INSA – Gaussian processes

Spectral representation and Bochner's theorem

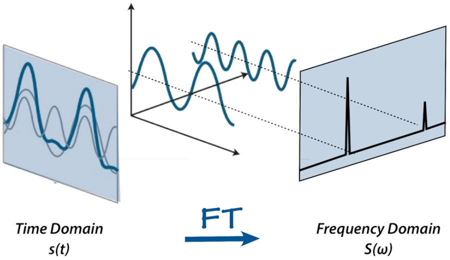
Andrés F. López-Lopera

The French Aerospace Lab ONERA, France
Information Processing and Systems Department (DTIS)
Multidisciplinary Methods, Integrated Concepts (M2CI) Research Unit

Spectral analysis

Spectral analysis

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

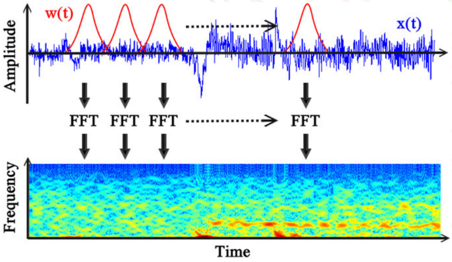


Fourier analysis

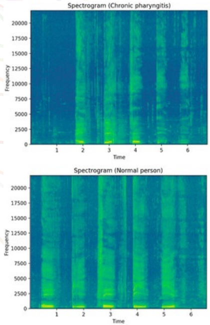
Spectral analysis

- 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

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

$$z(\boldsymbol{x}) = u(\boldsymbol{x}) + iv(\boldsymbol{x}),$$

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

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

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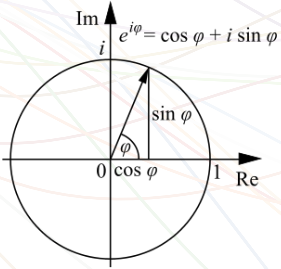
with $\boldsymbol{x} \in \mathbb{R}^d$, $i = \sqrt{-1}$ (imaginary number), and u, v real-valued functions.

· 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 $z : \mathbb{R}^d \to \mathbb{C}$ is given by the **Fourier transform (FT)**:

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

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

· The **inverse Fourier transform** of $S(\boldsymbol{\omega})$ is given by

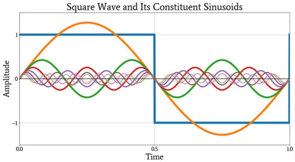
$$\mathcal{F}^{-1}[S](\boldsymbol{x}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(i\langle \boldsymbol{\omega}, \boldsymbol{x}\rangle)\, S(\boldsymbol{\omega}) d\boldsymbol{\omega}.$$

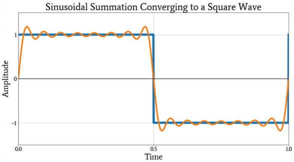
Fourier analysis

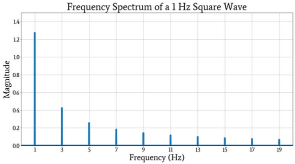
Fourier series (sine-cosine form):

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

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





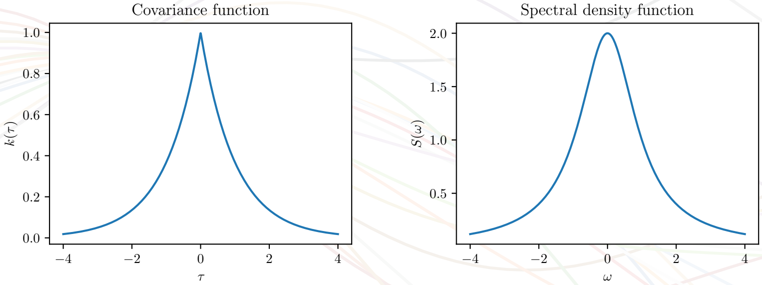


Fourier representation of the square wave function

[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 $k(\boldsymbol{\tau})$ have a spectral density $S(\boldsymbol{\omega})$
  - All spectral densities $S(\boldsymbol{\omega})$ define a covariance function

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Outline

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

Outline

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

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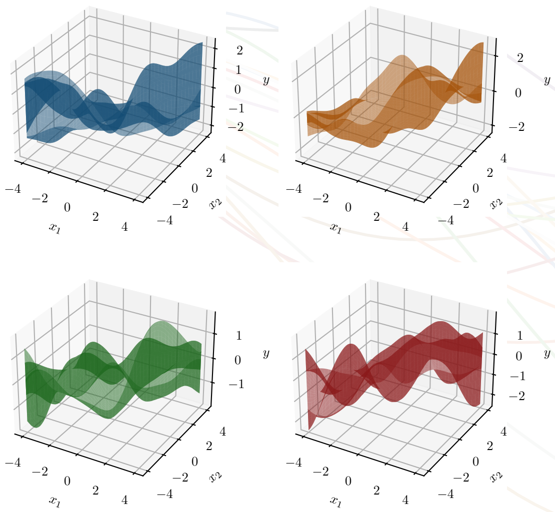
Complex-valued random fields

Random fields

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

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



Complex-valued random fields

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

$$Z(\boldsymbol{x}) = U(\boldsymbol{x}) + iV(\boldsymbol{x}),$$

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

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

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

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

$$\mathsf{Re}\{Z(\boldsymbol{x})\} = U(\boldsymbol{x}), \qquad \mathsf{Im}\{Z(\boldsymbol{x})\} = V(\boldsymbol{x}).$$

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Expectation of complex-valued random fields

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

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

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

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

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Covariance operation of complex-valued random fields

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

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

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

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

Positive semidefiniteness condition

Definition (positive semidefiniteness for complex-valued functions)

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

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

Definition (positive semidefiniteness for real-valued functions)

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

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

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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 $\boldsymbol{x}$ if:

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

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

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

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

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

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Exercise. Suppose $\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_n \in \mathbb{R}^d$ and let $Z_1, \ldots, Z_n$ be zero-mean complex random variables with $\mathbb{E}\left\{Z_p \overline{Z_q}\right\} = 0$ for $p \neq q$ and $\mathbb{E}\left\{|Z_p|^2\right\} = f_p < \infty$. Consider

$$\widetilde{Z}(\boldsymbol{x}) = \sum_{p=1}^{n} Z_p \exp(i\langle \boldsymbol{\omega}_p, \boldsymbol{x}\rangle).$$

Show that $\widetilde{Z}$ is weakly stationary.

Spectral representation of random fields

· $\widetilde{Z}(\boldsymbol{x}) = \sum_{p=1}^{n} Z_p \exp(i\langle \boldsymbol{\omega}_p, \boldsymbol{x}\rangle)$ is an example of a spectral representation.

· Generally, spectral representations of mean square continuous weakly stationary random fields can be obtained [Stein, 1999]:

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

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 $\widetilde{Z}$.

Exercise. Suppose that for some positive finite measure μ:

$$\mathbb{E}\left\{M(\Delta)\right\} = 0$$
$$\mathbb{E}\left\{|M(\Delta)|^2\right\} = \mu(\Delta)$$
$$\mathbb{E}\left\{M(\Delta_1), \overline{M(\Delta_2)}\right\} = 0, \quad \text{for disjoint Borel sets } \Delta_1, \Delta_2$$

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

Solution.

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

$\square$

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Bochner's theorem

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 $\mathbb{R}^d$ iif it can be represented as*

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

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

Proof. See previous exercise.

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

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

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:*

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

· *If S exists, we have the inversion formula:*

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

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

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

□

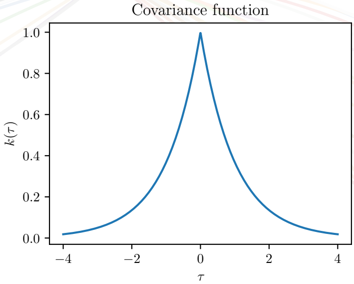
Exercise. Compute the spectral density of the kernel:

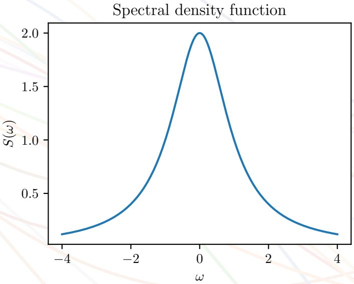
$$k(\tau) = \exp\left(-\frac{|\tau|}{\ell}\right),$$

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

Spectral density

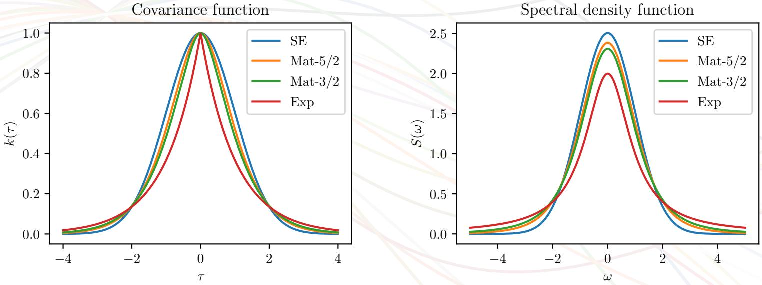
$$k(\tau) = \exp\left(-\frac{|\tau|}{\ell}\right) \qquad S(\omega) = \frac{2}{\frac{1}{\ell}+\ell\omega^2}$$





Spectral representation of the exponential kernel

Spectral density



Examples of spectral density functions [Heinonen, 2017]

Spectral density

- 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.

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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	$\sigma^2 \frac{\sin(\pi\tau)}{\pi\tau}$	Uniform
Squared Exponential	$\sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\}$	Gaussian
Exponential	$\sigma^2 \exp\left\{-\frac{\lvert\tau\rvert}{\ell}\right\}$	Student $t_{1/2}$
Matérn 3/2	$\sigma^2 \left(1+\sqrt{3}\frac{\lvert\tau\rvert}{\ell}\right)\exp\left\{-\sqrt{3}\frac{\lvert\tau\rvert}{\ell}\right\}$	Student $t_{3/2}$
Matérn 5/2	$\sigma^2 \left(1+\sqrt{5}\frac{\lvert\tau\rvert}{\ell}+\frac{5}{3}\frac{\tau^2}{\ell^2}\right)\exp\left\{-\sqrt{5}\frac{\lvert\tau\rvert}{\ell}\right\}$	Student $t_{5/2}$

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

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Extension to non-stationary kernels

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

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

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

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

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

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

- If S exists, we have the inversion formula:

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

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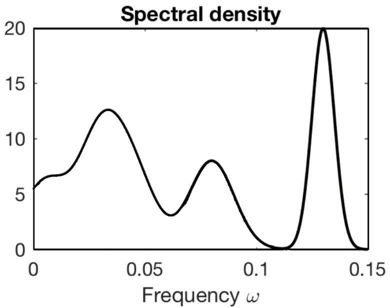
Spectral kernel design

Spectral kernel design

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



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 $\omega_1, \ldots, \omega_Q \in \mathbb{R}$

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

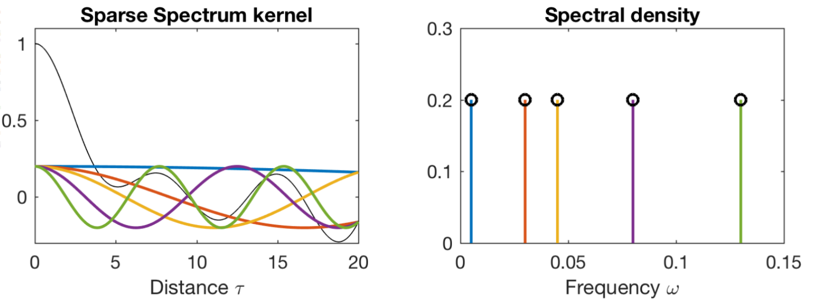
$$\widetilde{S}(\omega) = \delta(\omega - \omega_0), \qquad \widetilde{k}(\tau) = \cos(\omega_0 \tau),$$

we have that

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

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

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



Spectral mixture kernel [Heinonen, 2017]

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

Spectral kernel design

Spectral mixture kernel [Wilson and Adams, 2013]:

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

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

with mean m_q and variance σ_q^2.

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

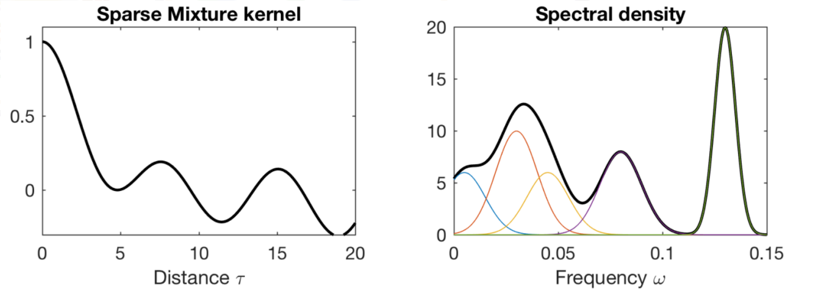
$$S(\boldsymbol{\omega}) = \sum_{q=1}^{Q} \alpha_q \mathcal{N}\left(m_q, \sigma_q^2\right).$$

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

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

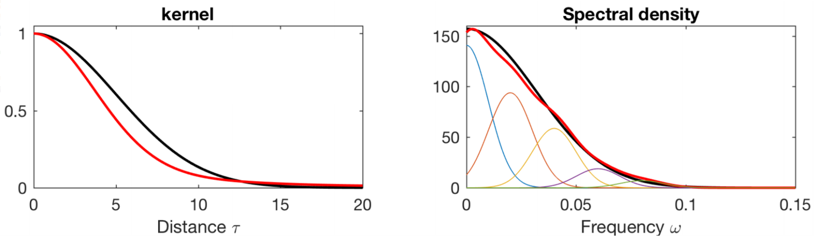
with $\tau \in \mathbb{R}$.

Spectral mixture kernel [Wilson and Adams, 2013]



Spectral mixture kernel [Heinonen, 2017]

Spectral mixture kernel [Wilson and Adams, 2013]



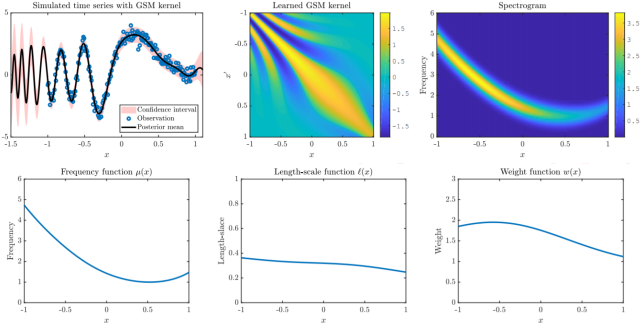
■ SE kernel vs ■ Spectral Mixture kernel with $Q = 5$ [Heinonen, 2017]

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

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

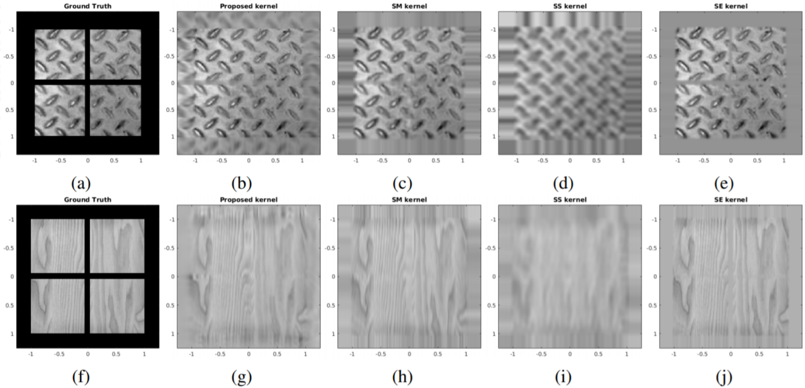
with $\psi_q(x) = [\cos(x\nu_q(x)), \sin(x\nu_q(x))]^\top$, and

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



Generalised spectral mixture (GSM) kernel [Heinonen et al., 2016]

Generalised spectral mixture kernel [Heinonen et al., 2016]



texture image examples [Heinonen et al., 2016]

Conclusions

Conclusions

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

$$Z(\boldsymbol{x}) = U(\boldsymbol{x}) + iV(\boldsymbol{x}).$$

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

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

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

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

- Spectral densities can be used for kernel design

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