

INSA – Gaussian processes

Spectral representation and Bochner's theorem

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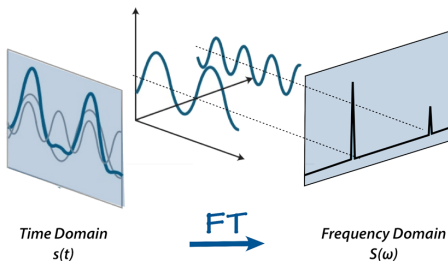
The French Aerospace Lab ONERA, France
Information Processing and Systems Department (DTIS)
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Spectral analysis

Spectral analysis

- Spectral methods are widely used for data analysis
- Analysis in terms of a spectrum of frequencies, energies, eigenvalues, etc

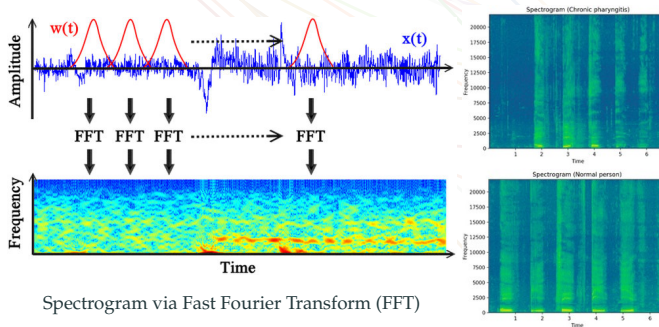


Fourier analysis

Spectral analysis

- Spectral analysis has its root in communications but it is also used in:
 - Electrical engineering
 - Acoustical engineering
 - Materials science
 - Geophysics
 - Atmospheric science & astronomy
 - ...

Speech spectrum of patients with chronic pharyngitis



Spectrogram via Fast Fourier Transform (FFT)

- Spectral analysis is a powerful tool to study complex-valued functions:

$$z(x) = u(x) + iv(x),$$

with $x \in \mathbb{R}^d$, $i = \sqrt{-1}$ (imaginary number), and u, v real-valued functions.

- Spectral analysis is a powerful tool to study complex-valued functions:

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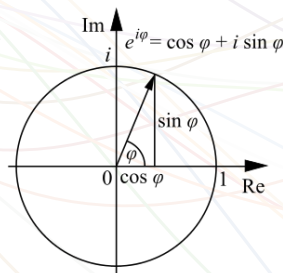
with $x \in \mathbb{R}^d$, $i = \sqrt{-1}$ (imaginary number), and u, v real-valued functions.

- An example of a complex-valued function is the **Euler's formula**:

$$z(\varphi) = \cos(\varphi) + i \sin(\varphi) = e^{i\varphi}, \quad \text{for } \varphi \in \mathbb{C}.$$

Euler's identity:

$$e^{i\varphi} - 1 = 0.$$



- In Fourier analysis, the spectral (frequency) representation of $z : \mathbb{R}^d \rightarrow \mathbb{C}$ is given by the **Fourier transform (FT)**:

$$S(\omega) := \mathcal{F}[f](\omega) = \int_{\mathbb{R}^d} \exp(-i\langle \omega, x \rangle) z(x) dx,$$

where $\langle \cdot, \cdot \rangle$ is the scalar product on \mathbb{R}^d .

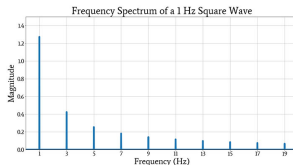
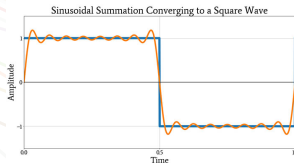
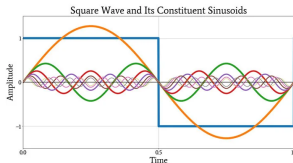
- The **inverse Fourier transform** of $S(\omega)$ is given by

$$\mathcal{F}^{-1}[S](x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(i\langle \omega, x \rangle) S(\omega) d\omega.$$

Fourier series (sine-cosine form):

$$z_{n_{\text{freq}}}(x) = \sum_{n=-n_{\text{freq}}}^{n_{\text{freq}}} c_n \exp(i\omega_n x) = \sum_{n=-n_{\text{freq}}}^{n_{\text{freq}}} c_n [\cos(\omega_n x) + i \sin(\omega_n x)]$$

with $x \in \mathbb{R}$ and $\omega_n = n\omega_0 = 2\pi n f_0$

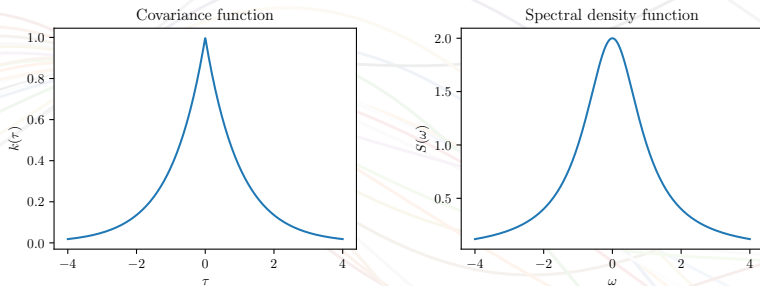


Fourier representation of the square wave function

[square wave] [sawtooth wave]

Spectral representation of kernels

- Fourier analysis can also be applied to random fields and kernels.



Spectral representation of the exponential kernel

- The spectral representation can be used for kernel design [Heinonen, 2017]:
 - All stationary kernels $k(\tau)$ have a spectral density $S(\omega)$
 - All spectral densities $S(\omega)$ define a covariance function

1. Complex-valued random fields
2. Spectral representation of random fields
3. Bochner's theorem
4. Spectral kernel design

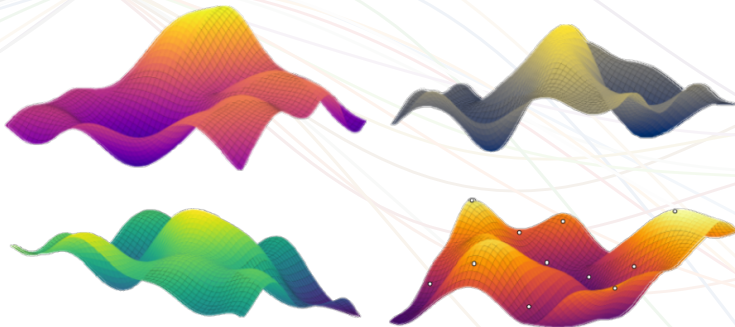
- In the following, we consider:
 - Stationary (centred) random fields $\{Y(\mathbf{x}); \mathbf{x} \in \mathbb{R}^d\}$ (e.g. a GP)
 - Stationary kernels $k(\boldsymbol{\tau}) := k(\mathbf{x}, \mathbf{x} + \boldsymbol{\tau})$ (abuse of notation)

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Complex-valued random fields

- A random field is a random function over an arbitrary domain, e.g. in \mathbb{R}^d :

Gaussian random field: $Y(x) \sim \mathcal{GP}(0, k)$.



2D Gaussian random fields

- A random field $\{Z(x); x \in \mathbb{R}^d\}$ is complex-valued if:

$$Z(x) = U(x) + iV(x),$$

where $i = \sqrt{-1}$ and U, V are real-valued random fields.

- We define \bar{Z} as the complex conjugate of Z :

$$\overline{Z(x)} = \overline{U(x) + iV(x)} = U(x) - iV(x)$$

- We denote $\text{Re}\{\cdot\}$ and $\text{Im}\{\cdot\}$ operators such that:

$$\text{Re}\{Z(x)\} = U(x), \quad \text{Im}\{Z(x)\} = V(x).$$

- The expectation of a complex-valued random field Z is given by:

$$\mathbb{E} \{Z(x)\} = \mathbb{E} \{U(x) + iV(x)\} = \mathbb{E} \{U(x)\} + i\mathbb{E} \{V(x)\}.$$

- Note that $\mathbb{E} \{Z(x)\}$ exists iff $\mathbb{E} \{U(x)\}$ and $\mathbb{E} \{V(x)\}$ exist.
- If $\mathbb{E} \{Z(x)\}$ exists, then the complex conjugation of $\mathbb{E} \{Z(x)\}$ is given by

$$\overline{\mathbb{E} \{Z(x)\}} = \mathbb{E} \left\{ \overline{Z(x)} \right\} = \mathbb{E} \{U(x)\} - i\mathbb{E} \{V(x)\}.$$

- The covariance of a operation of complex-valued random field Z is given by:

$$\text{cov} \left\{ Z(x), \overline{Z(x')} \right\} = \mathbb{E} \left\{ Z(x) \overline{Z(x')} \right\}$$

Exercise. Compute $k(\tau) = \text{cov} \left\{ Z(x + \tau), \overline{Z(x)} \right\}$.

Exercise. Show that $k(-\tau) = \overline{k(\tau)}$.

Definition (positive semidefiniteness for complex-valued functions)

A kernel $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C}$ is a p.s.d. complex function if for all $n \in \mathbb{N}$, and for all $c_1, \dots, c_n \in \mathbb{C}, \forall \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$,

$$\sum_{p=1}^n \sum_{q=1}^n c_p \bar{c}_q k(\mathbf{x}_p - \mathbf{x}_q) \geq 0.$$

Definition (positive semidefiniteness for real-valued functions)

A kernel $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is a p.s.d. function if for all $n \in \mathbb{N}$, and for all $a_1, \dots, a_n \in \mathbb{R}, \forall \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$,

$$\sum_{p=1}^n \sum_{q=1}^n a_p a_q k(\mathbf{x}_p - \mathbf{x}_q) \geq 0.$$

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Spectral representation of random fields

Spectral representation of random fields

- The spectral representation requires the following conditions:

Definition (Mean square continuity – see, e.g., [Stein, 1999])

A complex-valued random field Z is mean square continuous at x if:

$$\lim_{x' \rightarrow x} \mathbb{E} \left\{ |Z(x) - Z(x')|^2 \right\} = 0.$$

Definition (Weak stationarity – see, e.g., [Stein, 1999])

A complex-valued random field $\{Z(x); x \in \mathbb{R}^d\}$ is called *weakly stationary* if:

- $\mathbb{E} \{Z(x)\}$ is constant
- $\mathbb{E}\{Z(x)\overline{Z(x)}\} < \infty$ (finite second-order moments)
- $\text{cov}\{Z(x), \overline{Z(x + \tau)}\} = k(\tau)$ (stationary kernel)

Note: a strictly stationary random field with finite second-order moments is also weakly stationary.

Exercise. Suppose $\omega_1, \dots, \omega_n \in \mathbb{R}^d$ and let Z_1, \dots, Z_n be zero-mean complex random variables with $\mathbb{E} \{Z_p \overline{Z_q}\} = 0$ for $p \neq q$ and $\mathbb{E} \{|Z_p|^2\} = f_p < \infty$. Consider

$$\tilde{Z}(x) = \sum_{p=1}^n Z_p \exp(i\langle \omega_p, x \rangle).$$

Show that \tilde{Z} is weakly stationary.

- $\tilde{Z}(x) = \sum_{p=1}^n Z_p \exp(i\langle \omega_p, x \rangle)$ is an example of a spectral representation.
- Generally, spectral representations of mean square continuous weakly stationary random fields can be obtained [Stein, 1999]:

$$Z(x) = \int_{\mathbb{R}^d} \exp(i\langle \omega, x \rangle) M(d\omega) \quad (1)$$

where M is a *complex random measure* on \mathbb{R}^d .

- The integral in (1) can be seen as a limit in L^2 of the sums used for \tilde{Z} .

Exercise. Suppose that for some positive finite measure μ :

$$\mathbb{E} \{M(\Delta)\} = 0$$

$$\mathbb{E} \left\{ |M(\Delta)|^2 \right\} = \mu(\Delta)$$

$$\mathbb{E} \left\{ M(\Delta_1), \overline{M(\Delta_2)} \right\} = 0, \quad \text{for disjoint Borel sets } \Delta_1, \Delta_2$$

Compute $k(\tau) = \text{cov} \left\{ Z(x), \overline{Z(x + \tau)} \right\}$.

Solution.

$$\begin{aligned} k(\tau) &= \text{cov} \left\{ \int_{\mathbb{R}^d} \exp(i\langle \omega, x \rangle) M(d\omega), \overline{\int_{\mathbb{R}^d} \exp(i\langle \nu, x + \tau \rangle) M(d\nu)} \right\} \\ &= \int_{\mathbb{R}^d} \exp(i\langle \omega, x \rangle) \int_{\mathbb{R}^d} \exp(i\langle \nu, x + \tau \rangle) \text{cov} \left\{ M(d\omega), \overline{M(d\nu)} \right\} \\ &= \int_{\mathbb{R}^d} \exp(i\langle \omega, \tau \rangle) \mu(d\omega) \end{aligned}$$

□

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Bochner's theorem

Theorem (Bochner's theorem – see, e.g., [Stein, 1999])

· A complex-valued function k on \mathbb{R}^d is the covariance function of a weakly stationary mean square continuous complex-valued random process on \mathbb{R}^d iff it can be represented as

$$k(\tau) = \int_{\mathbb{R}^d} \exp(i\langle \omega, \tau \rangle) \mu(d\omega),$$

where the positive finite measure μ is known as the *spectral measure*.

Proof. See previous exercise.

· **Exercise.** Let k be a real function on \mathbb{R}^d . Verify that the kernels of the form

$$k(x, x') = \int_{\mathbb{R}^d} \cos(2\pi \langle s, x - x' \rangle) \mu(ds),$$

are positive semidefinite (p.s.d.).

Theorem (Wiener-Khintchine theorem – see, e.g., [Chatfield, 2016])

· If μ has a density S (known as the spectral density of k), then:

$$k(\tau) = \int_{\mathbb{R}^d} \exp(i\langle \omega, \tau \rangle) S(\omega) d\omega.$$

· If S exists, we have the inversion formula:

$$S(\omega) = \int_{\mathbb{R}^d} \exp(-i\langle \omega, \tau \rangle) k(\tau) d\tau.$$

Proof. Apply Bochner's theorem and the Fourier's formulas.

Example. Consider the spectral density:

$$S(\omega) = \delta(\omega - \omega_0),$$

with $\omega \in \mathbb{R}$. Compute the corresponding valid kernel $k(\tau)$.

Solution.

$$k(\tau) = \int_{\mathbb{R}} \exp(i\omega\tau) \delta(\omega - \omega_0) d\omega = \exp(i\omega_0\tau) = \cos(\omega_0\tau) + i \sin(\omega_0\tau).$$

Note that, if considering a real-valued random field, then

$$k(\tau) = \cos(\omega_0\tau).$$

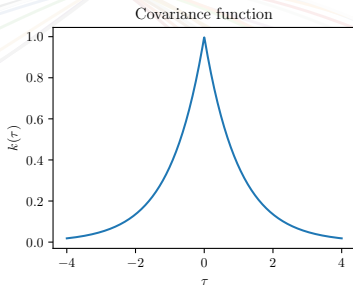
□

Exercise. Compute the spectral density of the kernel:

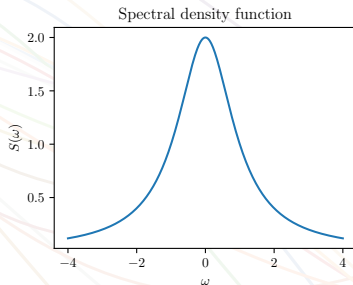
$$k(\tau) = \exp\left(-\frac{|\tau|}{\ell}\right),$$

with $\tau \in \mathbb{R}$ and $\ell > 0$.

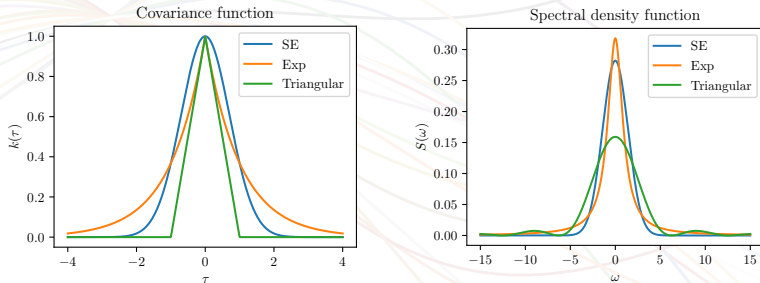
$$k(\tau) = \exp\left(-\frac{|\tau|}{\ell}\right)$$



$$S(\omega) = \frac{2}{\frac{1}{\ell} + \ell\omega^2}$$



Spectral representation of the exponential kernel



Examples of spectral density functions [Heinonen, 2017]

- Bochner's theorem can be used to prove p.s.d. of usual stationary kernels
 - The SE is the FT of a Gaussian function, i.e. it is p.s.d.
 - Matérn kernels are FT of Student t functions, i.e. they are p.s.d.
- It can also be generalised to distributions:
 - $\delta_{x-x'}$ is the FT of the constant functions, i.e. it is p.s.d.
 - The constant function is the FT of $\delta_{x-x'}$, i.e. it is p.s.d.

1D stationary kernel functions

- Some classic kernels for stationary processes:

Stationary kernel name	$k(\tau) := k(x, x + \tau)$	Spectral density
Cosine	$\sigma^2 \cos(2\pi\tau)$	Dirac delta
Sinc	$\sigma^2 \frac{\sin(\pi\tau)}{\tau}$	Uniform
Squared Exponential	$\sigma^2 \exp\left\{-\frac{1}{2} \frac{\tau^2}{\ell^2}\right\}$	Gaussian
Exponential	$\sigma^2 \exp\left\{-\frac{ \tau }{\ell}\right\}$	Student $t_{1/2}$
Matérn 3/2	$\sigma^2 \left(1 + \sqrt{3} \frac{ \tau }{\ell}\right) \exp\left\{-\sqrt{3} \frac{ \tau }{\ell}\right\}$	Student $t_{3/2}$
Matérn 5/2	$\sigma^2 \left(1 + \sqrt{5} \frac{ \tau }{\ell} + \frac{5}{3} \frac{\tau^2}{\ell^2}\right) \exp\left\{-\sqrt{5} \frac{ \tau }{\ell}\right\}$	Student $t_{5/2}$

Exercise. Compute the spectral density $S(\omega)$ for the previous kernels.

Extension to non-stationary kernels

- Non-stationary assumptions imply: $k(x, x') \neq k(x - x')$
- Examples of non-stationary kernels are [Heinonen et al., 2016]

$$k(x, x') = \langle x, x' \rangle^d \quad (\text{polynomial kernel})$$

$$k(x, x') = w(x)w(x') \sqrt{\frac{2\ell(x)\ell(x')}{\ell^2(x) + \ell^2(x')}} \exp\left(\frac{\|x - x'\|^2}{\ell^2(x) + \ell^2(x')}\right) \quad (\text{Gibbs kernel})$$

Definition (Bochner's theorem for non-stationary kernels [Heinonen, 2017])

- If μ has a spectral density S of k), then:

$$k(x, x') = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \exp(i[\langle \omega, \tau \rangle - \langle \omega', \tau' \rangle]) S(\omega, \omega') d\omega d\omega'.$$

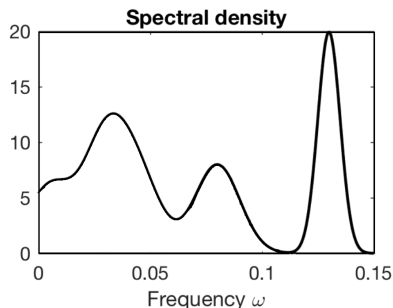
- If S exists, we have the inversion formula:

$$S(\omega, \omega') = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \exp(-i[\langle \omega, \tau \rangle - \langle \omega', \tau' \rangle]) k(x, x') dx dx'.$$

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Spectral kernel design

- Remember that all the spectral densities $S(\omega)$ define a covariance function
- Then one can use $S(\omega)$ for the design of stationary kernels $k(\tau)$



Example of a spectral density [Heinonen, 2017]

Sparse-spectrum kernel [Lázaro-Gredilla et al., 2010]:

- One can consider the spectral density given by

$$S(\omega) = \frac{1}{Q} \sum_{q=1}^Q \delta(\omega - \omega_q),$$

with real frequencies $\omega_1, \dots, \omega_Q \in \mathbb{R}$

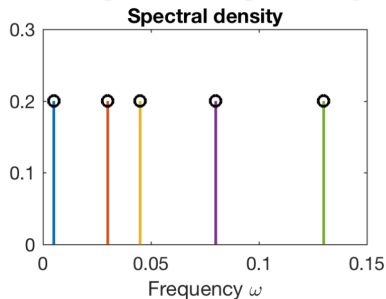
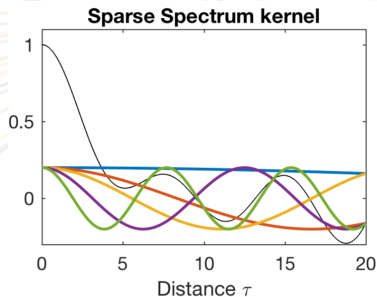
- By applying the Wiener-Khintchine theorem, and using the Fourier dual

$$\tilde{S}(\omega) = \delta(\omega - \omega_0), \quad \tilde{k}(\tau) = \cos(\omega_0 \tau),$$

we have that

$$k(\tau) = \frac{1}{Q} \sum_{q=1}^Q \cos(\omega_q \tau),$$

with $\tau \in \mathbb{R}$.



Spectral mixture kernel [Heinonen, 2017]

Note. Highly structured covariance (prone to overfitting) [Heinonen, 2017].

Spectral mixture kernel [Wilson and Adams, 2013]:

- Define the real frequencies $\omega_1, \dots, \omega_Q \in \mathbb{R}$ as Gaussian r.v.'s:

$$\omega_q \sim \mathcal{N}(m_q, \sigma_q^2), \quad \text{for } q = 1, \dots, Q,$$

with mean m_q and variance σ_q^2 .

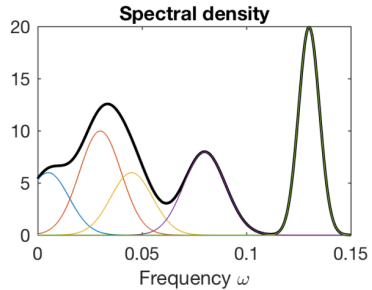
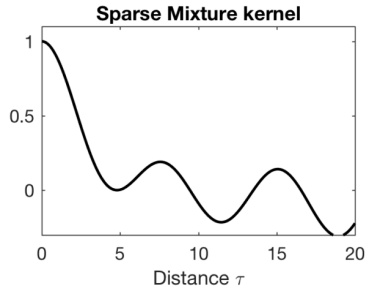
- Then, one can define the spectral density as a mixture of Gaussians:

$$S(\omega) = \sum_{q=1}^Q \alpha_q \mathcal{N}(m_q, \sigma_q^2).$$

- By applying the Wiener-Khintchine theorem, we have that

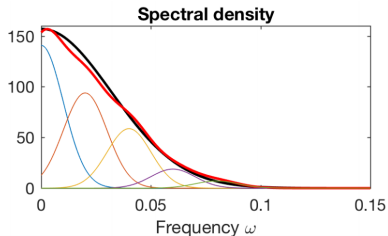
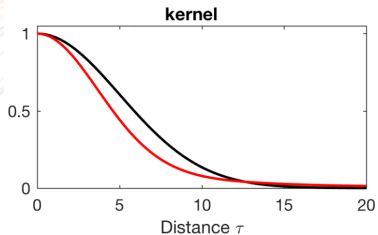
$$k(\tau) = \sum_{q=1}^Q \alpha_q \underbrace{\exp(-\sigma_q^2 \tau^2)}_{\text{smooth decay}} \underbrace{\cos(m_q \tau)}_{\text{periodic}},$$

with $\tau \in \mathbb{R}$.



Spectral mixture kernel [Heinonen, 2017]

Spectral mixture kernel [Wilson and Adams, 2013]



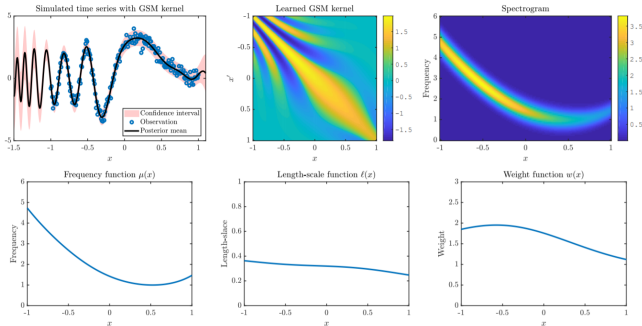
■ SE kernel vs ■ Spectral Mixture kernel with $Q = 5$ [Heinonen, 2017]

- A non-stationary version of the spectral mixture kernel is given by

$$k(x, x') = \sum_{q=1}^Q \underbrace{w_q(x)w_q(x')}_{\text{smooth decay}} \underbrace{\exp(-[x\rho_q^2(x) + x'\rho_q^2(x')])}_{\text{smooth decay}} \underbrace{\langle \psi_q(x), \psi_q(x') \rangle}_{\text{periodic}},$$

with $\psi_q(x) = [\cos(x\nu_q(x)), \sin(x\nu_q(x))]^\top$, and

$$\log w_q(x) \sim \mathcal{GP}(0, k_w), \quad \log \rho_q(x) \sim \mathcal{GP}(0, k_\rho) \quad \log \nu_q(x) \sim \mathcal{GP}(0, k_\nu)$$



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Conclusions

- Spectral analysis is a powerful tool to study complex-valued random fields

$$Z(x) = U(x) + iV(x).$$

- An example of a spectral representation is the Fourier transform
- All stationary kernels $k(\tau)$ have a spectral density $S(\omega)$

$$S(\omega) = \int_{\mathbb{R}^d} \exp(-i\langle \omega, \tau \rangle) k(\tau) d\tau.$$

- All spectral densities $S(\omega)$ define a covariance function (Bochner's theorem)

$$k(\tau) = \int_{\mathbb{R}^d} \exp(i\langle \omega, \tau \rangle) S(\omega) d\omega.$$

- Spectral densities can be used for kernel design

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