 \end{pmatrix}.$$

After some algebra, $\mathbf{a}_2^\top \partial^4 K(x\mathbf{u}) \mathbf{a}_2 = 25\sigma^2 \phi^4 e^{-\sqrt{5}\phi|x|} \{1 - 2\sqrt{5} \phi |x| \mathbf{u}_1^\perp \mathbf{u}_2^\perp (\mathbf{u}_1 \mathbf{u}_2 + \mathbf{u}_1^\perp \mathbf{u}_2^\perp)\}$. Observe that $\mathbf{u}_1^\perp = \mathbf{u}_2$ and $\mathbf{u}_2^\perp = -\mathbf{u}_1$, substituting we get $k_{22}(t^*, t^*) = 10\sqrt{5}\sigma^2 \phi^3 t^* G(1, \sqrt{5}\phi t^*)$.

For the Gaussian kernel, $k_{11}(t^*, t^*) = 2\sigma^2 \phi^2 t^* \int_{-t^*}^{t^*} e^{-\phi^2 x^2} dx = 2\sigma^2 \sqrt{\pi} \phi t^* \{2\Phi(\sqrt{2}\phi t^*) - 1\}$.

Note that $\mathbf{a}_1^\top \partial^3 K(x\mathbf{u}) \mathbf{a}_2 = 4\sigma^2 \phi^4 e^{-\phi^2 x^2} x \{\mathbf{a}_1^\top \mathbf{A}_1 \mathbf{a}_2 - 2\phi^2 x^2 \mathbf{a}_1^\top \mathbf{A}_2 \mathbf{a}_2\}$. Again, the first and second terms equate to 0 implying $k_{21}(t^*, t^*) = -k_{12}(t^*, t^*) = 0$. Next, $\mathbf{a}_2^\top \partial^4 K(x\mathbf{u}) \mathbf{a}_2 = 4\sigma^2 \phi^4 e^{-\phi^2 x^2} \{\mathbf{a}_2^\top \mathbf{A}_3 \mathbf{a}_2 - 2\phi^2 x^2 \mathbf{a}_2^\top \mathbf{A}_4 (2\phi^2 x^2) \mathbf{a}_2\}$. After some algebra, $\mathbf{a}_2^\top \partial^4 K(x\mathbf{u}) \mathbf{a}_2 = 12\sigma^2 \phi^4 e^{-\phi^2 x^2} \{1 - 4 \phi^2 x^2 \mathbf{u}_1^\perp \mathbf{u}_2^\perp (\mathbf{u}_1 \mathbf{u}_2 + \mathbf{u}_1^\perp \mathbf{u}_2^\perp)\}$. Substituting, we get $k_{22}(t^*, t^*) = 12\sigma^2 \sqrt{\pi} \phi^3 t^* \{2\Phi(\sqrt{2}\phi t^*) - 1\}$ resulting in the required expression for $\mathbf{V}_\Gamma(t^*)$. $\square$

?? interestingly shows that the posited cross-covariance matrix, $\mathbf{V}_\Gamma(t^*)$, reduces to a *variance-covariance matrix*. It has a simpler form for the Gaussian case when compared to Matérn with $\nu = \frac{5}{2}$. Finally, considering the covariance between $Z(\mathbf{s}_i)$, $i = 1, \dots, N$ and the wombling measures—in the Gaussian case, closed-forms are available (see, e.g., ?, end of Section 3). The inferential exercise of wombling does not require quadrature when using a Gaussian kernel however, only one-dimensional quadrature is required for the same when using a Matérn kernel.

Bibliography

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