Correction to Spectral Mixture (SM) Kernel Derivation for Multidimensional Inputs

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Abstract

This note corrects a typo in the spectral mixture kernel in Wilson and Adams (2013) for the case of multidimensional inputs.

Spectral densities $S(s)$ and stationarity kernels $k(x, x') = k(x - x') = k(\tau)$ are Fourier duals:

$$k(\tau) = \int_{\mathbb{R}^P} S(s) e^{2\pi i s^\top \tau} ds \,. \tag{1}$$

Wilson and Adams (2013) derive the *spectral mixture* kernel by modelling $S(s)$ as a symmetrized scale-location mixture of Gaussians:

$$S(s) = \sum_q w_q [\mathcal{N}(s; \mu_q, \Sigma_q) + \mathcal{N}(-s; \mu_q, \Sigma_q)] \,. \tag{2}$$

Substituting Eq. (2) into Eq. (1) we find

$$k_{\text{spectral mixture}}(x - x') = \sum_q w_q \frac{|\Sigma_q|^{\frac{1}{2}}}{(2\pi)^{\frac{P}{2}}} \exp\left(-\frac{1}{2} \left\| \Sigma_q^{\frac{1}{2}} (x - x') \right\|^2 \right) \cos \langle x - x', 2\pi \mu_q \rangle \tag{3}$$

In Wilson and Adams (2013), for multidimensional inputs, and a diagonal covariance $\Sigma_q = \text{diag}(v_q^{(1)}, \ldots, v_q^{(P)})$, the spectral mixture kernel is **incorrectly** written as

$$k(\tau) = \sum_{q=1}^{Q} w_q \prod_{p=1}^{P} \exp\{-2\pi^2 \tau_p^2 v_q^{(p)}\} \cos(2\pi \tau_p \mu_q^{(p)}) \tag{4}$$

Eq. (4) **is incorrect**. The cosine should be outside of the product. **The correct form for a diagonal covariance scale-location Gaussian mixture is**:

$$k_{\mathrm{SM}}(\tau) = \sum_{q=1}^{Q} w_q \cos(2\pi\tau^\top \mu_q) \prod_{p=1}^{P} \exp\{-2\pi^2 \tau_p^2 v_q^{(p)}\} \tag{5}$$

The corrected version can be found in Wilson (2014) and Yang et al. (2015). **Note that the typo in Eq. (4) does not make any difference for $P = 1$ dimensional inputs**. The correct multivariate version of the the spectral mixture kernel is implemented as `covSM.m` in the GPML toolbox (Rasmussen and Nickisch, 2010).

References

Rasmussen, C. E. and Nickisch, H. (2010). Gaussian processes for machine learning (GPML) toolbox. *Journal of Machine Learning Research (JMLR)*, 11:3011–3015.

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