Elucidating appealing features of differentiable auto-correlation functions: a study on the modified exponential kernel

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Abstract

Research on stochastic processes in recent decades has pointed out that, in the context of modelling spatial or temporal uncertainties, auto-correlation functions that are differentiable at the origin have advantages over functions that are not differentiable. For instance, the non-differentiability of e.g., single exponential auto-correlation functions yields non-smooth sample paths. Such sample paths might not be physically possible or may yield numerical difficulties when used as random parameters in partial differential equations (such as encountered in e.g., mechanical equilibrium problems). Further, it is known that due to the non-differentiability of certain auto-correlation functions, more terms are required in the series expansion representations of the associated stochastic processes. This makes these representations less efficient from a computational standpoint.

This paper elucidates some additional appealing features of auto-correlation functions which are differentiable at the origin. Further, it focuses on enhancing the arguments in favor of these functions already available in literature. Specifically, attention is placed on single exponential, modified exponential and squared exponential auto-correlation functions, which can be shown to be all part of the Whittle-Matérn family of functions. To start, it is shown that the power spectrum of differentiable kernels converges faster to zero with increasing frequency as compared to non-differentiable ones. This property allows capturing the same percentage of the total energy of the spectrum with a smaller cut-off frequency, and hence, less stochastic terms in the harmonic representation of stochastic processes. Further, this point is examined with reqards to the Karhunen-Loève series expansion and first and second order Markov processes, generated by auto-regressive representations. The need for finite differentiability is stressed and illustrated.

Keywords:

1. Introduction

Many of the loads on engineering components, structures, and systems, as well as the constitutive properties of these assets exhibit a stochastic nature. This assertion is based on the observation that these quantities exhibit apparent variability in time and/or space. In this context, the theoretical framework of stochastic process, and by extension, of random fields [19] has proven an excellent means for capturing inherent (aleatory) uncertainty [6]. Stochastic processes represent in essence jointly distributed random variables whose correlation function depends on time and/or space. Throughout literature, efficient methods have been introduced to effectively and accurately sample from these potentially high-dimensional joint distributions.

Typically, the auto-correlation of such stochastic process is governed by a pre-defined auto-correlation function (also often referred to as 'kernel'). This function describes the correlation between two random variables in the stochastic process as a function of the distance in time/space between them. Alternatively, in case the process is stationary, the auto-correlation is governed by the relative distance between two points. This paper focuses on auto-correlation functions that belong to the Whittle-Matérn family of functions. Special attention is given to the single exponential, modified exponential and squared exponential auto-correlation functions. The generation of samples from these stochastic processes is usually done using the well-known Karhunen-Loève series expansion [13, 21] or the spectral representation method as introduced by [7], [8] and later by [6]. Also extended versions of these techniques have been introduced. Examples of such methods include the Stochastic Harmonic Function representation by [1].

The single exponential auto-correlation kernel has been used extensively in engineering applications. For instance, [5] applied this kernel to represent a stochastic process to model the permeability in resin transfer molding simulation. Further, in [3], Bayesian updating in a geo-technical context was done based on a single exponential kernel. In fact, the overview paper of [4] shows that the single exponential model is most popular in geotechnical engineering, with a total of 47% of examined papers reporting usage of this auto-correlation model. The single exponential kernel is often selected due to the availability of analytical solutions to the eigenvalue problem corresponding to the Karhunen-Loève series expansion. However, the appropriate selection of the auto-correlation function is of large importance for the correct modelling and simulation of the phenomenon or property under consideration.

More relevantly to the problem discussed herein, [2] studied the effect of the auto-correlation function on the probability of failure in several geo-technical examples. In this work, the authors showed that the smoothness of a sample path had a significant effect on the probability of failure. This is particularly true when no spatial averaging is present in the considered problem capable of smoothing out local variations. Further, it was shown that the sample path smoothness depends on the functional form of the auto-

correlation function, and, more precisely, on the differentiability of such function at zero-lag. Thus, this work clearly illustrated that the auto-correlation function ends up affecting the probability of failure.

Furthermore in this context, [18] noted that the application of the single exponential auto-correlation kernel tends to underestimate the failure risk in the unsaturated slope risk assessment. In addition, they pointed out how the differentiability of the auto-correlation function affects the truncation order of the Karhunen-Loève series expansion. Also in this regard, [14] showed that square exponential kernels are preferable over single exponential kernels, allowing for a highly exact series expansion representation with far fewer terms in the expansion. Similar observations were made by [15] in the context of modelling stochastic ocean waves. In essence, they showed that fewer stochastic variables are required to describe stochastic processes with a narrow spectral bandwidth (i.e., spectra that converge relatively fast to zero away from the "central" frequency). A comprehensive study of the convergence of second order statistics of KL-simulated stochastic processes in function of the correlation length, functional form of the auto-correlation function and solution method is given by [22], indicating similar conclusions. However, the modified exponential kernel is not studied in this paper.

As a final note to this overview of the wide-spread application of single exponential kernels (versus less frequently used kernels), examination of the literature showed that non-differentiable auto-correlation functions are used to represent a random 'stiffness' term in partial differential equations. To address this, in [16] the "modified exponential kernel" was introduced to alleviate the shortcomings of the traditional single exponential kernel caused by non-differentiability. Further, this kernel maintains the enticing properties of the single exponential kernel, such as the availability of analytical solutions and the possibility to characterize quickly varying spatial or temporal phenomena. Also, this kernel is more efficient in terms of the required number of stochastic quantities as compared to the single exponential kernel. These properties are obtained by addressing the issue of non-differentiability at zero-lag in the single exponential kernel, while maintaining its functional form to a great extent.

This paper builds upon the work that was presented in [16] in three ways. First, it provides additional explanations of why this particular kernel is highly effective by analytically deriving the energy error rate convergence in the frequency domain. Second, it compares the modified exponential kernel to another widely used auto-correlation kernel, namely the squared exponential kernel. Finally, it provides additional numerical evidence for the effectiveness of the modified exponential kernel in conjunction with the Karhunen-Loève series expansion, and auto-regressive model representations. The paper is structured as follows. Section 2 starts by introducing some basic concepts related to the modelling and simulation of stochastic processes. Section 3 discusses the convergence of the considered auto-correlation kernels both in the frequency and time domain and discusses the implications hereof for numerical analysis purposes.

Finally, Section 4 briefly comprises the conclusions that can be drawn from this work.

2. Spectral stochastic process representation

2.1. Definition and stochastic properties

A finite-dimensional stochastic process $f(\boldsymbol{t}, \theta)$ describes a set of correlated random variables $f(\theta)$ that are assigned to a countable number of locations $\boldsymbol{t} \in \Omega$ in the model domain $\Omega \subset \mathbb{R}^d$ with dimension $d \in \mathbb{N}$. Each such a random variable $f(\theta) : (\Theta, \varsigma, P) \mapsto \mathbb{R}$, with $\theta \in \Theta$ a coordinate in sample space Θ and ς the sigma-algebra, as such maps from a complete probability space to the real domain. This map holds as long as $f(\boldsymbol{t}, \theta) \in \mathcal{L}^2(\Theta, P)$, with $L^2(\Theta, P)$ the Hilbert space of second-order random variables (i.e., finite variance). For a given event $\theta_i \in \Theta$, $f(t, \theta_i)$ is a realization of the stochastic process. A stochastic process is considered Gaussian if the distribution of $(f(\boldsymbol{t}_1, \theta), f(\boldsymbol{t}_2, \theta), \ldots, f(\boldsymbol{t}_n, \theta))$ is jointly Gaussian $\forall \boldsymbol{t} \in \Omega$.

Consider $f(t, \theta)$ to be a zero-mean one-dimensional univariate stochastic process (i.e, $\Omega \subset \mathbb{R}$) with constant variance over the domain and auto-correlation function $R_{ff}(t, \tau) : \Omega \times \Omega \mapsto [0, 1]$ and $\tau \subset \Omega$ a lag parameter. The auto-correlation $R_{ff}(t, \tau)$ of such a stochastic process represents the correlation between two random variables $f(t, \theta)$ and $f(t + \tau, \theta)$, separated by a lag τ. That is,

$$R_{ff}(t, \tau) = \frac{CV\left[f(t, \theta) f(t + \tau, \theta)\right]}{\sqrt{V\left[f(t, \theta)\right]} \sqrt{V\left[f(t + \tau, \theta)\right]}}, \tag{1}$$

with $CV[\cdot, \cdot]$ denoting an operator that returns the covariance and $V[\cdot]$ an operator returning the variance of the argument. In this regard, τ may represent a distance in time or space. In the remainder of this paper, only homogeneous auto-correlation functions, i.e., $R_{ff}(\tau)$ are considered.

In practical applications, often analytical models for the auto-correlation are applied [2]. In this context, particularly the auto-correlation functions belonging to the family of Whittle-Matérn type of functions are popular, the formulation of which is given as:

$$R_{ff}^{\nu}(\tau) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{\tau}{b}\right)^{\nu} K_{\nu} \left(\sqrt{2\nu} \frac{\tau}{b}\right), \tag{2}$$

where ν is the so-called "smoothness" parameter, Γ denotes the Gamma function, K_{ν} is the modified Bessel function of the second kind and b is the correlation length. It can be shown that for $\nu = p + 0.5$, with $p \in \mathbb{N}^+$, the Whittle-Matérn correlation function family can be represented as the product of an exponential and of a polynomial of order p. That is,

$$R_{ff}^{p+0.5}(\tau) = \exp\left(-\frac{\sqrt{2p+1}\tau}{b}\right) \frac{p!}{(2p)!} \sum_{i=1}^{p} \frac{(p+i)!}{i!(p-i)!} \left(\frac{2\sqrt{2p+1}\tau}{b}\right)^{p-i}. \tag{3}$$

From this equation, it is straightforward to show that the cases of $p = 0$, $p = 1$ and $p \to \infty$ give rise to the so-called single exponential, modified exponential and squared exponential auto-correlation functions. Namely, the single exponential auto-correlation function is given as

$$R_{ff}^{0.5}(\tau) = \exp(-|\tau|/b); \tag{4}$$

the modified exponential auto-correlation function [16] is given as

$$R_{ff}^{1.5}(\tau) = \exp(-|\tau|/b)(1 + |\tau|/b); \tag{5}$$

and the squared-exponential auto-correlation function is given as

$$R_{ff}^{\infty}(\tau) = \exp(-\tau^2/b^2). \tag{6}$$

As a final note, it is worthy to mention that the sample paths of a Gaussian process with a Whittle-Matérn kernel are $\lceil \nu \rceil - 1$ times differentiable. In the available literature, single and squared exponential functions are commonly used in various application domains. As discussed in [2], the main difference between these two auto-correlation functions is the smoothness of the resulting sample paths; related applications to soil engineering can be found in references such as [9] and [10]. The main advantage of a single exponential kernel is the availability of analytical solutions in terms of its Karhunen–Loève expansion [20], and the capability to characterize quickly varying phenomena. However, it exhibits non-differentiability at zero-lag, which causes non-differentiable sample paths (i.e., $C - 0$ continuity).

On the other hand, the squared exponential provides infinitely differentiable sample paths, but does not provide analytical solution for the terms of the expansion. Further, as Stein [11] argues, the infinite differentiability yields unrealistic results for physical processes, since observing only a small continuous fraction of space/time should, in theory, yield the whole process sample [11]. It should be pointed out, that for all practical reasons, a Whittle-Matérn function with $p = 3.5$ can be considered to be *almost* equal to $p \to \infty$ [12].

The modified exponential auto-correlation function aims at combining the strengths of both the aforementioned kernels, as it provides the temporal/geometric characteristics of the sample paths of a single exponential kernel, it solves the problem of the zero-lag discontinuities, and it provides analytical solutions for its Karhunen-Loève expansion [16]. Further, for many physical processes arising in mechanical or civil engineering, first-order differentiability is sufficient , as for instance illustrated in [10] in the case of soil mechanics. For instance, taking a practical standpoint, when considering certain input quantities to a Finite Element model in a quasi-static context, no higher-order differentiability due to the

approximations of the functional solution spaces made. In this context, note that Gaussian processes that are governed by a Whittle-Matérn kernel are $\lceil \nu \rceil - 1$ times differentiable in a mean-square sense [17]. This property makes this family of auto-correlation functions particularly appealing to model physical processes in a realistic and mathematically rigorous way.

Alternatively, the auto-correlation of $(f(t_1, \theta), f(t_2, \theta), \ldots, f(t_n, \theta))$ can be represented in the frequency domain by means of a two-sided power spectrum $S_{ff}(\omega) : \Gamma \times \Gamma \mapsto \mathbb{R}$, with $\Gamma \subset \mathbb{R}$ the frequency domain. The Wiener-Khintchine theorem allows for the calculation of the auto-correlation function $R_{ff}(\tau)$ of a stochastic process from its two-sided power spectrum $S_{ff}(\omega)$ and vice versa based on the following Fourier transforms:

$$S_{ff}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} R_{ff}(\tau) e^{-i\omega\tau} d\tau, \tag{7}$$

and

$$R_{ff}(\tau) = \int_{-\infty}^{+\infty} S_{ff}(\omega) e^{i\omega\tau} d\omega. \tag{8}$$

Applying the Wiener-Khintchine theorem to the auto-correlation function defined in Eq. (2) yields the form

$$S_{ff}^{\nu}(\omega) = \frac{2\pi^{0.5}\Gamma(\nu + 0.5)(2\nu)^{\nu}}{\Gamma(\nu) b^{2\nu}} \left(\frac{2\nu}{b^2} + 4\pi^2\omega^2 \right)^{-\nu+0.5} \tag{9}$$

for the corresponding power spectrum.

The power spectra corresponding to the auto-correlation functions in Eqs. 4–6 can be similarly shown to be given by the equations

$$S_{ff}^{0.5}(\omega) = \frac{1}{\pi} \frac{b}{b^2\omega^2 + 1}, \tag{10}$$

$$S_{ff}^{1.5}(\omega) = \frac{1}{\pi} \frac{2b}{(b^2\omega^2 + 1)^2}, \tag{11}$$

and

$$S_{ff}^{\infty}(\omega) = \frac{1b}{2\sqrt{\pi}} \exp \frac{-b^2\omega^2}{4}. \tag{12}$$

Close inspection of Eq. (9) reveals that the "smoothness" parameter, which is also critical for the differentiability of R_{ff}^{ν} for $\tau \to 0$, determines the range over which the energy content of the spectrum is spread out. Indeed, since ν determines the order of the denominator, it affects the rate with which $S_{ff}^{\nu}(\omega)$ tends to 0 for increasing ω values. Take for instance the case of Eq. 10. It is clear that in this case, due to the lack of higher order terms in the denominator, the energy content is broadly distributed over ω. Similarly, it can be seen that the energy content of the modified exponential kernel decreases quadratically with respect to the term $b^2\omega^2+1$ in Eq. 11. As such, the bandwidth of the single exponential kernel is wider as compared to the modified exponential. Finally, the $\exp(\cdot)$ term in Eq. 12 suggests that

most of the energy content is located in the lower frequencies for the squared exponential kernel. Thus, it is shown that the power-spectra of the zero-lag differentiable kernels, i.e., the modified and squared exponential kernel, converge faster to zero as $\omega \to \infty$.

2.2. Simulation of stochastic processes

2.2.1. Spectral representation

Following the power spectral representation of the auto-correlation of a stochastic process, the simulation of paths of this process can be done according to [7, 6] using the equation

$$f(t,\theta) = \sqrt{2}\sum_{n=0}^{N-1} A_n \cos(\omega_n t + \psi_n(\theta)), \tag{13}$$

where

$$A_n = \sqrt{2S_{ff}(\omega_n)\Delta\omega}, \tag{14}$$

and ω_n is defined as

$$\omega_n = n\Delta\omega, \tag{15}$$

where $n = 1, \ldots, N-1$ and $\Delta\omega = \omega_u/N$. The phase angles $\psi_n(\theta)$ are considered random and distributed as $\mathcal{U}(0, 2\pi)$, with $\mathcal{U}$ the uniform distribution. Thus, samples $f(t, \theta_i)$ of the stochastic process can be generated by sampling from $\mathcal{U}(0, 2\pi)$. The parameter ω_u represents the cut-off frequency, beyond which the power spectral density function $S_{ff}(\omega)$ may be assumed to be zero for either mathematical or physical reasons. In practice, an energy criterion is commonly used. That is,

$$\int_0^{\omega_u} S_{ff}(\omega_n)d\omega = (1 - e_S)\int_0^{\infty} S_{ff}(\omega_n)d\omega, \tag{16}$$

with e_S a measure for the error, which is typically a small value, e.g., $e_S = 0.01$ or $e_S = 0.001$. In this regard, the appropriate selection of ω_u is important for the accuracy of the analysis. In essence, it represents the degree of approximation of the energy content used in the representation of the stochastic process. As such, if ω_u is selected too small, a significant fraction of the energy of the modelled signal is lost. This might lead to an underestimation of the magnitude of the physical quantity under consideration, which can lead to severe limitations, e.g., underestimation of probability of failure. Further, ω_u cannot be selected arbitrarily larger for numerical reasons. Specifically, extremely high values of ω_u require a corresponding quite high number of random variables $\psi_n(\theta)$, leading to computationally costly procedures. Further, note that while herein attention is focused on the spectral representation, these arguments are also pertinent to other simulation methods based in the frequency domain, e.g., the Stochastic Harmonic

Function representation [1].

2.2.2. Karhunen-Loève expansion

The Karhunen-Loève expansion is a potent tool for representing stochastic processes [20]. Specifically, following the Karhunen-Loève (KL) series expansion, a stochastic process $f(t,\theta)$ is represented as:

$$f(t,\theta) = \mu_x(t) + \sigma_f \sum_{i=1}^{\infty} \sqrt{\lambda_i}\boldsymbol{\psi}_i(t)\xi_i(\theta), \tag{17}$$

where σ_f is the standard deviation of the random field. The quantities $\lambda_i \in (0,\infty)$ and $\boldsymbol{\psi}_i(t) : \Omega \mapsto \mathbb{R}$ are respectively the eigenvalues and eigenfunctions of the continuous, bounded, symmetric and positive (semi-) definite auto-correlation function $R_{ff}(\tau)$. The decomposition of $R_{ff}(\tau)$ is performed in accordance with Mercer's theorem. That is,

$$R_{ff}(\tau) = \sum_{i=1}^{\infty} \lambda_i \boldsymbol{\psi}_i(t)\boldsymbol{\psi}_i(t'). \tag{18}$$

These quantities are in practice obtained by solving the homogeneous Fredholm integral equation of the second kind. That is,

$$\int_{\Omega} R_{ff}(\tau)\boldsymbol{\psi}_i(t')dt' = \lambda_i \boldsymbol{\psi}_i(t), \tag{19}$$

with $t' = t + \tau$. Analytical solutions to this equation exist only for a limited number of auto-correlation functions. In general, discretization schemes are used to solve this equation, as explained in [21]. Since $R_{ff}(\tau)$ is bounded, symmetric, positive semi-definite, and, in most practical cases, can be even assumed positive definite, the eigenvalues λ_i are non-negative and the eigenfunctions $\boldsymbol{\psi}_i(t)$ satisfy the orthogonality condition

$$\langle \boldsymbol{\psi}_i(t), \boldsymbol{\psi}_j(t) \rangle = \int_{\Omega} \boldsymbol{\psi}_i(t)\boldsymbol{\psi}_j(t)dt = \delta_{ij}, \tag{20}$$

with δ_{ij} the Kronecker delta. $\langle \cdot, \cdot \rangle : \Omega \times \Omega \mapsto \mathbb{R}$ denotes the inner product in the functional space. Hence, the eigenfunctions form a complete orthogonal basis on an $\mathcal{L}_2$ Hilbert space. In this case, the series expansion in Eq. 18 can be shown to be optimally convergent [20].

For practical reasons, the infinite series expansion in Eq. 17 must be truncated after a finite number of terms $n_{KL} \in \mathbb{N}$. That is,

$$f(t,\theta) = \sigma_f \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i}\boldsymbol{\psi}_i(t)\xi_i(\theta), \tag{21}$$

where n_{KL} should be selected such that following inequality holds:

$$1 - \frac{1}{|\Omega|}\frac{1}{\sigma_f^2}\sum_{i=1}^{n_{KL}} \lambda_i \leq e_\sigma, \tag{22}$$

with e_σ the so-called mean error variance [21] and $|\Omega|$ denoting the length of the simulation domain.

In contrast to e_S introduced in Eq. (16), the quantity e_σ does not represent some sort of energy loss measure. Instead, e_σ represents the percentage of the variance of the original process that is captured by the truncated Karhunen-Loève expansion. In this respect, if n_{KL} is selected too small, it will lead to a loss of the variance in the representation. Hence, the magnitude of the physical quantity under consideration will be underestimated. Finally, similarly to the spectral representation, setting n_{KL} too large will render the computational cost of the corresponding analysis untractable due to the high dimension of the parameter input space.

2.2.3. Auto-regressive models

A third commonly used approach to simulate stochastic processes and fields is the auto-regressive representation (AR) method [23]. According to the AR framework, the value of a stochastic process $f(t,\theta)$ at time t_k with order m can be computed as

$$f(t_k,\theta) = -\sum_{i=1}^{m} a_i f(t_{k-i}) + b_0 w(t_k,\theta), \tag{23}$$

where a_i are the AR parameters and b_0 is the gain factor of the AR model. $w(t_k)$ is a band limited $[-\omega_b,\omega_b]$ white-noise process that satisfies

$$E\left[w(t_k)w(t_l)^T\right] = 2\omega_b I_n \delta_{kl}, \tag{24}$$

where $E[\bullet]$ and $\bullet^T$ denotes the operators of mathematical expectation and transpose respectively, ω_b is the cut-off frequency, I_n is the identity matrix and δ_{kl} the Kronecker delta. The representation in Eq. (23) is the best linear estimator of $f(t_k,\theta)$ by using the m previous values $[f(t_k), f(t_{k-1}), \ldots, f(t_{k-m})]$. The corresponding error ϵ can be expressed as:

$$\epsilon = \frac{\triangle t}{2\pi} E\left[\left(f(t_k,\theta) + \sum_{i=1}^{m} a_i f(t_{k-I})\right)\right] = b_0^2. \tag{25}$$

The parameters a_i in the series expansion defined in Eq. (23) can generally be determined by minimizing ϵ. This leads to the so-called Yule-Walker equations that relate the stationary target auto-correlation function $R_{ff}(\tau) \equiv R_{ff}(t_k - t_i)$ to the AR parameters via a Toeplitz system of equations:

$$\sum_{i=1}^{m} R_{ff}(t_k - t_i) a_i = -R_{ff}(t_k) \quad k = 1,\ldots,m \tag{26}$$

Alternative approaches used to fit an AR model to a predefined auto-correlation model interpret

Eq. (23) as the response of a discrete linear system to a white-noise excitation. For a thorough explanation of the fitting of an AR model to a predefined auto-correlation function or power spectral density, the reader is referred to the work of [23] or [24].

3. Convergence of the stochastic process representations

In this section analytical expressions are derived for the energy approximation error of the spectral stochastic representation of the three considered auto-correlation kernels. Then, the paper provides additional illustrations regarding the improved convergence behavior of the modified exponential kernel over the single exponential when they are used in the context of a KL expansion. Finally, a comparison of AR models for these three auto-correlation functions is included for the sake of completeness.

3.1. Spectral stochastic representation

The convergence behavior of the auto-correlation functions in Eqs. 4-6 is studied with respect to Eq. 16. In this context, analytical expressions for the approximation error e_s are derived with respect to the cut-off frequency ω_u. Note that similar expressions can be derived for all members of the Whittle-Matérn class of auto-correlation functions that abide $\nu = p + 0.5$. A general expression of the error in function of ν is far from trivial to obtain and falls outside the scope of this paper. To determine the cut-off frequency ω_u using Eq. (16), the power spectra $S_{ff}(\omega)$ in Eqs. 10-12 needs to be integrated. The right hand side integral of $S_{ff}(\omega)$ w.r.t. ω is obtained by means of substitution and given for these power spectra by the equations

$$\int_0^\infty S_{ff}^{0.5}(\omega)d\omega = \left[\frac{1}{\pi}\tan^{-1}(b\omega)\right]_0^\infty = \frac{1}{2}, \tag{27}$$

$$\int_0^\infty S_{ff}^{1.5}(\omega)d\omega = \left[\frac{1}{\pi}4b\left(\frac{\omega}{2(\omega^2b^2+1)} + \frac{1}{2b}\tan^{-1}(b\omega)\right)\right]_0^\infty = 1, \tag{28}$$

and

$$\int_0^\infty S_{ff}^{\infty}(\omega)d\omega = \left[\mathrm{erf}\left(\frac{b\omega}{2}\right)\right]_0^\infty = 1, \tag{29}$$

where $\mathrm{erf}(x) = \frac{1}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$ is the error function.

Similarly, the left-hand side of Eq. (16) for the considered auto-correlation functions can be determined as

$$\begin{aligned}\int_0^{\omega_u} S_{ff}^{0.5}(\omega)d\omega &= \left[\tfrac{1}{\pi}\tan^{-1}(b\omega)\right]_0^{\omega_u} \\ &= \tfrac{1}{\pi}\tan^{-1}(b\omega_u),\end{aligned} \tag{30}$$

$$\int_0^{\omega_u} S_{ff}^{1.5}(\omega)d\omega = \left[\frac{1}{\pi}4b\left(\frac{\omega}{2(\omega^2b^2+1)} + \frac{1}{2b}\tan^{-1}(b\omega)\right)\right]_0^{\omega_u}$$
$$= \frac{1}{\pi}4b\left(\frac{\omega_u}{2(\omega_u^2b^2+1)} + \frac{1}{2b}\tan^{-1}(b\omega_u)\right), \tag{31}$$

and

$$\int_0^{\omega_u} S_{ff}^{\infty}(\omega)d\omega = \left[\mathrm{erf}\left(\frac{b\omega}{2}\right)\right]_0^{\omega_u}$$
$$= \mathrm{erf}\left(\frac{b\omega_u}{2}\right). \tag{32}$$

Using these equations in conjunction with Eq. (16), and isolating the desired truncation error e_S provides relations between the error and the cut-off frequency as. Specifically,

$$e_{S,0.5} = 1 - \frac{2}{\pi}\tan^{-1}(b\omega_u), \tag{33}$$

$$e_{S,1.5} = 1 - \frac{2}{\pi}\left(\frac{b\omega_u}{b^2\omega_u^2+1} + \tan^{-1}(b\omega_u)\right), \tag{34}$$

and

$$e_{S,\infty} = 1 - \mathrm{erf}\left(\omega_u\frac{b}{2}\right). \tag{35}$$

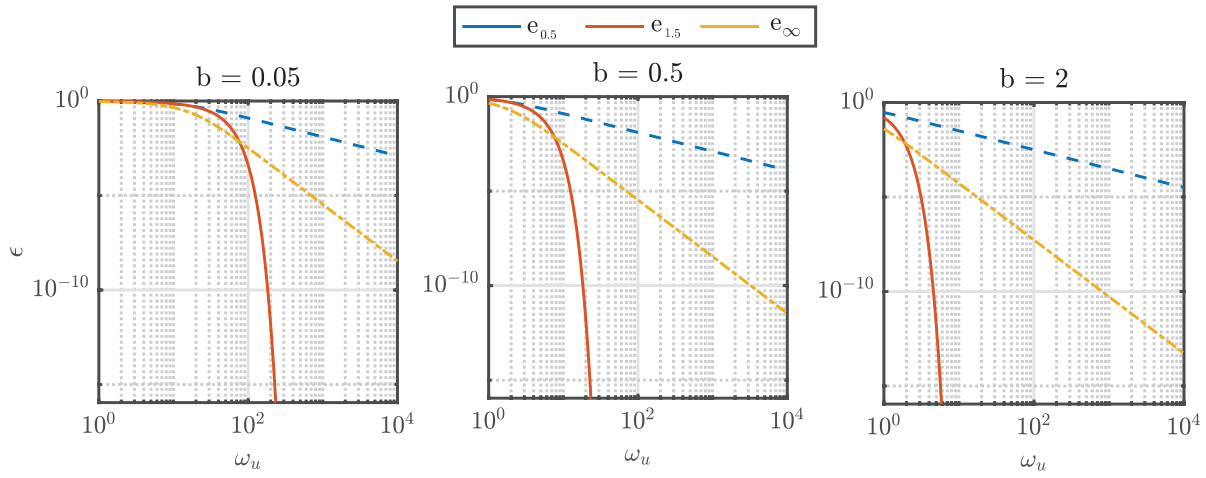

Figure 1: Decay of the energy approximation error e as a function of the truncation frequency ω_u. Plots for different values of the correlation length b are given.

Figure 1 shows the decay of the truncation error of the energy e_S as a function of the selected ω_u for the considered auto-correlation models, for several different values of the correlation lengths $b = [0.05, 0.5, 2]$. The decay function is calculated according to Eq. (33) to (35). In particular, a zero-mean Gaussian stochastic process with unit variance on a domain $t \in [0, 5]$ is considered for this purpose. From this

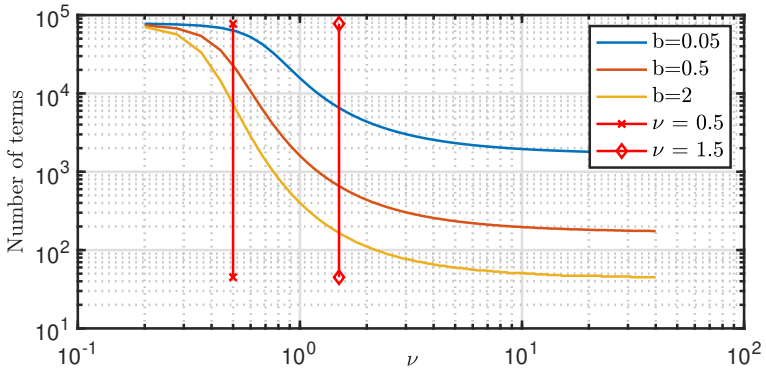

Figure 2: Number of terms in the spectral expansion as a function of the smoothness parameter of the Matérn kernel.

Figure, it is clear that this approximation error decays significantly faster in squared and modified exponential kernels as compared to a single exponential kernel. Specifically, the squared exponential kernel converges super-linearly, the modified exponential kernel converges linearly with a slope of 2.13 and the single exponential kernel converges linearly with a slope of 0.87. These findings are valid for all correlation lengths tested. The difference in the convergence rate between the modified and the single exponential kernels originates from the $\frac{b\omega_u}{b^2\omega_u^2+1}$-term in Eq. (34). This term ensures that the error for the modified exponential kernel decreases faster versus the single exponential case when $w_u \to \infty$. Nevertheless, note that the shape of the decay of the error with respect to ω_u is similar for both single and modified exponential curves.

These considerations are further elucidated in Figure 2, which shows the number of terms in the spectral expansion (see also Eq. (13)) that are required to represent 99.9% of the energy of the power spectrum. Also from this figure, it is clear that higher ν values and hence, a higher-order differentiability of the auto-correlation function at zero lag, yields more efficient representations of the random field. It is furthermore clear that the number of terms converges after approx. $\nu = 10$.

In Figure 3 sample paths of the corresponding Gaussian stochastic processes are shown for different values of the truncation error e_S. Each sample path is created with all the three correlation structures in the time $t \in [0, 5]$, but only $t \in [0, 0.1]$ is shown to better visualize the local characteristic of the samples. This Figure shows how the sample path from the exponential correlation exhibits non-negligible high frequency oscillations and noise when compared with the other two correlations when lower values of e_S are used. This is a direct result of the slower convergence of the single exponential kernel in energy content, which in it's turn is related to the non-differentiability of R_{ff} at zero lag. As pointed out in the literature, these high-frequency oscillations potentially impact the engineering analysis affected by the properties modeled with this kernel.

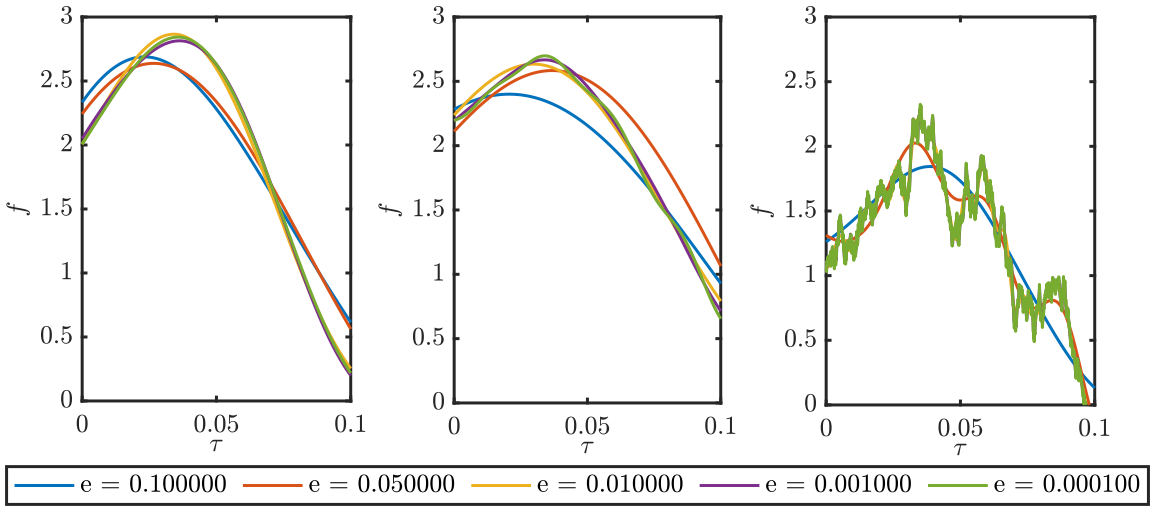

Figure 3: Sample paths of a one-dimensional Gaussian stochastic process, where the auto-correlation is governed by a Squared exponential (left), Modified exponential (middle) and Single exponential (right) kernel function, for different values of the truncation error.

3.2. Karhunen-Loève expansion

The advantage of using the modified exponential kernel over a single exponential one in terms of required terms in the Karhunen-Loève expansion has been illustrated in [16]. In this section, additional insights into this topic are attempted. In particular, it is shown that the reduction in the requisite number of stochastic terms holds consistently for the entire process series expansion. Further, this property also holds for a wide range of correlation length values. Figure 4 shows the convergence of the mean error variance as a function of the number of terms that are retained in the KL expansion for the same stochastic process considered in Section 3.1. Herein, the solution of the Fredholm integral equation in Eq. 19 is obtained using a Galerkin procedure with Legendre basis functions. Clearly, the convergence of the mean error variance corresponding to the squared exponential process is the fastest of the three considered auto-correlation functions. These results further confirm the findings of [16], namely that the modified exponential kernel converges faster than the single exponential kernel when considering the KL expansion for a wide range of correlation length values. This can be also explained by the differentiability of the auto-correlation function at zero-lag.

3.3. AR model representation

For the study of the applicability of the considered auto-correlation functions in conjunction with an AR representation, an analytical approach is used. In particular, the required AR models are derived based on the considered auto-correlation functions.

Regarding the single exponential covariance kernel $R_{ff}^{0.5}(\tau)$, it can be shown that an AR(1) process, i.e., an AR process with $m = 1$ is capable of directly representing a Gaussian process with $R_{ff}^{0.5}(\tau)$ [19].

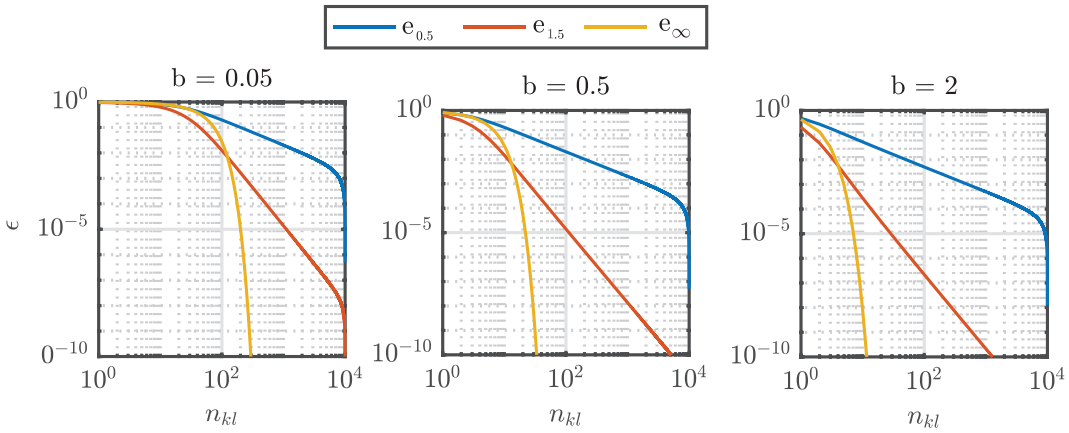

Figure 4: Convergence of the mean error variance with respect to the number of terms in the KL Expansion for the three considered auto-correlation kernels.

To capture this, write out Eq. (23) for $m = 1$ and subtract $f(t, \theta)$ from both sides. That is,

$$[f(t+1,\theta) - f(t,\theta)] + (1-a)f(t,\theta) = b_0 w(t,\theta). \tag{36}$$

The associated first-order differential equation to this finite-difference equation is

$$\frac{d}{dt}f(t,\theta) + \alpha f(t,\theta) = b_0 w(t,\theta), \tag{37}$$

which can be interpreted as a linear model that links $f(t, \theta)$ to a white-noise excitation. In the limit state for infinitesimally small τ, the transfer function corresponding to Eq.(37) is

$$H(\omega) = \frac{1}{i\omega + \alpha}, \tag{38}$$

that in combination with a constant spectral density S_0 gives rise to the power spectral density $S_{ff}(\omega)$:

$$S_{ff}(\omega) = \frac{S_0}{\omega^2 + \alpha^2}, \tag{39}$$

for $f(,\omega)$. This can be related through Eq. (8) to the auto-correlation function:

$$R_{ff}(\tau) = 1 \exp(-|\tau|\alpha), \tag{40}$$

which corresponds to a single exponential auto-correlation function.

Following a similar procedure, it can be shown that an AR(1) model of the following form:

$$f(t,\theta) = a\,[f(t-1,\theta) + f(t+1,\theta)] + b_o 2(t,\theta) \tag{41}$$

corresponds to a stationary Gaussian process with power spectral density:

$$S_{ff}(\omega) = \frac{4\alpha^3}{\pi(\omega^2 + \alpha^2)^2}, \tag{42}$$

and hence with auto correlation function

$$R_{ff}(\tau) = \exp(-\alpha|\tau|)(\alpha|\tau| + 1), \tag{43}$$

that corresponds to the modified exponential kernel. For the squared exponential auto-correlation function, a one-on-one exact relationship with a corresponding AR model is not trivial to establish and requires the solution of the Yule-Walker equations. This falls outside the scope of this paper.

4. Concluding remarks

In this paper, certain aspects relating to the mathematical behavior of common auto-correlation functions have been studied. Specifically, the convergence of the spectral density of the process to zero as the frequency tends to infinity has been examined. In particular, attention has been focussed on the comparison of the spectral convergence of functions that are differentiable at zero-lag versus those that are not-differentiable. In this regard, some selected functions from the Whittle-Matérn family were considered: the exponential, modified exponential and squared exponential function. This family has the appealing feature that the differentiability of the sample-paths is tuneable by tuning the differentiability of the auto-correlation function. The most popular member of this family is the single exponential auto-correlation function due to the availability of analytical solutions. However, as explained, the resulting sample paths are non-differentiable and the convergence of the stochastic representation is conparatively slow when compared to other functions. Of this family of auto-correlation functions, the squared exponential auto-correlation function was found to be the most efficient in terms of convergence properties. However, both the lack of analytical solutions, as the infinite differentiability of the sample paths make its application questionable from an application and physical standpoint.

It has been shown, both analytically and numerically, that the number of stochastic components required to represent a stochastic process with the single exponential kerne is considerably larger when compared to a modified or squared exponential kernel. This statement holds for both stochastic spectral representation methods, as well as for the well-known Karhunen-Loève series expansion. In this context, note that the single exponential kernel is not differentiable at zero lag, whereas, the modified and squared exponential kernel are completely differentiable. Squared exponential auto-correlation functions on the other hand show the fastest convergence. However, their infinite differentiability poses impor-

tant limitations with respect to their physical interpretation. It is found that auto-correlations from the Whittle-Matérn family with half-integer values pose an interesting trade-off between efficiency and physical interpretability. Of this family, the so-called modified exponential auto-correlation function stands out due to the availability of analytical solutions to the Fredholm integral equation of the second kind.

Further, in the paper AR models have been considered, for which it has been shown that for both a single and modified exponential kernel, a closed form expression for an AR(1) model can be derived. This proves that AR models are highly suited to represent these types of stochastic processes. Further work beyond this initial study can explore the relationship between the differentiability of the auto-correlation function at zero lag, and the convergence of the corresponding spectral density to zero as the frequency tends to infinity.

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