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:

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

Spectral Mixture Kernel (3)

- Equivalent generative model as a truncated Fourier series:

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

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

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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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– Unclear how many components needed
– 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**:

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

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

Multi-Output Spectral Mixture Kernel (3)

- Inverse Fourier transform gives kernel:

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

- Equivalent generative model as truncated Fourier series:

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

$$
\begin{aligned}
&\mathbb{E}[c_{ik}^{(p)}(t) c_{jl}^{(q)}(t')] \\
&\quad = \begin{cases} \frac{\alpha_{ij}^{(q)}}{w_i^{(q)} w_j^{(q)}} \exp\Big(-\frac{1}{2}(t-t')^{\mathsf{T}} \Sigma_{ij}^{(q)} (t-t')\Big) & \text{if } k = l,\, p = q, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}
$$

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- Uses the *Gibbs kernel* (Gibbs, 1997):

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

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- Construction of EQ from basis functions:

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f(t) \,|\, n &= \int_{-\infty}^{\infty} \phi(t; c) n(c) \,\mathrm{d}c, \quad n(t) \sim \mathcal{GP}(0, \delta(t - t')), \\
\mathbb{E}[f(t) f(t')] &= \int_{-\infty}^{\infty} \phi(t; c)\phi(t'; c) \,\mathrm{d}c \\
&= \exp\left(-\frac{1}{2\ell^2}(t - t')^2\right).
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$$

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Generalised Spectral Mixture Kernel (4)

- GSMK replaces the EQs with Gibbs kernels:

$$k^{(\mathrm{GSMK})}(t,t') = \sum_{q=1}^{Q} w^{(q)}(t) w^{(q)}(t') k_q^{(\mathrm{Gibbs})}(t,t') \\ \times \cos\Big(\mu^{(q)\mathsf{T}}(t)t - \mu^{(q)\mathsf{T}}(t')t'\Big).$$

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- $(w^{(q)}, \ell^{(q)} \mu^{(q)})_{q=1}^{Q}$ given log-GP priors.
- Estimated using MAP.

- Equivalent generative model as truncated Fourier series:

$$
\begin{aligned}
f^{(\mathrm{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)),
\end{aligned}
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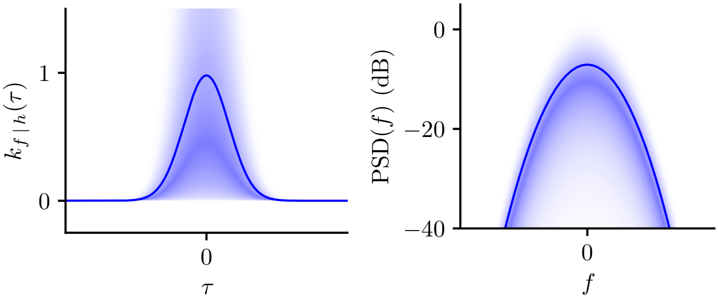
  - $\int_{-\infty}^{\infty} k_h(t, t)\,\mathrm{d}t < \infty$ (finite trace).

Gaussian Process Convolution Model (2)

- Nonparametric prior over kernels and PSDs.



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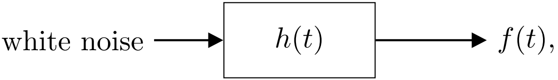

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- Inference complicated.

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