Analysis of parametric models
— linear methods and approximations*

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Abstract

Parametric models in vector spaces are shown to possess an associated linear map. This linear operator leads directly to reproducing kernel Hilbert spaces and affine- / linear- representations in terms of tensor products. From the associated linear map analogues of covariance or rather correlation operators can be formed. The associated linear map in fact provides a factorisation of the correlation. Its spectral decomposition, and the associated Karhunen-Loève- or proper orthogonal decomposition in a tensor product follow directly. It is shown that all factorisations of a certain class are unitarily equivalent, as well as that every factorisation induces a different representation, and vice versa.

A completely equivalent spectral and factorisation analysis can be carried out in kernel space. The relevance of these abstract constructions is shown on a number of mostly familiar examples, thus unifying many such constructions under one theoretical umbrella. From the factorisation one obtains tensor representations, which may be cascaded, leading to tensors of higher degree. When carried over to a discretised level in the form of a model order reduction, such factorisations allow very sparse low-rank approximations which lead to very efficient computations especially in high dimensions.

Key words: parametric models, reproducing kernel Hilbert space, correlation, factorisation, spectral decomposition, representation

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1 Introduction

Parametric models are used in many areas of science, engineering, and economics, etc. They appear in cases of design of some systems, where the parameters may be design variables of some kind, and the variation of the parameters may show different possibilities, or display the envelope of the system over a range of possible parameter values. Other possibilities arise when one wants to control the behaviour of some system, and the parameters are control variables. This is closely connected with situations where one wants to optimise the behaviour of some system more generally by changing some parameters. Another important area is where some of the parameters may be uncertain, i.e. they could be random variables, and with respect to these one wants to perform uncertainty quantification. Of course it is also possible that the parameter set has many-fold purposes, for example that some of the parameters model design variables, while others are uncertain, cf. [49].

Often the problem of having to deal with a parametric system is compounded by the fact that one also has to approximate the system behaviour through a reduced order model due to high computational demands of the full system. This reduced model then therefore becomes a parametrised reduced order model. The survey [3] and the recent collection [4] as well as the references therein provide a good view not only of reduced order models which depend on parameters, but also of parametric problems in general and some of the areas where they appear. So for further information on parametrised reduced order models and how to generate them we refer to these references.

Here, we want to concentrate on a certain topic illuminating the theoretical background of such parametrised models. This is the connection between separated series representations, associated linear maps, the singular value (SVD) and proper orthogonal decomposition (POD), and tensor products. This then immediately opens the connections to reduced order models and low-rank tensor approximations. It will be seen that the distribution of singular values of the associated linear map determines how many terms are necessary for a good approximation with a reduced order model. For higher order tensor representations in the context of hierarchical tensor approximations, it is the SVD structure of the tensor product splittings associated with the tree structure of the index set partitions.

Typically, the parameters are assumed to be tuples of independent real numbers, but here no assumptions are made about the parameter set. The geometry and topology of the parameter set is reflected by set of real functions defined on the parameter set, which can be viewed like co-ordinates in this context.

In some cases, like design evaluations and uncertainty quantification, the parameter set in itself is not important, but only the range or distribution of the parametric model. Here the analysis of the associated linear map allows the re-parametrisation of the parametric model with the parameters taken from a different set. The principal result is then that within a certain class of representations of parametric models and associated linear maps there is a one-to-one correspondence between separated series representations and factorisations of the associated linear map. But in general the representation through a linear map is much more general, and allows the modelling of weak or generalised models.

As a possible starting point to introduce the subject, assume that some physical system
is investigated, which is modelled by an evolution equation for its state:

\[
\frac{d}{dt}u(t) = A(q; u(t)) + f(q; t); \quad u(0) = u_0,
\]

where \( u(t) \in \mathcal{U} \) describes the state of the system at time \( t \in [0, T] \) lying in a Hilbert space \( \mathcal{U} \) (for the sake of simplicity), \( A \) is an operator modelling the physics of the system, and \( f \) is some external influence (action / excitation / loading). Assume that the model depends on some quantity \( q \), and assume additionally that for all \( q \) of interest the system Eq. (1) is well-posed. One part of these parameters \( q \) may describe the specific nature of the system Eq. (1), whereas another part of the parameters, here denoted by \( p \in \mathcal{P} \) has to be varied for one reason or another in the analysis.

One is often interested in how the system changes when these parameters \( p \) change. The parameter \( p \) can be for example

- just the quantity, \( p = q \); or
- the quantity and the action, \( p = (q, f) \); or
- as before, but including the initial condition, \( p = (q, f, u_0) \); or
- many other combinations.

To deal with all these different possibilities under one notation, the state Eq. (1) can be rewritten as

\[
\frac{d}{dt}u(t) = A(p; u(p; t)) + f(p; t); \quad u(0) = u_0,
\]

with a solution \( u(p; t) \) denoting the explicit dependence on the parameter \( p \in \mathcal{P} \).

Frequently, the interest is in functionals of the state \( \Psi(p, t) = \Psi(p, u(p; t)) \), and the functional dependence of \( u \) on \( p \) becomes important. Such situations arise in design, where \( p \) may be a design parameter still to be chosen, and one may seek a design such that a functional \( \Psi(p, t) \) or some kind of temporal integral or average \( \psi(p) = \int_0^T \Psi(p, t) \rho(t) \, dt \) is, e.g., maximised. Optimal control is a special case of this, as one may try to influence the time evolution in such a way that \( \Psi(p, T) \) (or \( \psi(p) \) above) is minimised or maximised. Another example is when the \( p \in \mathcal{P} \) are uncertain parameters, modelled by random variables. In the process of uncertainty quantification one then may want to compute expected values \( \mathbb{E}_p(\Psi(p, t)) \). It may also be that the parameters have to be determined or identified to allow the model to match some observed behaviour, this is called an inverse problem, see and the references therein. Another case is a general design evaluation, where one is interested in the range of \( u(p; t) \) — or \( \Psi(p, t) \) or \( \psi(p) \) — as \( p \) varies over \( \mathcal{P} \).

The situation just sketched involves a number of objects which are functions of the parameter values \( p \). While evaluating \( A(p) \) of \( f(p) \) in Eq. (2) for a certain \( p \) may be straightforward, one may easily envisage situations where evaluating \( u(p; t) \) or \( \Psi(p, t) \) may be very costly as it may involve some very time consuming simulation or computation. Therefore one is interested in representations of \( u(p; t) \) or \( \Psi(p, t) \) which allow the evaluation in a cheaper way. These simpler representations are called by many names, some are proxy- or surrogate-model. As will be shown in the following Section 2 any such parametric object may be represented in many different ways, many of which can be analysed by
linear maps which are associated with such representations. It will be shown that these representations may be seen as an element of a tensor product space. This in turn can be used to find very sparse approximations to those objects, and in turn much cheaper ways to evaluate the functional $\Psi$ or $\psi$ for other parameter values.

This association of parametric models and linear mappings has probably been known for a long time. The first steps which the authors are aware of in this direction of using linear methods are [31, 32]. A seminal work in this kind of inquiry is [23] (with English [26] and Spanish [25] translations available online), which contains a first rather thorough exploration in the context of probability on infinite dimensional vector or function spaces, and many influential ideas, see also [22, 24] for similar work. The name Karhunen-Loève expansion for approximations of this kind in the context of probability theory was coined after the authors of [23] and [31, 32]. This name is used in this context, in other areas that representation is now often known under the name proper orthogonal decomposition (POD), which is firmly connected with the singular value decomposition (SVD) of the associated linear map. In following publications, see [44, 45, 19, 46], the terms generalised processes, linear process, weak distribution or equivalently weak measure or weak process appear for the associated linear map. This is indicative of the generalisation possible with these linear methods, see also the monographs [16, 33, 28].

A first step of reviving and also connecting these methods of analysis with the theory of low-rank tensor approximations [20] was undertaken in [37] in the context of uncertainty quantification and inverse problems. It is furthermore also connected with non-orthogonal decompositions which are easier to compute, like the proper generalised decomposition (PGD) [7]. Here we continue that endeavour of showing the connection of parametric models, model reduction of parametric models, and sparse numerical approximations to a certain extent in a more general setting. It is on this theoretical background that one may analyse modern numerical methods which allow the numerical handling of very high-dimensional objects, i.e. where one has to deal with an essentially high-dimensional space for the parameters $p \in \mathcal{P}$.

Whereas the parametric map may be quite complicated, the association with a linear map translates the whole problem into one of linear functional analysis, and into linear algebra upon approximation and actual numerical computation. Also, whereas the set $\mathcal{P}$ might have a quite arbitrary structure, this is replaced by a subspace of the vector space $\mathbb{R}^\mathcal{P}$ of real valued functions on $\mathcal{P}$, in some sense this is a ‘problem oriented coordinate system’ on the set. This is a frequent technique in mathematics, and it replaces the quite arbitrary set by a vector space, which is much more accessible. Let us recall a situation which is similar and may be well-known to many readers. When the need arose to deal with very singular functions, especially when Dirac needed an ‘ideal’ object like the $\delta$-‘function’, for this and other so-called generalised functions or distributions a fruitful mathematical formulation turned out to be the model of a linear map into real numbers on a space of smooth regular functions, see e.g. [13, 15].

The association with a linear map is quickly shown to be related to representations connected with the adjoint of the map, and the precise definition and properties of the associated linear map are given in Section 2. The connection with reproducing kernel Hilbert spaces (RKHS) [5] also appears naturally here, and it is shortly sketched. From the map and its adjoint we obtain the ‘correlation’, which will be analysed in Section 3. Here the spectral analysis and factorisation of the correlation will become important [47, 43, 42, 11]. This also connects the whole idea of linear methods for representation
with tensor representations, which appear naturally in the spectral analysis. The kernel, which on the RKHS is the reproducing kernel, now appears in another context than the one already alluded to in Section 2, and in Section 3 the kernel side of the representation is analysed, which is the classical domain of integral transforms and integral equations as already envisaged in 23. Some examples and interpretations are explained in Section 5 to give an idea of the breadth of possible applications of the theory. Here the connection of these linear methods to both linear model reduction and nonlinear model reduction in the form of low-rank tensor approximations [20] is mentioned and briefly explained. The last Section 6 before the conclusion in Section 7 deals very shortly with certain refinements which are possible when some a priori structure of the represented spaces is known; we have connected it here with vector- and tensor-fields.

2 Parametric problems

Let \( r : \mathcal{P} \rightarrow \mathcal{U} \) be a parametric description of one of the objects alluded to in the introduction, or the state or response of some system, where \( \mathcal{P} \) is some set, and \( \mathcal{U} \) is assumed — for the sake of simplicity — as a separable Hilbert space with inner product \( \langle \cdot | \cdot \rangle_\mathcal{U} \). More general locally convex vector spaces are possible, but the separable Hilbert space is in many ways the simplest model.

The situation in its purest form may be thought of in an abstract way as follows: \( F : \mathcal{U} \times \mathcal{P} \rightarrow \mathcal{U} \) is some parameter dependent mapping like Eq. (2) in Section 1, which is well-posed in the sense that for each \( p \in \mathcal{P} \) it has a unique solution \( r(p) \) satisfying

\[
F(r(p), p) = 0,
\]

implicitly defining the function \( r(p) \) alluded to above. The mapping \( F \) is representative for the conditions which \( r(p) \) has to satisfy. What we desire is a simple representation / approximation of that function, which avoids solving Eq. (4) every time one wants to know \( r(p) \) for a new \( p \in \mathcal{P} \), i.e. a proxy- or surrogate model.

Of course the relation Eq. (3) or its possible source Eq. (2) not only defines \( r(p) \), but they can be an important relation each candidate has to satisfy as well as possible, and possibly other such relations. This is important, as a proxy-model will often be used also in the sense of a model order reduction, so that the computed \( r_c(p) \) will be an approximation. Then the degree to which a relation like Eq. (3) is satisfied can be the basis for estimating how good a particular approximation \( r_c(p) \) is.

One relatively well-known way when dealing with random models [15, 19, 16, 16, 28] turns the problem into one of consideration and ultimately of approximation of a linear mapping. The details in the simplest case are as follows.

2.1 Associated linear map

Assume without significant loss of generality that \( \text{span} \, r(\mathcal{P}) = \text{span} \, \text{im} \, r \subseteq \mathcal{U} \), the subspace of \( \mathcal{U} \) which is spanned by all the vectors \( \{ r(p) \mid p \in \mathcal{P} \} \), is dense in \( \mathcal{U} \).

Definition 1. Then to each such function \( r : \mathcal{P} \rightarrow \mathcal{U} \) one may associate a linear map

\[
R : \mathcal{U} \ni u \mapsto \langle r(\cdot) | u \rangle_\mathcal{U} \in \mathbb{R}^\mathcal{P},
\]

(4)
where \( \mathbb{R}^P \) is the space of real valued functions on \( P \) and \( (r(\cdot)|u)_U \) is the real valued map on \( P \) given by \( P \ni p \mapsto (r(p)|u)_U \in \mathbb{R} \).

**Lemma 2.** By construction, \( R \) restricted to span \( \text{im} \, r = \text{span} \, r(P) \) is injective, and hence has an inverse on its restricted range \( \tilde{R} := R(\text{span} \, \text{im} \, r) \).

**Proof.** Assume that for \( u \in \text{im} \, r = r(P), u \neq 0 \), it holds that \( Ru = 0 \). This means that \( \exists p_1 \in P \) such that \( u = r(p_1) \), and \((Ru)(p) = (r(p)|u)_U = (r(p)|r(p_1))_U = 0 \) for all \( p \in P \).

Taking \( p = p_1 \), this means that \( (r(p_1)|u)_U = (r(p_1)|r(p_1))_U = \|r(p_1)\|^2_U = \|u\|^2_U = 0 \). This can only hold for \( u = 0 \), contradicting the assumption \( u \neq 0 \), and so \( R \) is injective on \( \text{im} \, r \) and by linearity also on \( \text{span} \, \text{im} \, r \). It is obviously also surjective from \( \text{span} \, \text{im} \, r \) to \( \tilde{R} \), therefore bijective, hence has an inverse \( \tilde{R}^{-1} \) on \( \tilde{R} \). \( \square \)

**Definition 3.** This may be used to define an inner product on \( \tilde{R} \) as

\[ \forall \phi, \psi \in \tilde{R} \quad \langle \phi|\psi \rangle_{\tilde{R}} := \langle R^{-1}\phi|R^{-1}\psi \rangle_U, \tag{5} \]

and to denote the completion of \( \tilde{R} \) with this inner product by \( \tilde{R} \).

From Lemma 2 and Definition 3 one immediately obtains

**Proposition 4.** It is obvious from Eq. [5] that \( R^{-1} \) is a bijective isometry between \( \text{span} \, \text{im} \, r \) and \( \tilde{R} \), hence continuous, and the same holds also \( R \). Hence extended by continuity to the completion Hilbert spaces, \( R \) and \( R^* = R^{-1} \) are unitary maps.

Up to now, no structure on the set \( P \) has been assumed, whereas on \( U \) the inner product is assumed to measure what is important for the state \( r(p) \in U \), i.e. vectors with large norm are considered important. This is carried via the map \( R \) defined in Eq. [4] onto the space of scalar functions \( \mathcal{R} \) on the set \( P \), and the inner product there measures essentially the same thing as the one on \( U \). The only thing that changes is that now one does not have to work with the space \( U \), as everything is mirrored by the real functions \( \phi \in \mathcal{R} \), which may be seen as a ‘problem-oriented co-ordinate system’ on \( P \).

### 2.2 Reproducing kernel Hilbert space

Given the maps \( r : P \to U \) and \( R : U \to \mathcal{R} \), one may define the reproducing kernel [5, 21]:

**Definition 5.** The reproducing kernel associated with \( r : P \to U \) and \( R : U \to \mathcal{R} \) is \( \kappa \in \mathbb{R}^{P \times P} \) is given by:

\[ \mathcal{P} \times \mathcal{P} \ni (p_1, p_2) \mapsto \kappa(p_1, p_2) := (r(p_1)|r(p_2))_U \in \mathbb{R}. \tag{6} \]

It is straightforward to verify that:

**Theorem 6.** For all \( p \in P \): \( \kappa(p, \cdot) \in \mathcal{R} \subseteq \mathcal{R} \), and \( \text{span}\{\kappa(p, \cdot) \mid p \in P\} = \mathcal{R} \), i.e. the kernel \( \kappa \) generates the space \( \mathcal{R} \).

The point evaluation functional \( \delta_p \) is a continuous map on \( \mathcal{R} \), given by the inner product with the reproducing kernel:

\[ \delta_p : \mathcal{R} \ni \phi \mapsto \delta_p(\phi) = \langle \delta_p, \phi \rangle_{\mathcal{R} \times \mathcal{R}} := \phi(p) = \langle \kappa(p, \cdot)|\phi \rangle_{\mathcal{R}} \in \mathbb{R}. \tag{7} \]

This reproduction of \( \phi \) leads to the name reproducing kernel.
achieved by mapping these subsets with an appropriate kernel. This is then referred to as the ‘kernel trick’, and classification may be done by mapping. Looking at the Karhunen-Loève representation of the maps \( \mathcal{R} \) \([5, 21]\). In other settings like classification or machine learning with support vector machines, where \( p \in \mathcal{P} \) has to be classified as belonging to a certain subsets of \( \mathcal{P} \), one can use such a map \( r : \mathcal{P} \to \mathcal{U} \), the so-called feature map, implicitly through using an appropriate kernel. This is then referred to as the ‘kernel trick’, and classification may be achieved by mapping these subsets with \( r \) into \( \mathcal{U} \) and separating them with hyperplanes—a linear classifier. Observe also that the set \( \mathcal{P} \) is isomorphic space \( \mathbb{R} \), one may now choose a basis \( \{ \varphi_m \}_{m \in \mathbb{N}} \) in \( \mathcal{R} \), which may be assumed to be a complete orthonormal system (CONS).

**Proof.** The first statement is due to the fact that \( \varphi(p, \cdot) = \langle r(p), r(\cdot) \rangle_{\mathcal{U}} = Rr(p)(\cdot) \). For the reproducing property, similarly as in Lemma 2 we take \( \phi \in \mathcal{R} \), i.e. \( \exists u \in \mathcal{U} \) with \( \phi(\cdot) = \langle r(\cdot)|u \rangle_{\mathcal{U}} = Ru(\cdot) \), and then extend by continuity to \( \mathcal{R} \). It holds for all \( p \in \mathcal{P} \):

\[
\delta_p(\phi) = \langle \varphi(p, \cdot) | \phi \rangle_{\mathcal{R}} = \langle Rr(p)|Ru \rangle_{\mathcal{R}} = \langle r(p)|u \rangle_{\mathcal{U}} = Ru(p) = \phi(p),
\]

which is the reproducing property. As \( \delta_p \) is defined via the inner product, it is obviously continuous in \( \phi \), hence this extends to the closure of \( \mathcal{R} \), which is \( \mathcal{R} \).

Hilbert spaces with such a reproducing kernel are called a reproducing kernel Hilbert space (RKHS) \([5, 21]\). In other settings like classification or machine learning with support vector machines, where \( p \in \mathcal{P} \) has to be classified as belonging to a certain subsets of \( \mathcal{P} \), one can use such a map \( r : \mathcal{P} \to \mathcal{U} \), the so-called feature map, implicitly through using an appropriate kernel. This is then referred to as the ‘kernel trick’, and classification may be achieved by mapping these subsets with \( r \) into \( \mathcal{U} \) and separating them with hyperplanes—a linear classifier. Observe also that the set \( \mathcal{P} \) is isomorphic space \( \mathbb{R} \), one may now choose a basis \( \{ \varphi_m \}_{m \in \mathbb{N}} \) in \( \mathcal{R} \), which may be assumed to be a complete orthonormal system (CONS).

**Corollary 7.** With the CONS \( \{ y_m | y_m = R^{-1}\varphi_m = R^*\varphi_m \}_{m \in \mathbb{N}} \) in \( \mathcal{U} \), the operator \( R \), and its adjoint or inverse \( R^* = R^{-1} \), and the parametric element \( r(p) \) become:

\[
R = \sum_m \varphi_m \otimes y_m; \quad R^* = R^{-1} = \sum_m y_m \otimes \varphi_m; \quad r(p) = \sum_m \varphi_m(p)y_m = \sum_m R^*\varphi_m. \tag{8}
\]

These decompositions may also be seen as the singular value decompositions of the maps \( R \) and \( R^* = R^{-1} \), and are akin to the Karhunen-Loève decomposition of \( r(p) \).

**Proof.** As \( R \) is unitary, its singular values are all equal to unity, and any CONS such as \( \{ \varphi_m \}_m \) is a set of right singular vectors, giving the SVD of \( R \) and hence of \( R^* = R^{-1} \). For any \( m, n \in \mathbb{N} \) one has from the CONS property of \( \{ \varphi_m \}_m \) that

\[
\langle y_m|y_n \rangle_{\mathcal{U}} = \langle Ry_m|Ry_n \rangle_{\mathcal{R}} = \langle \varphi_m|\varphi_n \rangle_{\mathcal{R}} = \delta_{m,n},
\]

and hence for any \( p \in \mathcal{P} \) and any \( n \in \mathbb{N} \) : \( \varphi_n(p) = \langle r(p)|y_n \rangle_{\mathcal{U}} = \langle Ry_n \rangle(p) \), due to Eq. \([8]\) and the definition of the CONS \( \{ y_m \}_m \). The last in Eq. \([8]\) follows from definition of \( R^* \).
on \( \mathcal{P} \), i.e. transforming \( \mathcal{P} \ni p \mapsto (\varphi_1(p), \ldots, \varphi_m(p), \ldots) \in \mathbb{R}^N \), one obtains a linear / affine representation on \( \mathbb{R}^N \).

## 3 Correlation

As already alluded to at the end of Subsection 2.1, the RKHS construction \( \mathcal{R} \) with the inner product \( \langle \cdot | \cdot \rangle_{\mathcal{R}} \) just mirrors or reproduces the inner product structure on the original space \( (\mathcal{U}, \langle \cdot | \cdot \rangle_{\mathcal{U}}) \) on the RKHS space of real-valued functions \( \mathcal{R} \). Up to now there is no way of telling what is important in the parameter set \( \mathcal{P} \). Closely connected to this question is the one which subset of functions to choose for model reduction. Unfortunately, up to now we have no indication which subset may be particularly good. For this one needs additional information, a topic which will be taken up now.

As a way of indicating what is important on the set \( \mathcal{P} \), assume that there is another inner product \( \langle \cdot | \cdot \rangle_{\mathcal{Q}} \) for scalar functions \( \phi \in \mathbb{R}^\mathcal{P} \), and denote the Hilbert space of functions with that inner product by \( \mathcal{Q} \). Abusing the notation a bit, we denote the map \( R : \mathcal{U} \to \mathcal{Q} \), defined as in Eq. (4) but with range \( \mathcal{Q} \) still by \( R \). Generally one would also assume that the subspace \( \text{dom} \ R = \{ u \in \mathcal{U} \mid \|Ru\|_{\mathcal{Q}} < \infty \} \) is, if not the whole space \( \mathcal{U} \), at least dense in \( \mathcal{U} \). Additionally, one would assume that the densely defined operator \( R \) is closed. For simplicity assume here that \( R \) is defined on the whole space and hence continuous. Furthermore, assume that the map \( R : \mathcal{U} \to \mathcal{Q} \) is still injective, i.e. for \( \phi \in \mathcal{R} \) one has \( \|\phi\|_{\mathcal{R}} \neq 0 \Rightarrow \|\phi\|_{\mathcal{Q}} \neq 0 \), and that \( R \) is closed. Without loss of generality we assume then that \( R \) is surjective—by restricting ourselves to the closed Hilbert subspace \( R(\mathcal{U}) \) which we may call again \( \mathcal{Q} \).

**Definition 8 (Correlation).** With this, one may define a densely defined map \( C \) in \( \mathcal{U} \) through the bilinear form

\[
\forall u, v \in \mathcal{U}: \quad \langle Cu | v \rangle_{\mathcal{U}} := \langle Ru | Rv \rangle_{\mathcal{Q}}.
\]  

The map \( C \), which may also be written as \( C := R^* R \), may be called the ‘correlation’ operator. By construction it is self-adjoint and positive. In case \( R \) is defined on the whole space and hence continuous, so is \( C \).

The last statements are standard results from the theory of linear operators. Observe that in contrast to Subsection 2.2 the adjoint is now different from the inverse as normally \( R \) is not unitary, i.e. the adjoint is of the map \( R : \mathcal{U} \to \mathcal{Q} \) w.r.t. the \( \mathcal{Q} \)-inner product \( \langle \cdot | \cdot \rangle_{\mathcal{Q}} \). Often the inner product \( \langle \cdot | \cdot \rangle_{\mathcal{Q}} \) comes from a measure \( \varpi \) on \( \mathcal{P} \), so that for two measurable scalar functions \( \phi \) and \( \psi \) on \( \mathcal{P} \) one has

\[
\langle \phi | \psi \rangle_{\mathcal{Q}} := \int_{\mathcal{P}} \phi(p)\psi(p) \varpi(dp),
\]

where the space \( \mathcal{Q} \) may then be taken as \( \mathcal{Q} := L_2(\mathcal{P}, \varpi) \); or more generally with some kernel \( \beta(p_1, p_2) \)

\[
\langle \phi | \psi \rangle_{\mathcal{Q}} := \int_{\mathcal{P} \times \mathcal{P}} \phi(p_1)\beta(p_1, p_2)\psi(p_2) \varpi(dp_1)\varpi(dp_2) = \langle \beta, \phi \otimes \psi \rangle.
\]

One important sub-class of such situations is when \( \varpi \) is a probability measure on \( \mathcal{P} \), i.e.
\( \varpi(P) = 1 \). This is where the name ‘correlation’ is borrowed from. In the first case
\[
C = R^* R = \int_P r(p) \otimes r(p) \, \varpi(dp).
\]

Often the set \( P \) has more structure, like being in a topological space, a differentiable (Riemann) manifold, or a Lie group, which then may induce the choice of \( \sigma \)-algebra or measure.

### 3.1 Spectral decomposition

Before, in Subsection 2.2 it was the factorisation of \( C = R^* R \) which allowed the RKHS representation in Eq. (9). For other representations, one needs other factorisations. Most common is to use the spectral decomposition (e.g. [14, 16, 47, 43, 42, 11]) of \( C \) to achieve such a factorisation. In case the correlation were defined on a finite-dimensional space, \( C - \lambda I \) is not invertible—and eigen-decomposition would be written with eigenvectors \( v_m \) and eigenvalues \( \lambda_m \) as
\[
C v_m = \lambda_m v_m, \quad C = \sum_m \lambda_m v_m v_m^T = \sum_m \lambda_m v_m \otimes v_m = \sum_m \lambda_m \Delta E_m = V \Lambda V^T. \tag{10}
\]

As \( C \) is self-adjoint and positive, this implies \( \lambda \in \mathbb{R} \) and \( \lambda_m \geq 0 \). The set of all eigenvalues \( \sigma(C) := \{\lambda_m\}_m \subset \mathbb{C} \) is called the spectrum of \( C \). Here we assume the ordering \( 0 \leq \lambda_1 \cdots \leq \lambda_m \), each eigenvalue counted with appropriate multiplicity. The \( v_m \) are normalised eigenvectors, and are mutually orthogonal \( (v_m^T v_n = \delta_{m,n}) \). The first two decompositions—which are only different notations—are into weighted sums of simple tensor products of orthonormal vectors, or one-dimensional orthogonal projections \( \Delta E_m := v_m v_m^T = v_m \otimes v_m \), which define the spectral resolution \( E_m := \sum_{k \leq m} \Delta E_k \). The \( E_m \) are hence the orthogonal projections onto the subspaces \( \{v_k \mid k \leq m\} \).

The columns of \( V = [v_1, \ldots, v_m, \ldots] \) are the normalised eigenvectors, so that \( V \) is unitary resp. orthogonal, and \( A = \text{diag}(\lambda_m) \) is a diagonal matrix [50], a ‘multiplication’ operator, as for \( A u = w \), each component \( u_m \) of \( u = [u_1, \ldots, u_m, \ldots]^T \) is just multiplied by \( \lambda_m \): \( w_m = \lambda_m u_m \). The last decomposition in Eq. (10) hence means that \( C \) is unitarily equivalent to a multiplication operator by a diagonal matrix with real non-negative entries.

In contrast, on infinite dimensional Hilbert spaces the decompositions in Eq. (10) are materially different formulations of the spectral theorem for self-adjoint operators, e.g. [14, 16, 47, 43, 42, 11]. A number \( \lambda \in \mathbb{C} \) is in the spectrum \( \sigma(C) \) iff \( C - \lambda I \) is not invertible as a continuous operator. But now there may be spectral values \( \lambda \in \sigma(C) \) which are not eigenvalues—this has to do with the possibility of a continuous spectrum—and the sums in Eq. (10) have to become integrals. Probably best known is the generalisation of the second last form in Eq. (10) \( (C = \sum_m \lambda_m \Delta E_m) \), namely [14, 16, 47, 43, 42, 11]:

**Theorem 9** (First spectral theorem). The self-adjoint and positive operator \( C : U \to U \), where \( C = R^* R \), may be decomposed into an integral of orthogonal projections \( E_\lambda \),
\[
C = \int_0^\infty \lambda \, dE_\lambda = \int_{\sigma(C)} \lambda \, dE_\lambda. \tag{11}
\]

Here \( E_\lambda \) is the corresponding projection-valued spectral measure corresponding to \( E_m \) in
Eq. (11), with a non-negative spectrum \( \sigma(C) \subseteq \mathbb{R}_+ \).

Observe that the factorised form \( C = R^* R \) is actually equivalent to the statement that \( C \) is self-adjoint and positive.

For the sake of brevity and simplicity of exposition let us assume that \( C \) has a pure point spectrum \( \sigma_p(C) = \sigma(C) \), i.e. all \( \lambda_m \in \sigma_p(C) \) are eigenvalues with eigenvector \( v_m \), \( Cv_m = \lambda_m v_m, m \in \mathbb{N} \), each eigenvalue repeated with appropriate finite multiplicity. In this case Eq. (11) becomes just a sum, and may be written with the CONS of unit-\( \mathcal{U} \)-norm eigenvectors \( \{v_m\}_m \subseteq \mathcal{U} \). Here we assume the opposite ordering of the \( \lambda_m \) as before in Eq. (11), namely \( \lambda_1 \geq \cdots \geq \lambda_m \cdots \geq 0 \), and set

\[
E_0 := I, \quad E_m := \sum_{k>m} v_k \otimes v_k; \quad \text{and for } m \geq 1 : \quad \Delta E_{\lambda_m} := E_{m-1} - E_m. \tag{12}
\]

The spectral projection-valued measure \( dE_\lambda \) in Eq. (11) becomes a point measure \( dE_\lambda = \sum_m \delta_{\lambda_m} \Delta E_{\lambda_m} \), where \( \delta_{\lambda_m} \) is the Dirac-\( \delta \). For the second part of the following Theorem 10, also assume that the correlation \( C \) is a trace class or nuclear operator, which means that the trace is finite \( (\text{tr} \ C = \sum_m \lambda_m < \infty) \), and \( C \) is then necessarily also a Hilbert-Schmidt and a compact operator.

**Theorem 10** (First spectral representation and Karhunen-Loève expansion). The spectral decomposition of Theorem 4, Eq. (11) becomes

\[
C = \sum_m \lambda_m (v_m \otimes v_m) = \sum_m \lambda_m \Delta E_{\lambda_m}. \tag{13}
\]

Define a new CONS \( \{s_m\}_m \) in \( \mathcal{Q} \): \( \lambda_m^{1/2} s_m := R v_m \), to obtain the corresponding singular value decomposition (SVD) of \( R \) and \( R^* \). The set \( \varsigma(R) = \{\lambda_m^{1/2}\} = \sqrt{\sigma(C)} \subseteq \mathbb{R}_+ \) are the singular values of \( R \) and \( R^* \).

\[
R = \sum_m \lambda_m^{1/2} (s_m \otimes v_m); \quad R^* = \sum_m \lambda_m^{1/2} (v_m \otimes s_m); \quad r(p) = \sum_m \lambda_m^{1/2} s_m(p)v_m = \sum_m R^* s_m. \tag{14}
\]

The last relation is the so-called Karhunen-Loève expansion or proper orthogonal decomposition (POD). If in that relation the sum is truncated at \( n \in \mathbb{N} \), i.e.

\[
r(p) \approx r_n(p) = \sum_{m=1}^n \lambda_m^{1/2} s_m(p) v_m = \sum_{m=1}^n R^* s_m(p), \tag{15}
\]

we obtain the best \( n \)-term approximation to \( r(p) \) in the norm of \( \mathcal{U} \).

**Proof.** The spectral decompositions Eq. (13)—analogues of the first three in Eq. (11)—are a consequence of the fact that for a point spectrum the projection-valued measure \( dE_\lambda \) in Eq. (11) becomes a discrete projection-valued measure \( \Delta E_{\lambda_m} \).

That the system \( \{s_m\}_m \) is a CONS follows from

\[
(C v_m | v_n)_\mathcal{U} = \lambda_m \delta_{m,n} = (R v_m | R v_n)_\mathcal{Q} = (\lambda_m^{1/2} s_m | \lambda_n^{1/2} s_n)_\mathcal{Q} = \lambda_m (s_m | s_n)_\mathcal{Q}.
\]

The representations in Eq. (13) are shown in the same way as in Corollary 7. It still remains to show that the function \( p \mapsto r(p) \) defined in Eq. (15) is in \( \mathcal{U} \otimes \mathcal{Q} \). For that,
using the orthonormality of \( \{s_m\}_m \) and \( \{v_m\}_m \), and the nuclearity of \( C \), one computes

\[
\|r\|_{U \otimes Q}^2 = \langle r | r \rangle_{U \otimes Q} = \sum_{m,n} \sqrt{\lambda_m} \lambda_n \langle s_m | s_n \rangle_Q \langle v_m | v_n \rangle_U = \sum_{m,n} \sqrt{\lambda_m} \delta_{m,n} \delta_{m,n} = \sum_m \lambda_m < \infty.
\]

The statement about the best-\( n \)-term approximation follows from the well-known optimality \([50, 21]\) of the SVD.

Observe that, similarly to Eq. (8), \( r \) is linear in the \( s_m \). This means that by choosing the ‘co-ordinate transformation’ \( P \ni p \mapsto (s_1(p), \ldots, s_m(p), \ldots) \in \mathbb{R}^N \) one obtains a linear \( / \) affine representation where the first co-ordinates are the most important ones, i.e. they catch most of the variability in that the best-\( n \)-term approximation in the norm \( \| \cdot \|_C \) requires only the first \( n \) co-ordinate functions \( \{s_m\}_{m \leq n} \). This is one possible criterion on how to build good reduced order models \( r_n(p) \), i.e. how to choose a good subspace for approximation.

Note that in case \( P \) is a probability space, the condition that \( C \) be a trace class or nuclear operator is also a necessary condition that \( r \) have finite variance and that the distribution of \( r \) be a probability measure on \( U \). When stating other series representations in the sequel, it will always be assumed that this condition of nuclearity is satisfied. Hence the definition of models via linear maps is much more general and allows one to consider generalised resp. weak, or in some way ideal representations \([15, 13, 16, 28]\).

### 3.2 Singular value decomposition

To treat the analogues of the first two decompositions of \( C \) in Eq. (10) in the case where \( C \) has a continuous spectrum directly requires technical tools such as Gel’fand triplets (rigged Hilbert spaces), direct integrals of Hilbert spaces \([14, 16, 11]\), and generalised eigenvectors, which are beyond the scope of this short note. This also applies to representations which go beyond the case of a nuclear correlation, and typically become some kind of integral transform. We contend ourselves with an alternative, and materially stronger, formulation of the spectral decomposition than Eq. (10) \( (C = VAV^T) \) which will lead us to the singular value decomposition, an analogue of Eq. (14). The results in this Subsection 3.2 do not require \( C \) to be nuclear, nor do they require \( C \) or \( R \) to be continuous.

**Theorem 11** (Second spectral theorem). The densely defined, self-adjoint and positive operator \( C : U \to U \) is unitarily equivalent with a multiplication operator \( M_\mu \),

\[
C = VM_\mu V^*;
\]  

(16)

where \( V : L_2(T) \to U \) is unitary between some \( L_2(T) \) on a measure space \( T \) and the Hilbert space \( U \), and \( M_\mu \) is a multiplication operator, multiplying any \( \psi \in L_2(T) \) with a real-valued function \( \mu : \L_2(T) \ni \psi \mapsto \mu \psi \in L_2(T) \). In case \( C \) is bounded, \( \mu \in L_\infty(T) \). As \( C \) is positive, \( \mu(t) \geq 0 \) for almost all \( t \in T \), and the essential range of \( \mu \) is the spectrum of \( C \). As \( M_\mu \) with a real valued non-negative \( \mu \) is self-adjoint and positive, one may define

\[
M_\mu^{1/2} := M_{\sqrt{\mu}} : \L_2(T) \ni \psi \mapsto \sqrt{\mu} \psi \in L_2(T),
\]  

(17)
from which one obtains the square-root of $C$ via its spectral decomposition

$$C^{1/2} = VM\sqrt{\mu}V^*.$$  \hfill (18)

The factorisation corresponding to $C = R^* R$ in Theorem 9 is here (with $M\sqrt{\mu} = M_{\sqrt{\mu}}$)

$$C = (VM_{\sqrt{\mu}})(VM_{\sqrt{\mu}})^* = (VM_{\sqrt{\mu}}I)(VM_{\sqrt{\mu}}I)^*. \hfill (19)$$

**Proof.** The statement about the unitary equivalence is a standard result [14, 47, 43, 11] for self-adjoint operators, as well as the positivity of the multiplier $\mu$. Computation of the square-root $M_{\sqrt{\mu}}$ is obvious, as $M_{\sqrt{\mu}}^2 = M_{\mu}$; on the other hand Eq. (18) is standard functional calculus of operators. In the last Eq. (19), it obviously holds that $(VM_{\sqrt{\mu}})(VM_{\sqrt{\mu}})^* = VM_{\sqrt{\mu}}M_{\sqrt{\mu}}V^* = VM_{\mu}V^*$; observe that $M_{\mu}^* = M_{\mu}$ and $M_{\sqrt{\mu}}^* = M_{\sqrt{\mu}}$ as $\mu$ is real. \hfill \Box

From this spectral decomposition follow decompositions of $R$ and some spectrally connected factorisations of $C$:

**Corollary 12** (Singular value decomposition and further factorisations). The singular value decomposition (SVD) of $R$ is

$$R = UM_{\sqrt{\mu}}V^*,$$ \hfill (20)

where $U : L_2(\mathcal{H}) \to Q$ is a unitary operator, $M_{\sqrt{\mu}}$ is from Eq. (17), and the unitary $V$ from Eq. (14). Further decompositions of $C$ arising from Theorem 11 are $C = G^*G$ with $G := IM_{\sqrt{\mu}}V^*$, and $C = (C^{1/2})^*C^{1/2} = C^{1/2}C^{1/2}$, with the SVD of $C^{1/2}$ given by Eq. (18).

**Proof.** The SVD of $R$ in Eq. (20) is a standard result [47, 43], and $U$ is unitary as $R$ was assumed surjective. The decomposition with $G$ follows directly from Eq. (19). The last decomposition $C = (C^{1/2})^*C^{1/2}$ follows from the fact that with $C$ also $C^{1/2}$ is self-adjoint, and as $C^{1/2}$ is also positive, its SVD is equal to its spectral decomposition Eq. (18). \hfill \Box

### 3.3 Other factorisations and representations

In the preceding Subsection 5.2 in Corollary 12 it was shown that there are several ways to factorise $C = R^* R$. Let us denote a general factorisation by $C = B^* B$, where $B : \mathcal{U} \to \mathcal{H}$ is a map to a Hilbert space $\mathcal{H}$ with all the properties demanded from $R$—see the beginning of this section. Sometimes such a factor $B$ is called a *square root* of $C$, but we shall reserve that name for the *unique* factorisation with the self-adjoint factor $C^{1/2}$ from Eq. (18), $C = (C^{1/2})^*C^{1/2} = C^{1/2}C^{1/2}$. In some way, all such factorisations are equivalent:

**Theorem 13** (Equivalence of factorisations). Let $C = B^* B$ with $B : \mathcal{U} \to \mathcal{H}$ be any factorisation satisfying the conditions at the beginning of this section. Any two such factorisations $B_1 : \mathcal{U} \to H_1$ and $B_2 : \mathcal{U} \to H_2$ with $C = B_1^*B_1 = B_2^*B_2$ are unitarily equivalent in that there is a unitary map $X_{12} : H_1 \to H_2$ such that $B_2 = X_{21}B_1$. Equivalently, each such factorisation is unitarily equivalent to $R$, i.e. for $C = B^* B$ there is a unitary $X : \mathcal{H} \to \mathcal{Q}$ such that $R = XB$. \hfill \Box

**Proof.** Let $C = B_1^*B_1 = B_2^*B_2$ be two such factorisations, each unitarily equivalent to $R = X_1B_1 = X_2B_2$. As $X_2^* = X_2^{-1}$, it follows easily that $B_2 = X_2^*X_1B_1$, so $B_1$ and $B_2$ are unitarily equivalent with the unitary $X_{21} := X_2^*X_1$. 

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So what is left is to show that an arbitrary factorisation is equivalent to \( R \). From the SVD of \( R \) in Eq. (20), one sees easily that \( R \) and \( G \) in Corollary 12 are unitarily equivalent, as \( R = UM_\sqrt{\mu}V^* = U(M_\sqrt{\mu}V^*) = U(IM_\sqrt{\mu}V^*) = UG \). Now let \( C = B^*B \) be an arbitrary factorisation with the required properties. Then, just as \( R \) in Corollary 12, the factor \( B \) has a SVD [17, 13], \( B = WM_\sqrt{\mu}V^* \), with \( M_\sqrt{\mu} \) and \( V \) from Corollary 12 and a unitary \( W : L_2(\mathcal{T}) \to \mathcal{H} \). Hence \( B = WG \) or \( G = W^*B \), and finally \( R = UG = UW^*B = XB \) with a unitary \( X := UW^* \). \( \square \)

For finite dimensional spaces, a favourite choice for such a decomposition of \( C \) is the Cholesky factorisation \( C = LL^T \), where \( B = L^T \). Now let us go back to the situation described in Theorem 11 where for the sake of simplicity of exposition we assume that \( C \) has a purely discrete spectrum and a CONS of eigenvectors \( \{v_m\}_m \) in \( \mathcal{U} \), and let us have a look how the results up to now may be used to build new representations. First transport the eigenvector CONS from \( \mathcal{U} \) to \( L_2(\mathcal{T}) \):

**Lemma 14.** Setting for all \( m \in \mathbb{N} \): \( \xi_m := V^*v_m \), the system \( \{\xi_m\}_m \) is a CONS in \( L_2(\mathcal{T}) \), and \( M_\mu\xi_m = \lambda_m\xi_m \), i.e. the \( \xi_m \) are an eigenvector CONS of \( M_\mu = V^*CV \).

**Proof.** Orthonormality and completeness are due to \( V^* \) being unitary. With Eq. (16) one computes

\[
M_\mu\xi_m = V^*CVv_m = \lambda_mV^*v_m = \lambda_m\xi_m,
\]

which shows the eigenvector property. \( \square \)

**Proposition 15.** With the help of the CONS \( \{s_m\}_m \) in \( Q \) or \( \{v_m\}_m \) in \( \mathcal{U} \), define a CONS \( \{h_m\}_m \) in \( \mathcal{H} \): \( \text{span}\{h_m \mid m \in \mathbb{N}\} = \mathcal{H} \):

\[
\forall m \in \mathbb{N} : \quad h_m := BC^{-1}R^*s_m = BC^{-1/2}v_m. \tag{21}
\]

The CONS \( \{h_m\}_m \) in \( \mathcal{H} \) is an eigenvector CONS of the operator

\[
C_\mathcal{H} := BB^* : \mathcal{H} \to \mathcal{H}, \tag{22}
\]

\[
\forall m \in \mathbb{N} : \quad C_\mathcal{H}h_m := \lambda_mh_m. \tag{23}
\]

**Proof.** The stated orthonormality of the \( \{h_m\}_m \) is easily computed, as with Theorem 11 Corollary 12 and the SVD of \( B = WM_\sqrt{\mu}V^* \) from Theorem 13 one obtains after a bit of computation \( BC^{-1}R^* = WU^* \), and \( BC^{-1/2} = WV^* \), hence \( h_m = WU^*s_m \), and therefore orthonormality follows from the unitarity of \( WU^* \) and orthonormality of the \( \{s_m\}_m \). Completeness follows from the completeness of \( \{s_m\}_m \) and surjectivity of \( B \).

Similarly to \( h_m = WU^*s_m \) one obtains with Lemma 13

\[
v_m = VU^*s_m \Rightarrow h_m = WU^*s_m = WV^*(VU^*s_m) = WV^*v_m = W\xi_m.
\]

From this follows, again with Lemma 13

\[
C_\mathcal{H}h_m = (BB^*)W\xi_m = WM_\mu\xi_m = \lambda_mW\xi_m = \lambda_mh_m.
\]

One may see the statement in Lemma 14 as a special case of Proposition 15 with \( B = IM_\sqrt{\mu}V^* \), as then \( \xi_m = V^*v_m = U^*s_m \). Collecting, an immediate consequence is:
Corollary 16. One has the following equivalent eigensystems

- on $\mathcal{U}$ with $C = R^* R - C v_m = \lambda_m v_m$, $v_m = VU^* s_m$ and $C = VM \mu V^*$;
- on $\mathcal{H}$ with $C_H = B B^* - C_H h_m = \lambda_m h_m$, $h_m = WV^* v_m$ and $C_H = WV^* CV W^*$;
- on $\mathcal{Q}$ with $C_Q = R R^* - C_Q s_m = \lambda_m s_m$, $s_m = UV^* v_m$ and $C_Q = UV^* CV U^*$;
- on $L_2(\mathcal{T})$ with $C_{L_2(\mathcal{T})} = M_{\mu} - C_{L_2(\mathcal{T})} \xi_m = \lambda_m \xi_m$, $\xi_m = V^* v_m$ and $C_{L_2(\mathcal{T})} = V^* C V$.

The last two statements are special cases of the second one with $\mathcal{H} = \mathcal{Q}$ and $B = R$, resp. $\mathcal{H} = L_2(\mathcal{T})$ with $B = M_{\sqrt{\mu}} V^*$. Hence each factorisation $C = B^* B$ with $B : \mathcal{U} \to \mathcal{H}$ gives a new equivalent eigensystem on $\mathcal{H}$ for the operator $C_H = BB^*$.

From Eq. (14) in Theorem 10 one has $r = \sum_m R^* s_m$. This in conjunction with another equivalent factorisation according to Theorem 13 immediately leads to new representations of $r(p)$, by replacing $R^* s_m$ in the Karhunen-Loève expansion in Theorem 10 by the equivalent $B^* h_m$.

Corollary 17 (Representation from factorisation). With a factorisation $C = B^* B$ and $\text{CONS } \{h_m\}_m$ in $\mathcal{H}$ as in Proposition 13 one obtains the following representation of $r(p)$:

$$ r(p) = \sum_m B^* h_m = \sum_m VM_{\sqrt{\mu}} W^* h_m, \quad \text{in particular also} \quad r(t) = \sum_m VM_{\sqrt{\mu}} \xi_m(t). \quad (24) $$

In the special case of a purely discrete spectrum we are dealing with here it is possible to formulate analogues of the decompositions in Corollary 7. This is an analogue of Theorem 10 for the general case $C = B^* B$ with $B : \mathcal{U} \to \mathcal{H}$.

Corollary 18. With a factorisation $C = B^* B$ and $\text{CONS } \{v_m\}_m$ in $\mathcal{U}$, $\text{CONS } \{h_m\}_m$ in $\mathcal{H}$ as in Proposition 13 one obtains the following tensor representations of the map $C_H = BB^*$:

$$ C_H = \sum_m \lambda_m h_m \otimes h_m. \quad (25) $$

Specifically, for $\mathcal{H} = \mathcal{Q}$ and $C_H = C_Q$,

$$ C_Q = \sum_m \lambda_m s_m \otimes s_m. \quad (26) $$

The corresponding expansions of $B$ and its adjoint are:

$$ B = \sum_m \lambda_m^{1/2} h_m \otimes v_m; \quad \text{and} \quad B^* = \sum_m \lambda_m^{1/2} v_m \otimes h_m. \quad (27) $$

In case the space $\mathcal{H}$ is a function space like $L_2(\mathcal{T})$ on a set $\mathcal{A}$, this results in the Karhunen-Loève expansions for the representation of $r(p)$:

$$ r(a) = \sum_m \lambda_m^{1/2} h_m(a) v_m, \quad \text{in particular also} \quad r(t) = \sum_m \lambda_m^{1/2} \xi_m(t) v_m. \quad (28) $$

In this last Eq. (28) the function $r(p)$ has become a function of the new parameter $a \in \mathcal{A}$ or $t \in \mathcal{T}$, having implicitly performed a transformation $\mathcal{P} \to \mathcal{A}$ or $\mathcal{P} \to \mathcal{T}$. The new parametrisation covers the same range as $r(p)$ before. As a summary of the analysis let us put everything together:
Theorem 19 (Equivalence of representation and factorisation). A parametric mapping \( r : \mathcal{P} \to \mathcal{U} \) into a Hilbert space \( \mathcal{U} \) with the conditions stated at the beginning of Subsection 2.1 and this section induces a linear map \( R : \mathcal{U} \to \mathcal{Q} \), where \( \mathcal{Q} \) is a Hilbert space of functions on \( \mathcal{P} \). The reproducing kernel Hilbert space is a special case of this.

Any other factorisation of the ‘correlation’ \( C = R^*R \) on \( \mathcal{U} \), like \( C = B^*B \) with a \( B : \mathcal{U} \to \mathcal{H} \) into a Hilbert space \( \mathcal{H} \) with the same properties as \( R \) is unitarily equivalent, i.e. there is a unitary \( W : \mathcal{Q} \to \mathcal{H} \) such that \( B = WR \). Any such factorisation induces a representation of \( r \). Especially if \( \mathcal{H} \) is a space of functions on a set \( \mathcal{A} \), one obtains a representation \( r(a), (a \in \mathcal{A}) \), such that \( r(\mathcal{P}) = r(\mathcal{A}) \).

The associated ‘correlations’ \( C_\mathcal{Q} = RR^* \) on \( \mathcal{Q} \) resp. \( C_\mathcal{H} = BB^* \) on \( \mathcal{H} \) have the same spectrum as \( C \), and factorisations of \( C_\mathcal{Q} \) resp. \( C_\mathcal{H} \) induce new factorisations of \( C \).

4 Kernel space

In this section we take a closer look at the operator defined in Eq. (22) in Proposition 15 especially for the case \( \mathcal{H} = \mathcal{Q} \) and \( B = R \), i.e. we analyse the operator \( C_\mathcal{Q} = RR^* \). We shall restrict ourselves again to the case of a pure point spectrum. From Corollary 16 and Eq. (26) in Corollary 18 one knows that in an abstract sense

\[
C_\mathcal{Q} = UV^*CVU^* = UM_\mu U^* = \sum_m \lambda_m s_m \otimes s_m. \tag{29}
\]

But the point is here to spell this out in more analytical detail especially for the case when, as indicated already at the beginning of Section 3 the inner product on \( \mathcal{Q} \) is given by a measure \( \varpi \) on \( \mathcal{P} \):

\[
\forall \varphi, \psi \in \mathcal{Q} : \langle \varphi | \psi \rangle_\mathcal{Q} = \int_\mathcal{P} \varphi(p)\psi(p) \varpi(dp). \tag{30}
\]

4.1 Kernel spectral decomposition

Then \( C \) is given by

\[
C = \int_\mathcal{P} r(p) \otimes r(p) \varpi(dp), \tag{31}
\]

and \( C_\mathcal{Q} \) is represented by the kernel

\[
\varpi(p_1, p_2) = \langle r(p_1) | r(p_2) \rangle_\mathcal{U}, \tag{32}
\]

so that for all \( \varphi, \psi \in \mathcal{Q} \)

\[
\langle C_\mathcal{Q} \varphi | \psi \rangle_\mathcal{Q} = \langle R^* \varphi | R^* \psi \rangle_\mathcal{U} = \iint_{\mathcal{P} \times \mathcal{P}} \varphi(p_1) \varpi(p_1, p_2) \psi(p_2) \varpi(dp_1) \varpi(dp_2), \tag{33}
\]

i.e. \( C_\mathcal{Q} \) is a Fredholm integral operator

\[
(C_\mathcal{Q} \psi)(p_1) = \int_\mathcal{P} \varpi(p_1, p_2) \psi(p_2) \varpi(dp_2). \tag{34}
\]

The abstract eigenvalue problem described in Corollary 16 for the operator \( C_\mathcal{Q} \), when taking into account the explicit description Eq. (34), is translated into finding an eigen-
function \( s \in Q \) and eigenvalue \( \lambda \) such that

\[
(C_Q s)(p_1) = \int \chi(p_1, p_2) s(p_2) \, dp_2 = \lambda s(p_1), \tag{35}
\]

a Fredholm integral equation \([10, 2]\).

**Proposition 20.** From Corollary \([16]\) and Eq. \((24)\) one knows that the eigenfunctions are \( \{s_m\}_m \subset Q \), hence, in particular with the kernel \( \chi \), Mercer’s theorem \([10]\) gives

\[
\int \chi(p_1, p_2) s_m(p_2) \, dp_2 = \lambda_m s_m(p_1); \quad \chi(p_1, p_2) = \sum_m \lambda_m s_m(p_1) s_m(p_2), \tag{36}
\]

giving a decomposition of \( \chi \), which is of course essentially identical to Eq. \((29)\).

In Section \(3\) the analysis was based to a large extent on factorisations of the operator \( C = R^* R \). Similarly, now one looks at factorisations of \( C_Q = RR^* \).

One example situation which occurs quite frequently fits nicely here, rather than in the later Section \(5\) which is the case when \( \mathcal{P} = \mathbb{R}^n \) with the usual Lebesgue measure, and the kernel is a convolution kernel, i.e. \( \chi(p_1, p_2) = \kappa(p_1 - p_2) \). This means that the kernel is invariant under arbitrary displacements or shifts \( z \in \mathbb{R}^n \): \( \chi(p_1, p_2) = \chi(p_1 + z, p_2 + z) = \kappa(p_1 - p_2) \). The eigenvalue equation Eq. \((35)\) becomes

\[
(C_Q s)(p_1) = \int_{\mathbb{R}^n} \kappa(p_1 - p_2) s(p_2) \, dp_2 = \lambda s(p_1). \tag{37}
\]

As is well known, the symmetry of \( \chi \) implies now that the function \( \kappa \) has to be an even function \([3]\), \( \kappa(z) = \kappa(-z) \).

It is clear that this form of equation can be treated by Fourier analysis \([10, 2]\); performing a Fourier transform on Eq. \((37)\) and denoting transformed quantities by a hat, e.g. \( \hat{s} \), one obtains for all \( \zeta \in \mathbb{R}^n \)

\[
(C_Q \hat{s})(\zeta) = \hat{\kappa}(\zeta) \hat{s}(\zeta) = \lambda \hat{s}(\zeta). \tag{38}
\]

In this representation, \( \hat{C_Q s} \) has become a multiplication operator \( M_\kappa \) with the positive multiplier function \( \hat{\kappa}(\zeta) \geq 0 \) on the domain \( \zeta \in \mathbb{R}^n \). This is a concrete version of the case in the second spectral Theorem \([11]\), the multiplier function \( \mu(t) \) in that theorem is \( \hat{\kappa}(\zeta) \) here. The unitary transformation which has effectively diagonalised the integral operator Eq. \((35)\) is the Fourier transform, and the essential range of \( \hat{\kappa} \) is the spectrum. This relates to the fact that the Fourier transform of the correlation \( \kappa \) — or more precisely the covariance, but we do not distinguish this here — is usually called the spectrum, or more precisely the spectral density. In the terminology here the spectrum is the values of \( \hat{\kappa} \). It is now also easy to see how a continuous spectrum appears: on an infinite domain the integral operator Eq. \((34)\) is typically not compact, and unless \( \kappa \) is almost-periodic the operator has no point spectrum. The Fourier functions are generalised eigenfunctions \([14, 16, 11]\), as they are not in \( L_2(\mathbb{R}^n) \). We shall not dwell further on this topic here.

If we denote the Fourier transform on \( L_2(\mathbb{R}^n) \) by

\[
F : f(p) \mapsto \hat{f}(\zeta) = (F f)(\zeta) = \int_{\mathbb{R}^n} \exp(-2\pi i p \cdot \zeta) f(p) \, dp, \tag{39}
\]
where \( p \cdot \zeta \) is the Euclidean inner product in \( \mathbb{R}^n \), then one may write this spectral decomposition and factorisation of \( C_Q \) in this special case corresponding to Corollary 18 in the following way.

**Corollary 21.** The operator \( C_Q = RR^* \) has in the stationary case of Eq. (37) the spectral decomposition

\[
C_Q = F^* M \hat{\kappa} F. \tag{40}
\]

As \( \hat{\kappa}(\zeta) \geq 0 \), the square-root multiplier is given by

\[
M_{\hat{\kappa}}^{1/2} = M \sqrt{\hat{\kappa}}. \tag{41}
\]

This induces the following factorisation of \( C_Q = RR^* \):

\[
C_Q = (M \sqrt{\hat{\kappa}} F)^*(M \sqrt{\hat{\kappa}} F). \tag{42}
\]

From Corollary 16 one has \( C_Q = UV^*CVU^* \), which gives further

\[
C_Q = UV^*CVU^* = UV^*VM \hat{\mu} V^*U^* = UM \mu U^*, \tag{43}
\]

meaning that essentially in this case \( U = F^* \), the inverse Fourier transform. This implies the well-known Fourier representations of stationary random functions. Denoting the shift operator for \( z \in \mathbb{R}^n \) as \( T_z \)

\[
f(p) \mapsto T_z f(p) = f(p + z),
\]

it is elementary that with \( \eta(\zeta) := \exp(2\pi i p \cdot \zeta) \)

\[
T_z \eta(\zeta) = T_z \exp(2\pi i p \cdot \zeta) = \exp(2\pi i p \cdot z) \eta(\zeta),
\]

which says that the \( \eta(\zeta) \) are ‘generalised’ eigenfunctions of \( T_z \). They are not true eigenfunctions as they are not in \( L^2(\mathbb{R}^n) \).

Shift-invariance means that \( T_z C_Q = C_Q T_z \), i.e. the operators commute. This implies that \( T_z \) and \( C_Q \) are effectively diagonalised by the Fourier transform \( F \). This particular case of covariance has been treated extensively in the literature [22, 24, 54, 16, 52, 53, 33, 28, 35]. As is well known, the functions \( \eta(\zeta) \) are formal or generalised eigenvectors of \( C_Q \), formally,

\[
r(p) = \int_{\mathbb{R}^n} \sqrt{\hat{\kappa} \eta(\zeta)} v_{\zeta} d\zeta = \int_{\mathbb{R}^n} \exp(2\pi i p \cdot \zeta) M \sqrt{\hat{\kappa}} v_{\zeta} d\zeta = F^*(M \sqrt{\hat{\kappa}} v_{\zeta}), \tag{45}
\]

or, in the most general case, a combination of Eq. (44) and Eq. (45). In that last Eq. (45), the formal term \( v_{\zeta} d\zeta \) may be interpreted as a vector-valued measure \( \bar{v}(d\zeta) \), in the case of a random process or field \( r(p) \) on \( p \in \mathbb{R}^n \) it is called a stochastic measure.
4.2 Kernel factorisations

The concrete realisation of the operator $C_Q$ as an integral kernel Eq. (34) opens the possibility to look for factorisations in the concrete setting of integral transforms.

If, on the other hand, one has some other factorisation of the kernel, for example on some measure space $(\mathcal{X}, \nu)$:

$$\kappa(p_1, p_2) = \int_{\mathcal{X}} g(p_1, x)g(p_2, x) \nu(dx) = \langle g(p_1, \cdot) | g(p_2, \cdot) \rangle_{L_2(\mathcal{X})},$$

(46)

then the integral transform with kernel $g$ will play the role of a factor as before the mappings $R$ or $B$. Let us recall that in the context of RKHS, cf. Subsection 2.2, such a factorisation is often used as a so-called feature map.

**Definition 22.** Define the integral transform $X : L_2(\mathcal{X}) \to Q$ with kernel $g$ as

$$X : \xi \mapsto \int_{\mathcal{X}} g(\cdot, x)\xi(x) \nu(dx).$$

(47)

This results immediately in a new factorisation of $C_Q$ and a new representation:

**Corollary 23.** The operator $C_Q = RR^*$ with decomposition Eq. (29) has the factorisation

$$C_Q = XX^*.$$  

(48)

Defining the orthonormal system $\{\chi_m\} \subset L_2(\mathcal{X})$ by

$$\lambda_m^{1/2} \chi_m = X^* s_m; \quad \lambda_m^{1/2} \chi_m(x) = \int_P g(p, x)s_m(p) \varpi(dp),$$

(49)

this induces the following Karhunen-Loève representation of $r(x)$ on $\mathcal{X}$:

$$r(x) = \sum_m \lambda_m^{1/2} \chi_m(x)v_m.$$  

(50)

**Proof.** To prove Eq. (48), compute for any $\phi \in Q$ its adjoint transform $(X^* \phi)(x) = \int_P g(p, x)\phi(p) \varpi(dp)$. Now for all $\varphi, \psi \in Q$ it holds that

$$\langle XX^* \varphi | \psi \rangle_Q = \langle X^* \varphi | X^* \psi \rangle_{L_2(\mathcal{X})} = \int_{\mathcal{X}} (X^* \varphi)(x)(X^* \psi)(x) \nu(dx) =$$

$$\int_{\mathcal{X}} \left( \int_P g(p_1, x)\varphi(p_1) \varpi(dp_1) \right) \left( \int_P g(p_2, x)\psi(p_2) \varpi(dp_2) \right) \nu(dx) =$$

$$\int_P \int_{\mathcal{X}} \left( \int_P g(p_1, x)g(p_2, x) \nu(dx) \right) \varphi(p_1)\psi(p_2) \varpi(dp_1)\varpi(dp_2) =$$

$$\int_P X(p_1, p_2)\varphi(p_1)\psi(p_2) \varpi(dp_1)\varpi(dp_2) = \langle C_Q \varphi | \psi \rangle_Q,$$

which is the bilinear form for Eq. (48). The rest follows from Corollary 18 with $\mathcal{H} = L_2(T)$ and $B = X^* UV^* : \mathcal{U} \to L_2(\mathcal{X}) = \mathcal{H}$, as from Eq. (29)

$$XX^* = C_Q = UV^* CVU^* \implies C = (UU^*)X(X^* UV^*) = B^* B.$$

$\square$
The decomposition in Proposition \[20\] may now also be seen in this light by setting \( \mathcal{X} = \mathbb{N} \) with counting measure \( \nu \), such that \( L_2(\mathcal{X}) = \ell_2 \), and \( X \)-transformation kernel \( g(p, m) := \lambda_m^{1/2}s_m(p) \). Then Eq. \[46\] becomes Eq. \[30\], the concrete version of Eq. \[29\].

The result in Eq. \[42\], \( C_Q = (M_{\sqrt{n}}F)^*(M_{\sqrt{n}}F) \) shows that the Fourier diagonalisation in Corollary \[21\] is a special case of such a kernel factorisation with \( X := (M_{\sqrt{n}}F)^* \). As \( \kappa \) is the inverse Fourier transform of \( \hat{\kappa} \),

\[
\kappa(p) = \int_{\mathbb{R}^n} \exp(2\pi i p \cdot \zeta) \hat{\kappa}(\zeta) \, d\zeta,
\]

remembering that with the Fourier transform one has to consider the complex space \( \mathcal{C} = L_2(\mathbb{R}^n, \mathbb{C}) \) with inner product

\[
\forall \varphi, \psi \in \mathcal{C} : \langle \varphi|\psi \rangle_\mathcal{C} := \int_{\mathbb{R}^n} \varphi(\zeta)\overline{\psi(\zeta)} \, d\zeta
\]

(\( \overline{\varphi(\zeta)} \) is the conjugate complex of \( \varphi(\zeta) \)), and by defining the \( X \)-transformation kernel \( \gamma(p, \zeta) := \exp(2\pi i p \cdot \zeta) \sqrt{\hat{\kappa}(\zeta)} \), one obtains the kernel factorisation

\[
x(p_1, p_2) = \kappa(p_1 - p_2) = \int_{\mathbb{R}^n} \exp(2\pi i (p_1 - p_2) \cdot \zeta) \hat{\kappa}(\zeta) \, d\zeta = \int_{\mathbb{R}^n} \left( \exp(-2\pi i p_2 \cdot \zeta) \sqrt{\hat{\kappa}(\zeta)} \right) \left( \exp(2\pi i p_1 \cdot \zeta) \sqrt{\hat{\kappa}(\zeta)} \right) \, d\zeta = \langle \gamma(p_2, \cdot)|\gamma(p_1, \cdot) \rangle_\mathcal{C}.
\]

### 5 Interpretations, decompositions, and reductions

After all the abstract deliberations it is now time to see some concrete examples, which will show that the above description is in many cases an abstract statement of already very familiar constructions.

An important example of these decompositions is when \( \mathcal{U} \) is also a space of functions. Imagine for example a scalar random field \( u(x, \omega) \), where \( x \in \mathcal{X} \subset \mathbb{R}^n \) is a spatial variable, and \( \omega \in \Omega \) is an elementary event in a probability space \( \Omega \) with probability measure \( \mathbb{P} \). Naïvely, at each \( x \in \mathcal{X} \) there is a random variable (RV) \( u(x, \cdot) \), and for each realisation \( \omega \in \Omega \) one has an instance of a spatial field \( u(\cdot, \omega) \). To make things simple, assume that \( u \in L_2(\mathcal{X} \times \Omega) \), which is isomorphic to the tensor product \( L_2(\mathcal{X}) \otimes L_2(\Omega) \equiv L_2(\mathcal{X} \times \Omega) \).

Now one may investigate the splitting \( p = x, \mathcal{P} = \mathcal{X} \) and \( r(p) = u(p, \cdot) \) with \( \mathcal{U} = L_2(\Omega) \) and \( \mathcal{Q} = L_2(\mathcal{X}) \), where for each \( p \in \mathcal{X} \) the model \( r(p) \) is a RV. Then the operator \( C \) is on \( \mathcal{U} = L_2(\Omega) \), and one usually investigates \( C_Q \) on \( \mathcal{Q} = L_2(\mathcal{X}) \), an operator on a spatial field. Turning everything around, one may investigate the splitting \( p = \omega, \mathcal{P} = \Omega \) and \( r(p) = u(\cdot, p) \) with \( \mathcal{U} = L_2(\mathcal{X}) \) and \( \mathcal{Q} = L_2(\Omega) \), where for each \( p \in \Omega \) the model \( r(p) \) is a spatial field. The operator \( C \) on \( \mathcal{U} = L_2(\mathcal{X}) \) is what was before the operator \( C_Q \) and vice versa.

#### 5.1 Examples and interpretations

1. Taking up this first example, assume that the Hilbert space \( \mathcal{U} \) is a space of centred (zero mean) random variables (RVs), e.g. \( \mathcal{U} = L_2(\Omega) \) with inner product \( \langle \xi|\eta \rangle_\mathcal{U} := \mathbb{E}(\xi\eta) = \int_\Omega \xi(\omega)\overline{\eta(\omega)} \, \mathbb{P}(d\omega) \), the covariance, and \( r \) is a zero-mean scalar random field.
and \( r(p) = u(p, \cdot) \) is a zero-mean RV, or a \((n=1)\) stochastic process indexed by \( p \in \mathcal{P} \subseteq \mathbb{R}^n \). Then \( R : \mathcal{U} = L_2(\mathcal{X}) \to \mathcal{Q} = L_2(\mathcal{Y}) \) maps the RV \( \xi \) to its spatial covariance with the random field, \( R\xi = (p \mapsto \mathbb{E}(\xi(\cdot)u(p, \cdot))) \). The representation operator \( R^* \) maps fields into random variables, \( R^*v = \int_\mathcal{X} v(x)u(x, \cdot) \, dx \). The operator \( C \) on \( \mathcal{U} = L_2(\Omega) \) is rarely investigated, more typically one looks at \( C \mathcal{Q} \) on \( \mathcal{Q} = L_2(\mathcal{X}) \), represented by its kernel \( \kappa \) as an integral equation Eq. (35) on the spatial domain \( \mathcal{X} \). The kernel is the usual covariance function \( \kappa(p_1, p_2) \). This is the application where the name Karhunen-Loève expansion was originally used. We have used it here in a more general fashion.

2. Similar to the previous example, but the random field is assumed to be stochastically homogeneous, which means that the covariance function \( \kappa(p_1, p_2) \) is shift invariant or translation invariant. This example has already been shortly described at the end of Subsection 4.1, and there is much literature on this subject, e.g. [22, 24, 54, 16, 52, 53, 33, 28, 35], so we will not further dwell on this.

3. Here we look at the second example’s interpretation of the random field described above. This is a special case of what has been described at the beginning of Section 3 where the measure \( \mathcal{P} \) on \( \mathcal{P} \) is the probability measure \( \mathcal{P} = \mathbb{P} \). For simplicity let \( r(p) \) be a centred \( \mathcal{U} \)-valued RV, and each \( r(p) = u(\cdot, p) \) is an instance of a spatial field. The associated linear operator \( R : \mathcal{U} = L_2(\mathcal{X}) \to \mathcal{Q} = L_2(\Omega) \) maps spatial fields to weighted averages, a RV; \( Rv = \int_\mathcal{X} v(x)u(x, \cdot) \, dx \in \mathcal{Q} = L_2(\Omega) \). It is what \( R^* \) was in the first example. And here the representation operator \( R^* \) is what \( R \) was in the first example. Then \( C \) is the covariance operator, operating on spatial fields. This was \( C \mathcal{Q} \) in the first example.

4. If \( \mathcal{P} = \{1, 2, \ldots, n\} \), then \( \mathcal{U} = \text{span}\{r(\mathcal{P})\} \cong \mathbb{R}^n \) is finite dimensional, and \( \mathbb{R}^\mathcal{P} = \mathbb{R}^n \) by definition. Hence both \( \mathcal{Q} = \mathbb{R}^n \) and \( \mathcal{Q} = \mathbb{R}^n \), possibly with different inner products. In any case, \( \kappa \) is the Gram matrix of the vectors \( \{r_1, \ldots, r_n\} \). The SVDs of \( R \) are matrix SVDs, and the representation map \( R^* \) is connected to the Karhunen-Loève expansion, which here is called the proper orthogonal decomposition (POD).

5. If \( \mathcal{P} = [0, T] \) and \( r(t)(t \in [0, T]) \) is the response of a dynamical system with state space \( \mathcal{U} \), one may take \( \mathcal{Q} = L_2([0, T]) \). The associated linear map \( R \) tells us the dynamics of certain components. To illustrate this, assume for the moment that \( \mathcal{U} = \mathbb{R}^n \), a dynamical system with \( n \) degrees of freedom. Taking each canonical unit vector \( e_j \) in turn, one sees that \( R e_j = (t \mapsto e_j^T u(t) = u_j(t)) \), i.e. the time evolution of the \( j \)-th component. The representation operator \( R^* : \mathcal{Q} \subseteq L_2([0, T]) \) maps scalar time-functions on their weighted average with the dynamics \( R^* \phi = \int_{[0,T]} \phi(t) u(t) \, dt \in \mathcal{U} \).

6. Combining the two previous examples gives the method of temporal snapshots, and the Karhunen-Loève expansion becomes the POD for a dynamical system.

7. If \( \mathcal{P} = \{\omega_s \mid \omega_s \in \Omega\} \) are samples from some probability space \( \Omega \), then one obtains the POD method for samples for some \( \mathcal{U} \)-valued RV.
5.2 Decompositions and model reduction

Let us go back to the example at the beginning in Section 4, where the quantity of interest is the time evolution of a dynamical system, \( t \mapsto v(t, q) \) with state space \( \mathcal{V} \), dependent on a parameter \( q \in \mathcal{S} \). Assume for simplicity that the whole process can be thought of as an element of \( \mathcal{V} \otimes L_2([0, T]) \times \mathcal{S} \cong \mathcal{V} \otimes L_2([0, T]) \otimes L_2(\mathcal{S}) \). One may take \( \mathcal{U} = \mathcal{V} \otimes L_2([0, T]) \), the time-histories in state space, and \( p = q, \mathcal{P} = \mathcal{S}, \) and \( \mathcal{Q} = L_2(\mathcal{S}) \).

But it is also possible to take \( \mathcal{U} = \mathcal{V} \) and \( p = (t, q), \mathcal{P} = [0, T] \times \mathcal{S}, \) \( \mathcal{Q} = L_2([0, T]) \otimes L_2(\mathcal{S}) \). Staying with the latter split, for example the representation Eq. (54) in Theorem 10 becomes

\[
\mathbf{r}(p) = \sum_m \lambda_m^{1/2} s_m(p)v_m = \sum_m \lambda_m^{1/2} s_m((t, q))v_m. \tag{51}
\]

Now each of the scalar function \( s_m((t, q)) \) may be seen as a parametric model \( q \mapsto s_m(\cdot, q) \) of time functions in \( L_2([0, T]) \). So now one may investigate the parametric model based on \( \mathcal{U}_* = L_2([0, T]) \) and \( \mathcal{Q}_* = L_2(\mathcal{S}) \) for each of the \( s_m \).

Frequently the parameter space is a product space

\[
\mathcal{S} = \mathcal{S}_I \times \mathcal{S}_{II} \times \ldots = \prod_K \mathcal{S}_K, \quad K = I, II, \ldots,
\]

with a product measure \( \mathcal{w} = \mathcal{w}_I \otimes \mathcal{w}_{II} \ldots \), with \( s_m(t, q) = s_m(t, (q_I, q_{II}, \ldots)) \). As then

\[
L_2(\mathcal{S}) = L_2(\prod_K \mathcal{S}_K) = L_2(\mathcal{S}_I) \otimes L_2(\mathcal{S}_{II}) \otimes \ldots = \bigotimes_K L_2(\mathcal{S}_K), \quad K = I, II, \ldots,
\]

one obtains

\[
\mathcal{Q} = \mathcal{U}_* \otimes \mathcal{Q}_* = \mathcal{U}_* \otimes \mathcal{Q}_I \otimes \mathcal{Q}_{II} \otimes \ldots, \tag{52}
\]

with \( \mathcal{Q}_K = L_2(\mathcal{S}_K) \) for \( K = I, II, \ldots \). It is clear that \( \mathcal{Q}_* = \otimes_K \mathcal{Q}_K \) may be further split by different associations depending on the value of \( J \):

\[
\mathcal{Q}_* = \mathcal{U}_{**} \otimes \mathcal{Q}_{**} = \left( \bigotimes_{K=I}^J \mathcal{Q}_K \right) \otimes \left( \bigotimes_{K>J} \mathcal{Q}_K \right). \tag{53}
\]

As will be seen, this leads to hierarchical tensor approximations, e.g. [20] [37].

The model space has now been decomposed to

\[
\mathcal{U} \otimes \mathcal{Q} = \mathcal{U} \otimes \mathcal{U}_* \otimes \mathcal{Q}_* = \mathcal{U} \otimes \mathcal{U}_* \otimes \left( \bigotimes_K \mathcal{Q}_K \right). \tag{54}
\]

Computations usually require that one chooses finite dimensional subspaces and bases in there, in the example case of Eq. (54) assume that these are

\[
\text{span } \{ u_n \}_{n=1}^N = \mathcal{U}_N \subset \mathcal{U}, \quad \dim \mathcal{U}_N = N, \tag{55}
\]

\[
\text{span } \{ \tau_j \}_{j=1}^J = \mathcal{U}_{*J} \subset L_2([0, T]) = \mathcal{U}_*, \quad \dim \mathcal{U}_{*J} = J, \tag{56}
\]

\[
\forall \ell_1 = 1, \ldots, L_K, \quad K = I, II, \ldots:
\]

\[
\text{span } \{ s_{\ell_k} \}_{\ell_k=1}^{L_k} = \mathcal{Q}_{K,L_K} \subset L_2(\mathcal{S}_K) = \mathcal{Q}_K, \quad \dim \mathcal{Q}_{K,L_K} = L_K. \tag{57}
\]
An approximation to \( u \in \mathcal{U} \otimes \mathcal{Q} \) in the space described in Eq. (54) is thus given by
\[
u(x,t,q_1,\ldots,\approx N \sum_{n=1}^{J} \sum_{j=1}^{L} \ldots \sum_{\ell \in \mathcal{L}_K} u_{n,j,\ldots,\ell}^{\ell_j,\ldots,\ell_K} \cdot w^{n}(x) \tau^j(t) \left( \prod_{K} s_{\ell_K} (\omega_m) \right) .
\]
(58)

Via the Eq. (58) one sees that the tensor
\[
u = \left( u_{n,j,\ldots,\ell \in \mathcal{L}_K}^{\ell_j,\ldots,\ell_K} \right) \in \mathbb{R}^{(N \times J \times \prod \mathcal{L}_K)} \cong \mathbb{R}^{N} \otimes \mathbb{R}^{J} \otimes \bigotimes_{K} \mathbb{R}^{L_K}
\]
represents the total parametric response \( u(x,t,q_1,\ldots) \).

One way to perform model reduction is to apply the techniques described before on the finite dimensional approximation space of the one described in Eq. (54)
\[\mathcal{U}_N \otimes \mathcal{Q}_M = \mathcal{U}_N \otimes \mathcal{U}_J \otimes \left( \bigotimes_{K} \mathcal{Q}_{K,L_K} \right) := \mathcal{U} \otimes \mathcal{U}_* \otimes \left( \bigotimes_{K} \mathcal{Q}_{K} \right),
\]
(60)
with \( \mathcal{Q}_M = \mathcal{U}_J \otimes \left( \bigotimes_{K} \mathcal{Q}_{K,L_K} \right) \) and dimension \( \text{dim} \mathcal{Q}_M = M = J \times \prod \mathcal{L}_K \) but not using the full dimension, as the spectral analysis of the ‘correlation’ operator \( C \) picks out the important parts.

Another kind of reduction works directly with the tensor \( \nu \) in Eq. (59). It has formally \( R' = N \times J \times \prod \mathcal{L}_K \) terms. Here we only touch on this subject, which is a nonlinear kind of model reduction, and that is to represent this tensor with many times fewer \( R \ll R' \) terms through what is termed a low-rank approximation, for a thorough treatment see the monograph [20].

Whereas the so called canonical polyadic (CP) decomposition uses the flat tensor product in Eq. (54) — under the name proper generalised decomposition (PGD) [39, 38, 1, 29] this is also a computational method to solve an effectively high-dimensional problem as Eq. (1) or Eq. (2), see the review [8] and the monograph [7] — the recursive use of splittings Eq. (53) leads to hierarchical tensor approximations, e.g. [17]. The index set can be thought to be partitioned and arranged into a binary tree, each time causing a split as in Eq. (53), or rather on the finite dimensional approximation Eq. (60), or equivalently in the concrete tensor in Eq. (59). Particular cases of this are the tensor train (TT) [40, 41] and more generally the hierarchical Tucker (HT) decompositions, see the review [18] and the monograph [20]. An example how this representation then allows also fast post-processing such as finding maxima is given in [12]. Let us also mention that these sparse or low-rank tensor representations are connected with the expressive power of deep neural networks [9, 27]. Neural networks are one possibility of choosing the approximation functions in Eq. (57). Obviously, a good reduced order model is one with only few terms. One recognises immediately that the SVD structure of the associated linear map of such a split determines how many terms are needed for a good approximation. Equivalently it is the structure of the spectrum of the appropriate correlation operator associated with the splitting.
6 Refinements

Often the parametric element has more structure than is resolved by saying that for each \( p \in \mathcal{P} \) one has \( r(p) \) in some Hilbert space \( \mathcal{U} \). Most of the preceding had to do with alternative ways of describing the dependence on the parameter \( p \). Here a short look is taken on the case when the Hilbert space \( \mathcal{U} \) has more structure, which one might want to treat separately. One big area, which we only entered slightly, are invariance properties as the invariance w.r.t. shifts for stationary or stochastically homogeneous random fields touched on in Subsection 4.2. We shall look only at two simple but instructive cases.

6.1 Vector fields

One of the simplest variations on the modelling in the previous sections is the refinement that the rôle of the Hilbert space \( \mathcal{Q} \) is taken by a tensor product \( \mathcal{W} = \mathcal{Q} \otimes \mathcal{E} \), where as before \( \mathcal{Q} \) is a Hilbert space of scalar functions and \( \mathcal{E} \) a finite-dimensional inner-product (Hilbert) space. The associated linear map is then a map

\[
R_E : \mathcal{V} \to \mathcal{W} = \mathcal{Q} \otimes \mathcal{E}.
\]

One possible situation where this occurs is when, similar to the third example in Subsection 5.1, the random field \( u(x, p) \) is not scalar- but vector valued, i.e. \( u(x, p) \in \mathcal{E} \). It could be that several correlated scalar fields have to be described which have been collected into a vector \( [u_a(x, p), \ldots, u_j(x, p)] \), or that \( u(x, p) \in \mathbb{R}^n \) is actually to be interpreted as a vector in the space \( \mathbb{R}^n \), e.g. a velocity vector field. Without loss of generality we shall assume that \( \mathcal{E} = \mathbb{R}^n \). This obviously also covers the case when \( \mathcal{E} \) is a space of tensors of higher degree; although for tensors of even degree we shall show a further simplification in Subsection 6.2.

In this case, when \( \mathcal{V} = \mathcal{U} \otimes \mathcal{E} \), the parametric map is

\[
r : \mathcal{P} \to \mathcal{V} = \mathcal{U} \otimes \mathcal{E}; \quad r(p) = \sum_k r_k(p) r_k,
\]

where as before \( r_k(p) \in \mathcal{U} \) — here in the motivating example a Hilbert space of scalar fields — and the \( r_k \in \mathcal{E} \). In this case the associated map \( R_E \) is chosen to be

\[
R_E = \sum_k R_k \otimes r_k : \mathcal{U} \ni u \mapsto \sum_k R_k(u) r_k = \sum_k (u \cdot r_k) U r_k \in \mathcal{Q} \otimes \mathcal{E}.
\]

where the maps \( R_k : \mathcal{U} \to \mathcal{Q} \) are just the maps from Eq. 4, but each \( R_k \) is the associated map to \( r_k(p) \).

The 'correlation' can now be given by a bilinear form, but not with values in \( \mathbb{R} \) as in Definition 8 but with values in \( \mathcal{E} \otimes \mathcal{E} \). For this we define on \( \mathcal{W}^2 = (\mathcal{Q} \otimes \mathcal{E})^2 \) a bilinear form \([ \cdot | \cdot ]\) with values in \( \mathcal{E} \otimes \mathcal{E} \) first on elementary tensors,

\[
\forall s = s \otimes s, t = \tau \otimes \tau \in \mathcal{W} = \mathcal{Q} \otimes \mathcal{E} : \quad [s \otimes s | \tau \otimes \tau] := \langle s | \tau \rangle \mathcal{Q} s \otimes \tau,
\]

and then extended by linearity. Concerning \( \mathcal{U} \) and \( \mathcal{Q} \) we make the same assumptions as before in Subsection 2.1 and Section 3.
Definition 24 (Vector-Correlation). Define a densely defined map \( C_E \) in \( V = U \otimes E \) on elementary tensors as
\[
\forall u = u \otimes u, v = v \otimes v \in V = U \otimes E : \\
\langle C_E u | v \rangle_U := u^T [R_k u | R_j v] = \sum_{k,j} \langle R_k(u) | R_j(v) \rangle_Q (u^T r_k) (r_j^T v)
\]
and extend it by linearity. It may be called the ‘correlation’ operator. By construction it is self-adjoint and positive.

The factorisations and decompositions then have to be of this operator. The eigenproblem on \( V \) is: Find \( \lambda \in \mathbb{R}, v \in U \otimes E \) such that
\[
C_E v = \sum_{k,j,\ell} \langle r_k(p_1) | r_j(p_2) \rangle_U r_k \otimes r_j.
\]
The kernel \( \kappa_E : P^2 \to (E \otimes E) \) for the eigenvalue problem on \( W = Q \otimes E \) is
\[
\kappa_E(p_1, p_2) = \sum_{k,j} \langle r_k(p_1) | r_j(p_2) \rangle_U r_k \otimes r_j.
\]
So \( \kappa \) is matrix-valued. These are actually ‘correlation’ matrices.

In case the function space \( Q \) has the structure of \( L^2(P) \) with measure \( \varpi \) on \( P \), the Fredholm eigenproblem has the following form: Find \( \lambda \in \mathbb{R}, s \in Q \otimes E \) with \( s = \sum_\ell \varsigma_\ell(\cdot) r_\ell \) such that
\[
\int_P \kappa_E(p_1, p_2) \left( \sum_\ell \varsigma_\ell(p_2) r_\ell \right) \varpi(dp_2) = \sum_{k,j,\ell} \left( \int_P \langle r_k(p_1) | r_j(p_2) \rangle_U \varsigma_\ell(p_2) \varpi(dp_2) \right) (r_k^T r_\ell) r_j = \lambda \sum_j \varsigma_j(p_1) r_j.
\]

Both of these eigenproblems then combine into a generalised Karhunen-Loève expansion, the analogue of Eq. (14) in Theorem 10:
\[
r(p) = \sum_k r_k(p) r_k = \sum_m \lambda_m^{1/2} \left( \sum_k \varsigma_m,k(p) v_m,k \right) = \sum_k \left( \sum_m \lambda_m^{1/2} \varsigma_m,k(p) v_m,k \right) r_k.
\]

6.2 Tensor fields

Some situations as described in the previous Subsection 6.1 allow an even somewhat simpler approach. This is the case when the vector space \( E \) in Eq. (61) consist of tensors of even degree. Formally this means that \( E = \mathcal{F} \otimes \mathcal{F} \) for some space of tensors \( \mathcal{F} \) of half the degree. A tensor of even degree can always be thought of as a linear map from a space of tensor of half that degree into itself. Namely, let for example \( A_{abc}^{def} \in E \) be a tensor of even degree—here six. Then this tensor acts as a linear map on the space of tensors of e.g. the form \( f^{ef}_{bf} \in \mathcal{F} \) (the Einstein summation convention for tensor contraction is used in this symbolic index notation):
\[
A_{abc}^{def} f_{bf} = q_{ac}^d.
\]
Often the particular application domain will dictate which space of tensors it acts on. Being a linear map, it can be represented as a matrix $A \in \mathbb{R}^{n \times n}$, which we shall assume from now on. Often these linear maps / matrices have to satisfy some additional properties, for example they have to be positive definite or orthogonal.

It is maybe now the opportunity to make an important remark: The representation methods which have been shown here are linear methods, which means they work best when the object to be represented is in a linear or vector space, essentially free from nonlinear constraints. Consider two illustrative examples:

As a first example, assume that $A$ has to be orthogonal, then one requires $A^T A = I = AA^T$, a nonlinear constraint. It is well known that the orthogonal matrices $O(n)$ form a compact Lie group, just as the sub-group of special orthogonal matrices $SO(n)$. Here it is important to notice that their Lie algebra $o(n) = so(n)$, the tangent space at the group identity $I$, are the skew symmetric matrices, a free linear space. And each $Q \in SO(n)$ can be represented with the exponential map $Q = \exp(S)$ with $S \in so(n)$ and ‘exp(·)’ the matrix exponential. This recipe, using the exponential map from the Lie algebra, which is a vector space, to its corresponding Lie group, is a very general one. One has to deal only with representations on free linear spaces, the Lie algebra, but models entities in the Lie group.

For another example, assume that the matrix $A \in Sym^+(n)$ has to be symmetric positive definite (spd), as is often required when one wants to model constitutive material tensors. One defining condition is that it can be factored as $A = G^T G$ with invertible $G \in GL(n)$. Both of these are nonlinear constraints. In fact the spd matrices are an open cone, a Riemannian manifold, in the space of all symmetric matrices $sym(n)$. There are different ways how to make $Sym^+(n)$ into a Lie group, but the important thing here is that any $A \in Sym^+(n)$ can be represented again with the matrix exponential as $A = \exp(H)$ with $H \in sym(n)$, a free linear space. Let us point out that this also important in the case $n = 1$, i.e. when $A$ is a positive scalar. Here $sym(1) = \mathbb{R}$ and the map $\exp(\cdot)$ is the usual exponential.

A parametric element in this special case of Eq. (62), let us say in the example of positive definite matrices $A(p) \in Q \otimes Sym^+(n)$, would be represented by an element $H(p) \in Q \otimes sym(n)$ and then exponentiated:

$$H(p) = \sum_k \varsigma_k(p) H_k, \quad H(p) \mapsto \exp(H(p)) = A(p).$$

(70)

This way one is sure that $A(p) \in Sym^+(n)$ for each $p \in \mathcal{P}$. Therefore we can now concentrate on the problem of representing $H(p)$.

Here everything is very similar to the previous Subsection 6.1. The associated linear map in Eq. (61) remains as it is, only that now $\mathcal{E} = sym(n)$. The parametric map would be written as

$$R(p) = \sum_k r_k(p) \otimes R_k \in \mathcal{U} \otimes \mathcal{E}, \quad \text{with} \quad R_k \in sym(n).$$

(71)

The correlation corresponding to Definition 24 is now defined as

**Definition 25** (Tensor-Correlation). Define a densely defined map $C_\mathcal{E}$ in $\mathcal{W} = \mathcal{U} \otimes \mathcal{F} = \mathcal{U} \otimes \mathbb{R}^n$ — observe, not $\mathcal{U} \otimes \mathcal{E} = \mathcal{U} \otimes sym(n) = \mathcal{U} \otimes \mathbb{R}^{n(n+1)/2}$ — on elementary tensors
through a bilinear form as

$$\forall (u = u \otimes v), (v = v \otimes v) \in W = U \otimes F :$$

$$\langle C_{\mathcal{F}}u | v \rangle_U := \sum_{k,j} \langle R_k(u) | R_j(v) \rangle_Q (R_ku)^T (R_jv), \quad (72)$$

and extend it by linearity. It may be called the ‘correlation’ operator. By construction it is self-adjoint and positive.

The eigenproblem for $C_{\mathcal{F}}$ corresponding to Eq. (66) is now formulated on $W = U \otimes F = U \otimes \mathbb{R}^n$, i.e. like Eq. (66) but with $\mathcal{E}$ replaced by $\mathcal{F}$, otherwise everything is as before and hence will not be spelled out in detail. The eigenvectors, analogous to Eq. (66), will look the same as there but with $v_{m,j} \in \mathcal{F}$:

$$W \ni v_m = \sum_j v_{m,j} \otimes v_{m,j} \in U \otimes F. \quad (73)$$

The kernel corresponding to Eq. (67) is

$$\kappa_{\mathcal{F}}(p_1, p_2) = \sum_{k,j} \langle r_k(p_1) | r_j(p_2) \rangle_u (R_k^T R_j), \quad (74)$$

with eigenvectors of the form $s_m(p) = \sum_j s_{m,j}(p) v_{m,j} \in Q \otimes \mathcal{F}$. So $\kappa_{\mathcal{F}}$ is matrix-valued here as well. From these the final representation, the analogue of Eq. (14) in Theorem 10 and Eq. (69), is obtained as:

$$R(p) = \sum_k r_k(p) R_k = \sum_m \lambda_m^{1/2} \left( \sum_j s_{m,j}(p) v_{m,j} \otimes v_{m,j} \right). \quad (75)$$

7 Conclusion

A parametric mapping $r : \mathcal{P} \rightarrow U$ has been analysed in a variety of settings. The basic idea is the associated linear map $R : U \rightarrow \mathbb{R}^\mathcal{P}$, which both generalises the parametric mapping and enables the linear analysis. This leads immediately to the RKHS setting, and a first equivalent representation on the RKHS in terms of tensor products. By choosing other inner products than the one coming from the RKHS one can analyse the importance of different features, i.e. subsets of the parameter set.

Importance is measured by the spectrum of the ‘correlation’ operator $C$, and the representation is again in terms of tensor products. The correlation is factored by the associated linear map, and it is shown that on one hand all factorisations are unitarily equivalent, and on the other hand that each factorisation leads to differently parametrised representations, indeed linear resp. affine representations, if the correlation is a nuclear or trace class operator. In fact, each such factorisation corresponds to a representation, and vice versa. This equivalence is due to our strict assumptions on the associated linear map, but in general the associated linear map is a truly more general concept.

These linear representations are in terms of real valued functions, which may be seen as some kind of ‘co-ordinates’ on the parameter set. In the RKHS case, they are truly co-ordinates or an embedding of the parameter set into the RKHS, as each parameter
point \( p \in \mathcal{P} \) can be identified with the evaluation functional \( \delta_p \) and hence the kernel \( \kappa(p, \cdot) \) at that point.

An equivalent spectral analysis can be carried out for the kernel space in terms of integral equations and integral transforms. These spectral decompositions or other factorisations also lend themselves to the construction of parametric reduced order models, as the importance of different terms in the representing Karhunen-Loève- or POD-series can be measured. But other factorisations also lead to, not necessarily optimal, reduced order models. For the sake of simplicity for the representation only orthonormal bases have been considered here as they appear quite natural in the Hilbert space setting, but obviously other bases can be considered. The tensor product nature of this series makes it natural to employ this factorisation in a recursive fashion and thereby to generate a representation through high-order tensors. These often allow very efficient low-rank approximations, which is in fact another, but this time nonlinear, model order reduction. Certain refinements are possible in case the representation space has the structure of a ‘vector’- or ‘tensor’-field, a point which is only briefly touched. It was also shown that the structure of the spectrum of the correlation operator attached to such a tensor-space factorisation, or equivalently the structure of the set of singular values of the associated linear map, determines how many terms are needed in a reduced order model to achieve a certain degree of accuracy.

Thus the functional analytic view on parametric problems via decompositions of linear maps gives a certain unity to seemingly different procedures which turn out to be closely related, at least if one looks for the similarities. This constitutes a natural introduction and background to low-rank tensor product representations, which are crucial for efficient computation. They are naturally employed in a functional approximation approach to parametric problems.

References

[1] A. Ammar, F. Chinesta, and A. Falcó, On the convergence of a greedy rank-one update algorithm for a class of linear systems, Arch Computat Methods Eng 17 (2010), 473–486, \( \text{doi:10.1007/s11831-010-9048-z} \).

[2] K. E. Atkinson, The numerical solution of integral equations of the second kind, Cambridge University Press, Cambridge, 1997.

[3] P. Benner, S. Gugercin, and K. Willcox, A survey of projection-based model reduction methods for parametric dynamical systems, SIAM Review 57 (2015), 483–531, \( \text{doi:10.1137/130932715} \).

[4] P. Benner, M. Ohlberger, A. T. Patera, G. Rozza, and K. Urban (eds.), Model Reduction of Parametrized Systems, MS&A — Modeling, Simulation & Applications, vol. 17, Berlin, Springer, 2017, \( \text{doi:10.1007/978-3-319-58786-8} \).

[5] A. Berlinet and C. Thomas-Agnan, Reproducing kernel Hilbert spaces in probability and statistics, Kluwer, Dordrecht, 2004.

[6] R. N. Bracewell, The Fourier transform and its applications, McGraw-Hill, New York, NY, 1978.

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[7] F. Chinesta, R. Keunings, and A. Leygue, *The proper generalized decomposition for advanced numerical simulations*, Springer, Berlin, 2014.

[8] F. Chinesta, P. Ladevèze, and E. Cueto, *A short review on model order reduction based on proper generalized decomposition*, Arch Computat Methods Eng 18 (2011), 395–404. [doi:10.1007/s11831-011-9064-7]

[9] N. Cohen, O. Sharri, and A. Shashua, *On the expressive power of deep learning: A tensor analysis* [online], arXiv: 1509.05009 [cs.NE], 2016, Available from: [http://arxiv.org/abs/1509.05009](http://arxiv.org/abs/1509.05009).

[10] R. Courant and D. Hilbert, *Methods of mathematical physics*, John Wiley & Sons, Chichester, 1989.

[11] R. Dautray and J.-L. Lions, *Spectral theory and applications*, Mathematical Analysis and Numerical Methods for Science and Technology, vol. 3, Springer, Berlin, 1990.

[12] M. Espig, W. Hackbusch, A. Litvinenko, H. G. Matthies, and E. Zander, *Efficient analysis of high dimensional data in tensor formats*, Sparse Grids and Applications (J. Garcke and M. Griebel, eds.), Lecture Notes in Computational Science and Engineering, vol. 88, Springer, Berlin, 2013, pp. 31–56. [doi:10.1007/978-3-642-31703-3_2]

[13] I. M. Gel’fand and G. E. Shilov, *Properties and operations*, Generalized Functions, vol. 1, Academic Press, New York, NY, 1964.

[14] ______, *Theory of differential equations*, Generalized Functions, vol. 3, Academic Press, New York, NY, 1967.

[15] ______, *Spaces of fundamental and generalized functions*, Generalized Functions, vol. 2, Academic Press, New York, NY, 1968.

[16] I. M. Gel’fand and N. Y. Vilenkin, *Applications of harmonic analysis*, Generalized Functions, vol. 4, Academic Press, New York, NY, 1964.

[17] L. Grasedyck, *Hierarchical singular value decomposition of tensors*, SIAM Journal on Matrix Analysis and Applications 31 (2010), 2029–2054. [doi:10.1137/090764189]

[18] L. Grasedyck, D. Kressner, and C. Tobler, *A literature survey of low-rank tensor approximation techniques*, GAMM-Mitteilungen 36 (2013), 53–78. [doi:10.1002/gamm.201310004]

[19] L. Gross, *Measurable functions on Hilbert space*, Transactions of the American Mathematical Society 105 (1962), no. 3, 372–390. [doi:10.2307/1993726]

[20] W. Hackbusch, *Tensor spaces and numerical tensor calculus*, Springer, Berlin, 2012.

[21] S. Janson, *Gaussian Hilbert spaces*, Cambridge Tracts in Mathematics, 129, Cambridge University Press, Cambridge, 1997.

[22] K. Karhunen, *Zur Spektraltheorie stochastischer Prozesse*, Ann. Acad. Sci. Fennicae. Ser. A. I. Math.-Phys. 34 (1946), 1–7.
[23] ______, Über lineare Methoden in der Wahrscheinlichkeitsrechnung, Ann. Acad. Sci. Fennicae. Ser. A. I. Math.-Phys. 37 (1947), 1–79.

[24] ______, Über die Struktur stationärer zufälliger Funktionen, Arkiv för Matematik 1 (1950), 141–160. doi:10.1007/BF02590624

[25] K. Karhunen, F. Oliva Santos (transl.), and S. Ferrer Martín (transl.), Metodos lineales en el calculo de probabilidades — Über lineare Methoden in der Wahrscheinlichkeitsrechnung — 1947, in Trabajos de Estadistica Y de Investigacion Operativa [23], 59–137, Spanish Translation — Traducción Español, doi:10.1007/bf03002862.

[26] K. Karhunen and I. Selin (transl.), On linear methods in probability theory — Über lineare Methoden in der Wahrscheinlichkeitsrechnung — 1947, U.S. Air Force — Project RAND T-131, The RAND Corporation, St Monica, CA, USA, August 1960, English Translation, Available from: https://www.rand.org/pubs/translations/T131.html.

[27] V. Khrulkov, A. Novikov, and I. Oseledets, Expressive power of recurrent neural networks [online], arXiv: 1711.00811 [cs.LG], 2018, Available from: http://arxiv.org/abs/1711.00811.

[28] P. Krée and C. Soize, Mathematics of random phenomena—random vibrations of mechanical structures, D. Reidel, Dordrecht, 1986.

[29] P. Ladevèze and L. Chamoin, On the verification of model reduction methods based on the proper generalized decomposition, Computer Methods in Applied Mechanics and Engineering 200 (2011), no. 23–24, 2032–2047, doi:10.1016/j.cma.2011.02.019.

[30] O. P. Le Maître and O. M. Knio, Spectral methods for uncertainty quantification, Scientific Computation, Springer, Berlin, 2010.

[31] M. Loève, Fonctions aléatoires de second ordre, C. R. Acad. Sci. 220 (1945), 295–296.

[32] ______, Fonctions aléatoires de second ordre, C. R. Acad. Sci. 222 (1946).

[33] M. Loève, Probability theory II, 4th ed., Graduate Texts in Mathematics, vol. 46, Springer, Berlin, 1978.

[34] D. G. Luenberger, Optimization by vector space methods, John Wiley & Sons, Chichester, 1969.

[35] H. G. Matthies, Uncertainty quantification with stochastic finite elements, Encyclopaedia of Computational Mechanics (E. Stein, R. de Borst, and T. J. R. Hughes, eds.), vol. 1, John Wiley & Sons, Chichester, 2007, Part 1. Fundamentals. Encyclopaedia of Computational Mechanics, doi:10.1002/0470091355.ecm071.

[36] ______, Uncertainty quantification and Bayesian inversion, Encyclopaedia of Computational Mechanics (E. Stein, R. de Borst, and T. J. R. Hughes, eds.), vol. 1, John Wiley & Sons, Chichester, 2nd ed., 2017, Part 1. Fundamentals. Encyclopaedia of Computational Mechanics, doi:10.1002/9781119176817.ecm2071.
[37] H. G. Matthies, A. Litvinenko, O. Pajonk, B. V. Rosić, and E. Zander, *Parametric and uncertainty computations with tensor product representations*, Uncertainty Quantification in Scientific Computing (A. Dienstfrey and R. Boisvert, eds.), IFIP Advances in Information and Communication Technology, vol. 377, Springer, Boulder, CO, 2012, pp. 139–150, doi:10.1007/978-3-642-32677-6.

[38] A. Nouy, *Proper generalized decompositions and separated representations for the numerical solution of high dimensional stochastic problems*, Archives of Computational Methods in Engineering 17 (2010), 403–434, doi:10.1007/s11831-010-9054-1.

[39] A. Nouy and O. P. Le Maître, *Generalized spectral decomposition for stochastic nonlinear problems*, Journal of Computational Physics 228 (2009), no. 1, 202–235, doi:10.1016/j.jcp.2008.09.010.

[40] I. Oseledets and E. Tyrtyshnikov, *TT-cross approximation for multidimensional arrays*, Linear Algebra and its Applications 432 (2010), 70–88, doi:10.1016/j.laa.2009.07.024.

[41] I. V. Oseledets, *Tensor-train decomposition*, SIAM J. Sci. Comput. 33 (2011), no. 5, 2295–2317, doi:10.1137/090752286.

[42] M. Reed and B. Simon, *Fourier analysis and self-adjointness*, Methods of modern mathematical Physics, vol. II, Academic Press, New York, NY, 1975.

[43] ______, *Functional analysis*, Methods of modern mathematical Physics, vol. I, Academic Press, New York, NY, 1980.

[44] I. E. Segal, *Tensor algebras over Hilbert spaces I*, Transactions of the American Mathematical Society 81 (1956), no. 1, 106–134, doi:10.2307/1993234.

[45] ______, *Distributions in Hilbert space and canonical systems of operators*, Transactions of the American Mathematical Society 88 (1958), no. 1, 12–41, doi:10.2307/1993234.

[46] ______, *Nonlinear functions of weak processes. I*, Journal of Functional Analysis 4 (1969), no. 3, 404–456, doi:10.1016/0022-1236(69)90007-X.

[47] I. E. Segal and R. A. Kunze, *Integrals and operators*, Springer, Berlin, 1978.

[48] R. C. Smith, *Uncertainty quantification: Theory, implementation, and applications*, Computational Science & Engineering, vol. 12, SIAM, Philadelphia, PA, 2014.

[49] C. Soize and C. Farhat, *A nonparametric probabilistic approach for quantifying uncertainties in low-dimensional and high-dimensional nonlinear models*, International Journal for Numerical Methods in Engineering 109 (2017), 837–888, doi:10.1002/nme.5312.

[50] G. Strang, *Introduction to applied mathematics*, Wellesley-Cambridge Press, Wellesley, MA, 1986.

[51] D. Xiu, *Numerical methods for stochastic computations: a spectral method approach*, Princeton University Press, Princeton, NJ, 2010.
[52] A. M. Yaglom, *Correlation theory of stationary and related random functions I*, Springer, Berlin, 1968.

[53] ———, *Correlation theory of stationary and related random functions II*, Springer, Berlin, 1968.

[54] ———, *An introduction to the theory of stationary random functions*, Dover, Mineola, NY, USA, 2004.

[55] K. Yosida, *Functional analysis*, 6th ed., Springer, Berlin, 1980.