Derivative of the Anisotropic Covariance Function (Matérn) in 2D and 3D

We consider an anisotropic covariance function of the form:

$$k(h) = C\left(r(h)\right), \quad \text{where } r(h) = \sqrt{h^\top T h}$$

with:

- $h \in \mathbb{R}^d$ is the spatial displacement vector,
- $T = R^\top \Lambda R \in \mathbb{R}^{d\times d}$ is a symmetric positive definite anisotropy tensor,
- $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, [\lambda_3])$, with $\lambda_i = \frac{1}{s_i^2}$,
- $R \in SO(d)$ is a rotation matrix.

We define the rotated coordinate $\tilde{h} = Rh$, so:

$$r(h)^2 = \tilde{h}^\top \Lambda \tilde{h}$$

2D Case

Let $d = 2$, and $R(\theta)$ be a rotation by angle θ:

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

Let $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ be the generator of infinitesimal rotations.

Derivative with respect to scale s_i

Since $\lambda_i = 1/s_i^2$, we obtain:

$$\frac{\partial k(h)}{\partial s_i} = -\frac{C'(r)}{r} \cdot \frac{\tilde{h}_i^2}{s_i^3}$$

Derivative with respect to angle θ

$$\frac{\partial k(h)}{\partial \theta} = \frac{C'(r)}{r} \cdot \tilde{h}^\top \Lambda J \tilde{h}$$

Behavior at $h = 0$

In both cases, the derivative tends to 0 as $h \to 0$, so:

$$\left.\frac{\partial k(h)}{\partial \xi}\right|_{h=0} = 0 \quad \text{for } \xi \in \{s_1, s_2, \theta\}$$

3D Case

Let $d = 3$, and $R \in SO(3)$ be a rotation matrix parameterized by Euler angles $(\theta_1, \theta_2, \theta_3)$ (e.g., ZYX convention: yaw, pitch, roll).

Derivative with respect to scale s_i

Same as in 2D:

$$\frac{\partial k(h)}{\partial s_i} = -\frac{C'(r)}{r} \cdot \frac{\tilde{h}_i^2}{s_i^3}$$

Derivative with respect to orientation parameters

Let $J_k \in \mathfrak{so}(3)$ be the skew-symmetric generator for infinitesimal rotation around axis k. Then:

$$\frac{\partial k(h)}{\partial \theta_k} = \frac{C'(r)}{r} \cdot \tilde{h}^\top \Lambda J_k \tilde{h}$$

Infinitesimal rotation matrices

The generators $J_1, J_2, J_3 \in \mathbb{R}^{3\times 3}$ are:

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad J_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad J_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Each corresponds to rotation around the x-, y-, and z-axes, respectively.

Note on parameterization

The matrices J_k apply directly for Lie algebra–based parametrization. If using Euler angles, chain rule must be applied:

$$\frac{\partial k}{\partial \theta_{\text{Euler}}} = \sum_{k=1}^{3} \frac{\partial k}{\partial \theta_k} \cdot \frac{\partial \theta_k}{\partial \theta_{\text{Euler}}}$$