

A representation theorem for stochastic processes with separable covariance functions, and its implications for emulation

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Abstract

Many applications require stochastic processes specified on two- or higher-dimensional domains; spatial or spatial-temporal modelling, for example. In these applications it is attractive, for conceptual simplicity and computational tractability, to propose a covariance function that is *separable*; e.g. the product of a covariance function in space and one in time. This paper presents a representation theorem for such a proposal, and shows that all processes with continuous separable covariance functions are second-order identical to the product of second-order uncorrelated processes. It discusses the implications of separable or nearly separable prior covariances for the statistical emulation of complicated functions such as computer codes, and critically reexamines the conventional wisdom concerning emulator structure, and size of design.

KEYWORDS: Stochastic process, spatial-temporal modelling, k th-order uncorrelated families, computer experiment, emulator

1 Introduction

Many statistical applications require covariance functions expressed over two or more dimensions. Spatial and spatial-temporal modelling are obvious applications, where the number of dimensions is typically two or three. Emulating

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deterministic functions with Gaussian processes, part of the general field of computer experiments (see, e.g., Santner et al., 2003), will often require five or ten dimensions—sometimes more.

Covariance functions, being non-negative definite symmetric, are highly structured, and one does not hit upon them by chance. In some cases, domain symmetry can be used to simplify the problem. Thus, if two of the dimensions are spatial and there is no preferential direction, then an isotropic covariance function can be defined on the basis of distance alone, reducing a two-dimensional problem to a one-dimensional one. This device is not available in computer experiments, where each dimension represents an input to the code, and there is no reason why two different inputs should even have the same units, let alone have a symmetric effect on the code output.

Therefore it is often attractive to take advantage of the general result that a p -dimensional covariance function can be built up as the product of p one-dimensional covariance functions. This product form is termed a ‘separable covariance function’. At the very least, all such covariance functions satisfy the necessary conditions of being non-negative definite symmetric. There are other advantages of this approach, discussed in section 2. Section 2 also presents the restrictions on the conditional and marginal correlation functions which follow directly from the separability of the covariance function.

Of more general interest is whether a separable covariance function provides any restrictions on the underlying stochastic process itself. Section 3 provides a complete answer to this question, giving a representation theorem on the underlying process which holds if and only if the covariance function is separable. There is also a close relationship between separable covariance functions and a product form for the underlying process, e.g. the situation in which $F(x, y)$ might be written as $F_x(x) \times F_y(y)$. It is well-known that if F_x and F_y are probabilistically independent, then F has a separable covariance function. Section 4 provides a converse result, in terms of second-order properties. This allows us to ‘explain’ the restrictions of the conditional and marginal correlations in terms of the product form for F .

The main implications of these results are for the emulation of complex computer codes, discussed in section 5. Here it is completely standard to use separable covariance functions as a large component of the emulator, and, indeed, the conventional wisdom is that the entire emulator may be constructed in this fashion. This advice is critically analysed using the representation theo-

rem, allowing us to identify why it might perform well in many applications, and when it breaks down. Finally, section 6 concludes with a brief summary.

2 Separable covariance functions

Consider a real-valued stochastic process F with domain $\mathcal{X} \times \mathcal{Y}$. The covariance function of F is denoted

$$\kappa\{(x, y), (x', y')\} := \text{cov}\{F(x, y), F(x', y')\}. \quad (1)$$

If F has a separable covariance function then κ factorises into the product of a function in (x, x') and a function in (y, y') , denoted

$$\kappa\{(x, y), (x', y')\} = \kappa_x(x, x') \kappa_y(y, y'). \quad (2)$$

For clarity, in this paper this is stated as “the covariance function is separable”, noting that separability as used here should not be confused with the property of separability of metric spaces (see, e.g., Kreyszig, 1978, chapter 1) and the related property of separability of stochastic processes (see, e.g., Loève, 1960, sec. 35). Nor should it be confused with the notion of separability used in Genton and Perrin (2004), which considers the case where $\kappa_x(x, x')$ can be written as $r_1(x)r_2(x')$.

There are two principal advantages when the covariance function is separable. First, it can be hard to specify a non-negative definite function jointly over a two- or higher-dimensional domain, and it is very useful that such functions can be built up as products of simpler functions. This is particularly true in the case where the covariance function contains parameters that need to be estimated, because in this case the parameters separate cleanly into x -parameters and y -parameters. This is the motivation for using separable covariance functions for emulating complex computer codes, as discussed in more detail in section 5. Note that separability of the covariance function is not preserved under rotation; it insists on a preferential set of directions in the input space, aligned with the axes. The exception is the squared exponential correlation function with a common correlation length, i.e. (for the stationary

case)

$$\begin{aligned}\kappa\{(x, y), (x', y')\} &= \sigma^2 \exp\{-\theta^2(x - x')^2\} \exp\{-\theta^2(y - y')^2\} \\ &= \sigma^2 \exp\{-\theta^2 h[(x, y), (x', y')]^2\}\end{aligned}\quad (3)$$

where $h[\cdot, \cdot]$ denotes Euclidean distance. This is a very popular choice in computer experiments, originating in the papers of Sacks et al. (1989) and Currin et al. (1991), although different correlation lengths are used in each direction.

Second, in situations where the process F is observed on a grid, the variance matrix of the observations has Kronecker product form, and hence is much more easily inverted. If the grid has $m \times n$ points, then this converts an $O((m+n)^3)$ calculation into a $O(m^3) + O(n^3)$ calculation. This result is widely used in space-time kriging. Genton (2007), for example, presents a method for finding separable approximations to space-time variance matrices, while Li et al. (2007) present a non-parametric test for separability (see also Li et al., 2008). Gneiting et al. (2007) review general approaches to modelling spatial-temporal processes, including an example of fitting a separable covariance function and a comparison with other structured approaches.

However, there is a price for these benefits: separability of the covariance function is a strong constraint on the nature of F . In the supporting material for Kennedy and O'Hagan (2001), O'Hagan (1998) considers the implication of a separable covariance function for the conditional covariance of a Gaussian process, namely that

$$\text{cov}\{F(x, y), F(x', y') \mid F(x', y)\} = 0 \quad (4)$$

(see Figure 1). O'Hagan is able to provide a representation theorem for the covariance function of processes having this type of conditional covariance structure. This is related to the separability of the covariance function of a transformed process. A similar result to (4) holds in the more general Bayes linear case, where conditioning is replaced by projection (Goldstein and Wooff, 2007).

Cressie and Huang (1999) consider the implications of the separability of the covariance function when F is a spatial-temporal process. In general,

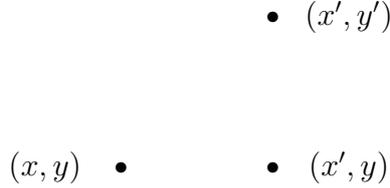


Figure 1: $\text{cov}\{F(x, y), F(x', y') \mid F(x', y)\} = 0$ when the covariance function is separable.

separability of the covariance function implies that

$$\text{corr}\{F(x, y), F(x, y')\} = \frac{\kappa_y(y, y')}{\sqrt{\kappa_y(y, y) \kappa_y(y', y')}} \quad (5)$$

for all values of x . In other words, if x represents location and y represents time, then the temporal correlation structure cannot vary spatially. Cressie and Huang conclude that this separable covariance function “does not model space-time interaction” (p. 1331). A general concern about the absence of interaction has led to substantial effort being devoted to developing flexible and parametric stochastic processes with non-separable covariance functions (see, e.g., Cressie and Huang, 1999; Iaco et al., 2002; Gneiting, 2002; Stein, 2005; Kent et al., 2011).

Note, to avoid confusion, that this type of interaction is different from that modelled in decompositions of the type

$$f(x, y) = \alpha_0 + \alpha_1(x) + \alpha_2(y) + \alpha_{12}(x, y) \quad (6)$$

where f is a deterministic function (see, e.g., Owen, 1997). Here $\alpha_{12}(x, y)$ would be the interaction term. But F is a stochastic process, *not* a deterministic function. If f is a realisation of F then it will almost certainly have an α_{12} term. When talking of interactions in the stochastic process F , we need to refer to the properties of the distribution of F . Hence, if the focus is on second-order properties, we must consider interactions in terms of the

properties of the covariance and correlation functions. So, ‘no interactions in F ’ means that the correlation function of F is invariant to the value of x when considered along y (and *vice versa*).

3 Representation theorem

These preliminaries are from Loève (1960), chapter 10. Consider the set of all real random quantities with finite second moments, denoted F, F', \dots . Identify each random quantity with its equivalence class, where two random quantities are equivalent if they are identical, or differ only on a set of measure zero. These equivalence classes represent points in a Hilbert space, with inner product $\langle F, F' \rangle = \mathbf{E}(FF')$. For simplicity, and without loss of generality, consider all random quantities to be centred, so that the inner product represents the covariance, and orthogonal random quantities are uncorrelated. In this case the Hilbert space has norm and distance

$$\|F\| = \text{sd}(F) \quad \text{and} \quad d(F, F') = \text{sd}(F - F'),$$

where ‘sd’ denotes ‘standard deviation’. (These are just for orientation, they are not used in what follows.) Convergence in this Hilbert space is equivalent to convergence in quadratic mean, written here as

$$F^{(n)} \xrightarrow{\text{q.m.}} F \iff \mathbf{E}\{(F^{(n)} - F)^2\} \rightarrow 0. \quad (7)$$

Now within this Hilbert space consider a family of random quantities indexed by the tuple $(x, y) \in \mathcal{X} \times \mathcal{Y}$, where \mathcal{X} and \mathcal{Y} are both closed and bounded intervals of the real line. This family is termed a *stochastic process*. The covariance function of this stochastic process is

$$\kappa\{(x, y), (x', y')\} = \langle F(x, y), F(x', y') \rangle = \mathbf{E}\{F(x, y)F(x', y')\} \quad (8)$$

where, necessarily, κ is symmetric and non-negative definite. This paper investigates the consequence of this covariance function having the separable form given in (2), where, necessarily, both κ_x and κ_y are symmetric and non-negative definite.

Consider the sequence of stochastic processes indexed by n ,

$$F^{(n)}(x, y) = \sum_{i=1}^n \sum_{j=1}^n Z_{ij} g_i(x) h_j(y) \quad (9)$$

where the $\{Z_{ij}\}$ are orthonormal, i.e. $\mathbb{E}(Z_{ij}) = 0$, $\mathbb{E}(Z_{ij}Z_{i'j'}) = \delta_{ii'}\delta_{jj'}$ (δ is the Kronecker delta), and where the functions in $\{g_i\}$ and $\{h_j\}$ are continuous on \mathcal{X} and \mathcal{Y} , respectively. While there are no restrictions on $\{g_i\}$ and $\{h_j\}$ beyond continuity, there is no loss of generality in removing obvious redundancies. Therefore we may assume that the functions are mutually scaled so that $\|g_1\|^2 := \int g_1(x)^2 dx = 1$, although in fact this property is not used below. Also, we could remove functions that are identically zero, but keeping them in allows us to use just one limit for both i and j , simplifying the notation slightly.

The following two propositions together establish the equivalence between (9) and separability of the covariance function of F .

Proposition 1. *If n is finite or $F^{(n)} \xrightarrow{q.m.} F$ uniformly on $\mathcal{X} \times \mathcal{Y}$ then F has a continuous separable covariance function.*

Proof. Only the $n \rightarrow \infty$ result needs to be proved; n finite is a special case. The convergence of $F^{(n)}(x, y)$ to $F(x, y)$ for each (x, y) implies the pointwise convergence of the covariance functions; this is a standard continuity property of Hilbert spaces (see, e.g., Kreyszig, 1978, Lemma 3.2-2). Thus

$$\kappa\{(x, y), (x', y')\} = \lim_{n \rightarrow \infty} \kappa^{(n)}\{(x, y), (x', y')\} \quad (10)$$

for each (x, y) and (x', y') , where

$$\begin{aligned} \kappa^{(n)}\{(x, y), (x', y')\} &= \langle F^{(n)}(x, y), F^{(n)}(x', y') \rangle \\ &= \sum_{i=1}^n \sum_{j=1}^n g_i(x) h_j(y) g_i(x') h_j(y') \\ &= \sum_{i=1}^n g_i(x) g_i(x') \sum_{j=1}^n h_j(y) h_j(y') \\ &= \kappa_x^{(n)}(x, x') \kappa_y^{(n)}(y, y'), \end{aligned} \quad (11)$$

say, where the second line follows from the orthonormality of the $\{Z_{ij}\}$, and the functions $\kappa_x^{(n)}$ and $\kappa_y^{(n)}$ in the final line are clearly symmetric and non-

negative definite (this proves the n finite case). The separability of κ follows immediately.

For continuity, $\kappa^{(n)}$ is uniformly convergent, because all random quantities have finite second moments and $F^{(n)}$ is uniformly convergent. As $\kappa^{(n)}$ is continuous, uniform convergence implies that the limit κ is continuous. \square

Note that $\{Z_{ij}\}$ must be uncorrelated, but the components do not have to be standardised. However, if the variance of Z_{ij} depends on (i, j) , then it must factorise as $\lambda_i \gamma_j$ in order for F to have a separable covariance function; but in that case the terms in the variance can be absorbed into $\{g_i\}$ and $\{h_j\}$.

The second proposition asserts the converse.

Proposition 2. *If F has a continuous separable covariance function, then there exist sets of continuous functions $\{g_i\}$ and $\{h_j\}$ in (9) such that $F^{(n)} \xrightarrow{\text{q.m.}} F$ uniformly on $\mathcal{X} \times \mathcal{Y}$.*

Proof. This follows from an application of Mercer's Theorem and the Karhunen-Loève expansion; these are both derived in Ash (1965, Appendix).

Mercer's Theorem states that if κ_x is continuous on $\mathcal{X} \times \mathcal{X}$ then

$$\kappa_x(x, x') = \lim_{n \rightarrow \infty} \sum_{i=1}^n \lambda_i \psi_i(x) \psi_i(x') \quad (12)$$

where $\{\lambda_i\}$ are the positive eigenvalues of κ_x and $\{\psi_i(x)\}$ are the corresponding eigenfunctions, which are continuous on \mathcal{X} ; the convergence is absolute and uniform on $\mathcal{X} \times \mathcal{X}$. Similarly, for κ_y ,

$$\kappa_y(y, y') = \lim_{n \rightarrow \infty} \sum_{j=1}^n \gamma_j \phi_j(y) \phi_j(y'). \quad (13)$$

If the covariance function κ is separable, then, in obvious notation,

$$\begin{aligned} \kappa\{(x, y), (x', y')\} &= \kappa_x(x, x') \kappa_y(y, y') \\ &= \left(\lim_{n \rightarrow \infty} \kappa_x^{(n)}(x, x') \right) \left(\lim_{n \rightarrow \infty} \kappa_y^{(n)}(y, y') \right) \\ &= \lim_{n \rightarrow \infty} \left(\kappa_x^{(n)}(x, x') \kappa_y^{(n)}(y, y') \right) \\ &= \lim_{n \rightarrow \infty} \sum_{i=1}^n \sum_{j=1}^n \lambda_i \gamma_j \psi_i(x) \phi_j(y) \psi_i(x') \phi_j(y'). \end{aligned} \quad (14)$$

The series for κ is absolutely convergent because both κ_x and κ_y are absolutely

convergent (according to Mercer's Theorem). The series is uniformly convergent because both κ_x and κ_y are uniformly convergent (according to Mercer's Theorem) and bounded.

It is easy to verify that, for every i and j , $\lambda_i\gamma_j$ is a positive eigenvalue for κ , and $\psi_i(x)\phi_j(y)$ a corresponding eigenfunction. Thus we can apply the Karhunen-Loève (KL) expansion. Therefore, define

$$Z'_{ij} := \iint_{\mathcal{X} \times \mathcal{Y}} F(x, y) \psi_i(x) \phi_j(y) \, dx \, dy \quad (15)$$

for which $\mathbb{E}(Z'_{ij}Z'_{i'j'}) = \lambda_i\gamma_j\delta_{ii'}\delta_{jj'}$. It follows that if

$$F^{(n)}(x, y) := \sum_{i=1}^n \sum_{j=1}^n Z'_{ij} \psi_i(x) \phi_j(y), \quad (16)$$

then $F^{(n)} \xrightarrow{\text{q.m.}} F$ uniformly on $\mathcal{X} \times \mathcal{Y}$. Eq. (16) has the required form, with $Z_{ij} := Z'_{ij}/\sqrt{\lambda_i\gamma_j}$, $g_i(x) := \sqrt{\lambda_i}\psi_i(x)$, and $h_j(y) := \sqrt{\gamma_j}\phi_j(y)$. \square

Putting these two Propositions together, we can conclude the following.

Proposition 3 (Representation theorem). *F has continuous separable covariance function if and only if it can be represented as $F^{(n)}$ in (9), or as its limit when $n \rightarrow \infty$.*

This result is straightforward to derive in the special case where both \mathcal{X} and \mathcal{Y} are finite, and F is Gaussian. The Hilbert space approach used here is necessary to lift these two restrictions. In the case where F is a Gaussian process, the $\{Z_{ij}\}$ are *independent* standard Gaussian quantities, and the convergence of $F^{(n)}$ to F at each (x, y) is almost sure; see, Loève (1960, p. 485), or Ash (1965, p. 279).

Generalisations. Two generalisations are immediate. First, the result is a special case of a more general result for complex F , for which the inner product is $\langle F, F' \rangle = \mathbb{E}(F\bar{F}')$, where \bar{F}' is the complex conjugate of F' . It is the complex case that is treated in Loève (1960, ch. 10). Second, the result extends to any domain of F with a finite number of dimensions, as can be seen by inspecting the two proofs. To apply directly the results, the domain must be the product of closed and bounded intervals of the real line. However, more general versions of Mercer's Theorem are available; see, e.g., Ferreira and Menegatto (2009).

4 Products of processes

This section considers the special case in which F can be written as the product of two stochastic processes, one in x and one in y :

$$F(x, y) = F_x(x) F_y(y). \quad (17)$$

First, though, it is necessary to digress briefly on independence and ‘uncorrelation’, where this neologism (which is not original) is shorter and also more direct than ‘lack of correlation’.

4.1 Probabilistic independence and uncorrelation

Consider two families of random quantities, $\{X_i\}$ and $\{Y_j\}$. Following Whittle (2000, ch. 4, sec. 3), we say that these two families are probabilistically independent if

$$E [g(\{X_i\}) \times h(\{Y_j\})] = E [g(\{X_i\})] \times E [h(\{Y_j\})] \quad (18)$$

for all scalar functions g and h for which the righthand product is defined. This property is far too strong (i.e. restrictive) for results that concern second-order properties such as covariances. But, as shown below, simple uncorrelation is too weak. Therefore consider an indexed sequence of properties that runs from one to the other.

Definition 4. *Two families of random quantities $\{X_i\}$ and $\{Y_j\}$ are k th-order uncorrelated if*

$$E \left(\prod_i X_i^{a_i} \times \prod_j Y_j^{b_j} \right) = E \left(\prod_i X_i^{a_i} \right) \times E \left(\prod_j Y_j^{b_j} \right)$$

for all tuples $\{a_i\}$ and $\{b_j\}$ comprising non-negative integers whose sum does not exceed k .

If the families are first-order uncorrelated, then every X_i is uncorrelated with every Y_j , but nothing else is implied. At the other end of the scale, ($k \rightarrow \infty$)th-order uncorrelated implies probabilistic independence, if g and h are restricted to functions with well-behaved Taylor Series expansions. Therefore, statements of probabilistic independence are stupendously stronger than those concerning second-order uncorrelation, noting that the set of second-degree

monomials is a vanishingly small fraction of the set of all possible functions used in (18).

4.2 Products of processes

Now we return to F s that are products of processes. It is a standard and immediate result that if F_x and F_y are probabilistically independent then F has a separable covariance function; see, e.g., the textbooks of Stein (1999, sec. 2.3), Santner et al. (2003, sec. 2.3), or Rasmussen and Williams (2006, sec. 4.2). But in fact probabilistic independence is far too strong: all that is required for F to have a separable covariance function is that the stochastic processes F_x and F_y are second-order uncorrelated, so that

$$\mathbf{E}\{F(x, y) \times F(x', y')\} = \mathbf{E}\{F_x(x)F_x(x')\} \times \mathbf{E}\{F_y(y)F_y(y')\}. \quad (19)$$

One might imagine that the class of processes with separable covariance functions contains many processes that cannot be represented as products of second-order uncorrelated processes. In general this is correct, but if we consider only the second-order properties of the process then in fact the two classes are equivalent.

Proposition 5. *Every stochastic process with a separable covariance function is second-order identical to the product of second-order uncorrelated processes.*

Proof. It suffices to consider processes indexed by the tuple (x, y) , as the extension to more than two indices is immediate, so let $F(x, y)$ be a stochastic process with a separable covariance function. By Proposition 3, $F(x, y)$ can be represented as (9), or its limit as $n \rightarrow \infty$. Now replace each Z_{ij} in (9) with $Z_i Z'_j$. In order to preserve the mean and covariance functions, these $\{Z_i\}$ and $\{Z'_j\}$ must satisfy $\mathbf{E}(Z_i Z'_j) = 0$ and $\mathbf{E}(Z_i Z_{i'} Z'_j Z'_{j'}) = \delta_{ii'} \delta_{jj'}$. The natural solution is that $\{Z_i\}$ are orthonormal, $\{Z'_j\}$ are orthonormal, and $\{Z_i\}$ and $\{Z'_j\}$ are second-order uncorrelated. At this point, the original $F^{(n)}$ has been replaced by a new function with the same (separable) covariance function. But this new function factorises into the product

$$\left(\sum_{i=1}^n Z_i g_i(x) \right) \times \left(\sum_{j=1}^n Z'_j h_j(y) \right)$$

and these two functions are second-order uncorrelated, because $\{Z_i\}$ and $\{Z'_j\}$

are second-order uncorrelated. \square

It is very important to appreciate that $\{Z_{ij}\}$ and $\{Z_i Z'_j\}$ do not have the same joint distribution, and so replacing the n^2 terms $\{Z_{ij}\}$ with the $2n$ terms $\{Z_i Z'_j\}$ changes the stochastic process to something other than F . But this new process has the same (zero) mean, and the same (separable) covariance function, and so it is identical in its second-order properties. In general, the step where we replace $\{Z_{ij}\}$ with $\{Z_i Z'_j\}$ shows that there are an infinite number of possible candidates for $F_x(x)F_y(y)$.

To give an important example of the difference between $F(x, y)$ with a separable covariance function and its second-order identical $F_x(x)F_y(y)$, consider the case where F is a Gaussian process. In this case, as mentioned in Section 3, $\{Z_{ij}\}$ are IID standard Gaussian random quantities. But if $Z_{ij} = Z_i Z'_j$ then Z_i and Z'_j *cannot* be Gaussian random quantities, and in this case the implied F_x and F_y are *not* Gaussian processes, and nor is the product $F_x(x)F_y(y)$. So a second-order identical process for a Gaussian process with a separable covariance function is *not* a Gaussian process. It is a different stochastic process that just happens to coincide with $F(x, y)$ in its mean and covariance functions.

Proposition 5 provides the explanation for the strong constraints implied by a separable covariance function, presented in Section 2. Both (4) and (5) concern second-order properties, and, according to Proposition 5, at this level F will behave identically to the product of second-order uncorrelated processes. When considering $F(x, y)$ along y at a given x , the product form shows that the only effect of x is to provide an uncertain scaling term $F_x(x)$, which cancels in the correlation, hence (5). The heuristic explanation of (4) is that under a product structure for F no information passes along diagonals in (x, y) . This emphasises the point made in section 2, that a separable covariance function insists on a preferential set of directions in the input space, aligned with the axes.

Figure 2 gives a summary of the results in this paper.

5 Implications for emulators

An emulator is a statistical representation of a function; denote this function as f , assuming, for simplicity, that it is a deterministic function of two arguments x and y . Typically, f would be a computer code and $f(x, y)$ would be expensive to run. An emulator offers the opportunity to augment the ensemble

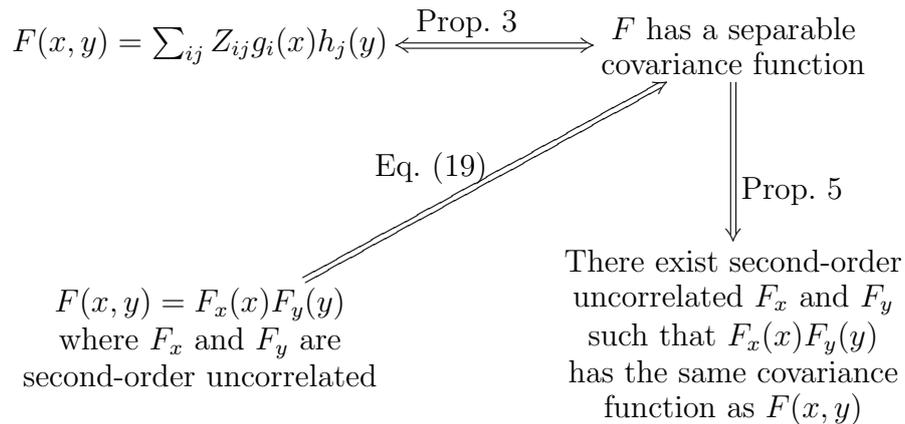


Figure 2: A summary of the results in this paper.

of runs with additional judgements, for example about the monotonicity and smoothness of f . In the Bayesian approach to emulation initiated by Currin et al. (1991), one proposes a prior stochastic process for f , F say, which represents these additional judgements, and then conditions this process on the ensemble of runs.

In the Bayesian approach, the prior stochastic process for f is written as the sum of two uncorrelated components, a set of regression terms and a ‘residual’:

$$F(x, y) = \sum_i \beta_i r_i(x, y) + E(x, y) \quad (20)$$

where $\{\beta_i\}$ are unknown regression coefficients, $\{r_i\}$ are specified regressors, and $E(x, y)$ is mean-zero stochastic process (see, e.g. Santner et al., 2003, ch. 2). The separability of the covariance function of E was proposed in the early papers of Sacks et al. (1989) and Currin et al. (1991), and is a crucial feature in screening experiments designed to identify important inputs (Welch et al., 1992). It is now a standard choice, although Rougier et al. (2009) provide an example where prior information about f leads to a non-separable covariance function for E . In multivariate emulation, Rougier (2008) proposed an E which is separable between inputs and outputs, but not necessarily separable within the inputs.

5.1 The role of the regressors

According to the representation theorem, including regressors with $\text{var}(\beta_i) > 0$ is sufficient to prevent the covariance function of F from being separable. However, conventional wisdom originating in the experiments of Welch et al. (1992, p. 16) suggests that regression terms beyond a mean effect are not required (see also Steinberg and Bursztyn, 2004). Furthermore, the mean effect is often estimated (e.g. with its updated mean) and then plugged in. This leaves us with a prior emulator with mean zero and a separable covariance function, or ‘nearly separable’ if E accounts for most of the prior variance of F .

This is where Proposition 5 comes in. If our judgements only extend to second-order—and it would be unusual to have higher-order judgements about a complex computer code—then this is akin to asserting that, as far as our judgements about the code are concerned, there exist functions f_x and f_y for which $f(x, y) \approx f_x(x)f_y(y)$.

Now consider the implications of this. Were I to believe that there existed f_x and f_y such that $f(x, y) \approx f_x(y)f_y(y)$ then I would see little need for multi-parameter perturbations in the ensemble of training runs. Instead, for an efficient design I would fix x at x_0 , and run the sequence $(x_0, y_1), (x_0, y_2), \dots$; this would give me an accurate picture of the function f_y up to the multiplicative constant $f_x(x_0)$. Then I would reverse the process, fixing y at y_0 .

But would anyone advocate this kind of experiment for a complex computer code? I doubt it: the standard experimental designs are multi-parameter perturbations such as Latin Hypercube Designs (LHDs, see, e.g., Santner et al., 2003, ch. 5). Now a LHD will perform no worse than single parameter perturbations in the case where $f(x, y) \approx f_x(x)f_y(y)$, and would be preferred for robustness. But few if any statisticians working in the field of computer experiments would believe that a LHC would perform *no better* than single parameter perturbations. And yet that is what is suggested by a prior for f with a separable covariance function.

This line of thought sheds some light on the $n = 10p$ rule (n being the number of runs, and p being the number of inputs), which has recently been reviewed, investigated, and advocated by Loepky et al. (2009, “a reasonable rule of thumb for an initial experiment”, p. 374). *A priori*, this seems rather a small number of runs, especially for more than six inputs (implying more corners than runs, so that it is impossible for the convex hull of the ensemble

to fill the input space). And so $n = 10p$ is an interesting and potentially very useful rule. However, its linearity in p is suggestive: this is exactly the kind of rule that would be appropriate if $f(x, y) \approx f_x(x)f_y(y)$. The value 10 sounds about right to fit a smooth curve for each of f_x and f_y .

A close examination of the Loepky et al. experiment (their section 5) reveals that all candidate functions on which this rule was evaluated were sampled from a Gaussian process with a separable covariance function. So this experiment only ever considered the case of functions that were second-order identical to $f_x(x)f_y(y)$. We must conclude that this experiment provides no support for $n = 10p$ in the general case.

5.2 The effect of conditioning

Let us put prior judgements aside, in favour of pragmatism. Ideally, the separability of the prior covariance function for F would be a property similar to prior stationarity: a convenient way to specify a stochastic process with a small number of hyperparameters, with possibly undesirable properties that are erased by conditioning on one or more members of the ensemble. This is in fact the case, as can easily be seen from the representation theorem. Conditioning the prior for F on a value for $f(x, y)$ induces a linear constraint across the $\{Z_{ij}\}$ in (9), and consequently the components of $\{Z_{ij}\}$ can no longer be uncorrelated.

Thus the use of a separable or nearly separable prior covariance function for the emulator is defensible even though we judge that $f(x, y)$ is much more complicated than $f_x(x)f_y(y)$, in the same way that the use of a stationary covariance function is defensible even though we are much more uncertain about f around the edges of the input space than in the middle (say).

Having said that, my personal view is that we should always include a reasonable number of regression terms with uncertain coefficients in the emulator, a point made in Rougier et al. (2009). Conditioning will erase second-order properties of the residual E in and around the convex hull of the ensemble of runs. However, away from this convex hull the updated E will revert gradually to its prior formulation. If we can be confident that the ensemble is large enough to fill the input space, then the prior choices we make for E (stationarity, separability of the covariance function) will not matter in practice.

But for really large applications, including many environmental science applications like climate modelling, long run times and large input spaces can

imply that most of the input space is outside the convex hull of the ensemble. In this case, an emulator without regression terms could revert to its prior around the edges of the input space, but an emulator with regression terms is able to carry the information in the ensemble all the way to the edges of the input space. An updated emulator without regressors would revert to a separable covariance function. It is not clear to me what the effect of this would be, e.g. in summaries that integrate over the input space (Oakley and O’Hagan, 2004). But since the representation theorem shows that separability of the covariance function is a strong constraint on the structure of F , it seems wise not to impose it *a priori*.

6 Summary

Probabilistic inference is extremely demanding, and we often find ourselves making pragmatic choices where our judgements are only partial. This is certainly the case in a fully probabilistic inference, but it is also true at second-order. This paper has examined choices about covariance functions, and, in particular, the effect of the pragmatic choice to treat the covariance function as separable—i.e. having a product structure. It is well-known that such a choice constrains conditional variances and marginal correlations. What was not known was the relationship between this choice and the underlying stochastic process. This paper has completely resolved this issue, by providing a representation theorem for stochastic processes with separable covariance functions. Briefly, the centred process F has a separable continuous covariance function *if and only if* it can be represented as $\sum_{ij} Z_{ij} g_i(x) h_j(y)$ where $\{Z_{ij}\}$ is a collection of mean zero, variance one, uncorrelated quantities, and $\{g_i\}$ and $\{h_j\}$ are collections of continuous functions.

One use of this representation theorem is to provide a partial converse to the standard result that if $F(x, y)$ can be represented as $F_x(x)F_y(y)$, where F_x and F_y are probabilistically independent, then F has a separable covariance function. By substituting $\{Z_i Z'_j\}$ for $\{Z_{ij}\}$ in the representation theorem it was shown that the second-order properties of an F with separable covariance function can be duplicated by the product of two uncorrelated processes. To get the most general statement of the converse result it was necessary to introduce ‘ k -fold uncorrelated’ families of random variables. This converse result clarifies the properties of stochastic processes with separable covariance func-

tions, by envisaging such processes as the product of uncorrelated processes. The theoretical results of this paper are summarised in Figure 2.

The main relevance of these results is in the emulation of complex computer simulators, part of the statistical field of computer experiments. In this application it is completely standard to represent a large chunk of the prior variance of the emulator in the form of a stochastic process with a separable covariance function. Indeed, the conventional wisdom is that the whole prior may be thus represented. The results of this paper suggests that this conventional choice is in fact highly restrictive, being equivalent to the judgement that the simulator $f(x, y)$ could be approximated by the product $f_x(x)f_y(y)$. This has practical implications for experimental design, and casts doubt upon the provenance of the $n = 10p$ rule for selecting sample size. The representation theorem also shows that it is very easy to construct emulators which do not have separable covariance functions (by including regression terms with uncertain coefficients), for which there is no *a priori* restriction to $f(x, y) \approx f_x(x)f_y(y)$.

These new theoretical results notwithstanding, in many applications the use of a prior emulator with a separable covariance function is innocuous and will continue. This is because updating the emulator with one or more runs of the computer code will erase the separability of the covariance function, in the same way that other properties such as stationary are also erased. This is demonstrated through the representation theorem. The main concern is then for large experiments, where the ensemble of simulator runs does not fill the input space, and for which emulators based around a separable covariance function may revert to their prior at the edges and corners of the input space (remembering that a high-dimensional space is all edges and corners).

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