Spectral Methods in Gaussian Modelling

Topic 2: Kernel Design

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How to parametrise a flexible kernel?

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- PSD:
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  - must be nonnegative and symmetric.
- Easier to flexibly parametrise PSD!

Spectral Mixture Kernel

- SSA (Lázaro-Gredilla et al., 2010) models PSD with symmetric average of lines:

$$s(\omega) = \frac{1}{2Q} \sum_{q=1}^{Q} (\delta(\omega - \mu^{(q)}) + \delta(\omega + \mu^{(q)})).$$

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- Strong parametric assumption: $f(t) =$ sum of sines.

Spectral Mixture Kernel (2)

- SMK (Wilson and Adams, 2013) models PSD with symmetric mixture of Gaussians:

$$s(\omega) = \frac{1}{2} \sum_{q=1}^{Q} w^{(q)} \Big(\mathcal{N}\Big(\omega; \mu^{(q)}, \Sigma^{(q)}\Big) + \mathcal{N}\Big(\omega; -\mu^{(q)}, \Sigma^{(q)}\Big) \Big).$$

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- Inverse Fourier transform gives kernel:

$$k^{(\mathsf{SMK})}(\tau) = \sum_{q=1}^{Q} w^{(q)} \exp\Big(-\tfrac{1}{2}\tau^{\mathsf{T}}\Sigma^{(q)}\tau\Big)\cos\Big(\mu^{(q)\mathsf{T}}\tau\Big).$$

Spectral Mixture Kernel (3)

- Equivalent generative model as a truncated Fourier series:

$$f^{(\mathsf{SMK})}(t) = \sum_{q=1}^{Q} \sqrt{w^{(q)}}(c_1^{(q)}(t)\cos(\mu^{(q)\mathsf{T}}t) + c_2^{(q)}(t)\sin(\mu^{(q)\mathsf{T}}t)),$$

$$c_1^{(q)}, c_2^{(q)} \sim \mathcal{GP}(0, \exp(-\tfrac{1}{2}\tau^{\mathsf{T}}\Sigma^{(q)}\tau)).$$

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- In SSA, $(c_1^{(q)}, c_2^{(q)})_{q=1}^{Q}$ are constant.
- SMK fattens spectral lines by allowing $c_1^{(q)}$ and $c_2^{(q)}$ to vary with time.

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– Hyperparameters difficult to optimise

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    - Must be nonnegative: $S(\omega) \geq 0$.

Multi-Output Spectral Mixture Kernel (2)

- MOSMK models PSD with symmetric mixture of outer products of vectors of Gaussians:

$$S(\omega) = \frac{1}{2}\sum_{q=1}^{Q}\Big(R^{(q)}(\omega)R^{(q)\dagger}(\omega) + R^{(q)}(-\omega)R^{(q)\dagger}(-\omega)\Big),$$

$$R_i^{(q)}(\omega) = w^{(q)}\exp\Big(-\tfrac{1}{4}(\omega-\mu_i^{(q)})\Sigma_i^{(q)-1}(\omega-\mu_i^{(q)}) - \iota(\theta_i^{(q)\mathsf{T}}\omega + \phi_i^{(q)})\Big).$$

Multi-Output Spectral Mixture Kernel (3)

- Inverse Fourier transform gives kernel:

$$K_{ij}^{(\mathsf{MOSMK})}(\tau) = \sum_{q=1}^{Q} \alpha_{ij}^{(q)} \exp\Big(-\tfrac{1}{2}(\tau + \theta_{ij}^{(q)})^{\mathsf{T}} \Sigma_{ij}^{(q)} (\tau + \theta_{ij}^{(q)})\Big) \\ \times \cos\Big((\tau + \theta_{ij}^{(q)})^{\mathsf{T}} \mu_{ij}^{(q)} + \phi_{ij}^{(q)}\Big).$$

Multi-Output Spectral Mixture Kernel (4)

- Equivalent generative model as truncated Fourier series:

$$
\begin{aligned}
f_i^{(\mathsf{MOSMK})}&(t) \\
&= \sum_{q=1}^{Q} w_i^{(q)} \Big(c_{i1}^{(q)}(t-\theta_i^{(q)}) \cos\Big(\mu_i^{(q)\mathsf{T}}(t-\theta_i^{(q)}) + \phi_i^{(q)}\Big) \\
&\qquad\qquad + c_{i2}^{(q)}(t-\theta_i^{(q)}) \sin\Big(\mu_i^{(q)\mathsf{T}}(t-\theta_i^{(q)}) + \phi_i^{(q)}\Big)\Big),
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{E}[c_{ik}^{(p)}&(t) c_{j\ell}^{(q)}(t')] \\
&= \begin{cases} \frac{\alpha_{ij}^{(q)}}{w_i^{(q)} w_j^{(q)}} \exp\Big(-\frac{1}{2}(t-t')^\mathsf{T}\Sigma_{ij}^{(q)}(t-t')\Big) & \text{if } k=\ell,\ p=q, \\ 0 & \text{otherwise.} \end{cases}
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- Uses the *Gibbs kernel* (Gibbs, 1997):

$$k^{(\mathsf{Gibbs})}(t,t') = \prod_{d=1}^{D} \sqrt{\frac{2\ell_d(t)\ell_d(t')}{\ell_d^2(t)+\ell_d^2(t')}} \exp\left(-\sum_{d=1}^{D} \frac{(t_d - t'_d)^2}{\ell_d^2(t)+\ell_d^2(t')}\right).$$

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Generalised Spectral Mixture Kernel (3): Nonstationary EQ Kernel

- Make length scale of ϕ dependent on t:

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$$= \sqrt{\frac{2\ell(t)\ell(t')}{\ell^2(t)+\ell^2(t')}} \exp\left(-\frac{(t-t')^2}{\ell^2(t)+\ell^2(t')}\right).$$

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- GSMK replaces the EQs with Gibbs kernels:

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k^{(\mathsf{GSMK})}(t, t') = \sum_{q=1}^{Q} & w^{(q)}(t) w^{(q)}(t') k_q^{(\mathsf{Gibbs})}(t, t') \\
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- $(w^{(q)}, \ell^{(q)} \mu^{(q)})_{q=1}^{Q}$ given log-GP priors.
- Estimated using MAP.

Generalised Spectral Mixture Kernel (5)

- Equivalent generative model as truncated Fourier series:

$$
\begin{aligned}
f^{(\mathsf{GSMK})}(t) = \sum_{q=1}^{Q} w^{(q)}(t)(c_1^{(q)}(t)\cos(\mu^{(q)\mathsf{T}}(t)t) \\
+ c_2^{(q)}(t)\sin(\mu^{(q)\mathsf{T}}(t)t)), \\
c_1^{(q)}, c_2^{(q)} \sim \mathcal{GP}(0, k^{(\mathsf{Gibbs})}(t, t')).
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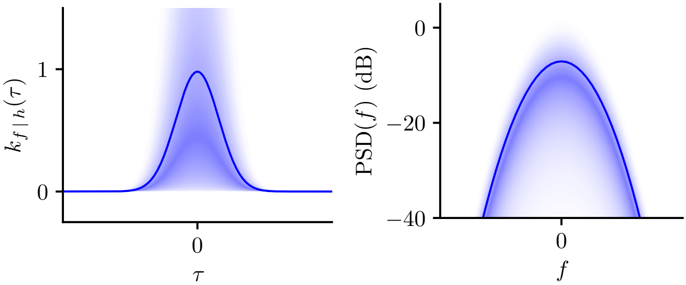
  - $\int_{-\infty}^{\infty} k_h(t, t)\,\mathrm{d}t < \infty$ (finite trace).

Gaussian Process Convolution Model (2)

- Nonparametric prior over kernels and PSDs.



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- Inference complicated.

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- Parametric approaches:
    - line spectrum (SSA),
    - mixture of Gaussians (SMK, MOSMK, GSMK).
- Nonparametric approach also possible (GPCM).

Appendix

References

Chen, K., Groot, P., Chen, J., & Marchiori, E. (2018). Generalized spectral mixture kernels for multi-task Gaussian processes. *arXiv preprint arXiv:1808.01132*. eprint: `https://arxiv.org/abs/1808.01132`

Gibbs, M. N. (1997). *Bayesian Gaussian processes for regression and classification*. (Doctoral dissertation, Computational and Biological Learning Laboratory, University of Cambridge).

Lázaro-Gredilla, M., Candela, J. Q., Rasmussen, C. E., & Figueiras-Vidal, A. R. (2010). Sparse spectrum Gaussian process regression.. *Journal of Machine Learning Research*, *11*, 1865–1881. Retrieved from `http://dblp.uni-trier.de/db/journals/jmlr/jmlr11.html#Lazaro-GredillaCRF10`

Parra, G., & Tobar, F. (2017). Spectral mixture kernels for multi-output Gaussian processes. *arXiv preprint arXiv:1709.01298*. eprint: `https://arxiv.org/abs/1709.01298`

References (2)

Tobar, F., Bui, T. D., & Turner, R. E. (2015). Learning stationary time series using Gaussian processes with nonparametric kernels. *Advances in Neural Information Processing Systems*, *29*, 3501–3509.

Wilson, A. G., & Adams, R. P. (2013). Gaussian process kernels for pattern discovery and extrapolation. *arXiv preprint arXiv:1302.4245*. eprint: `https://arxiv.org/abs/1302.4245`