Karhunen-Loève Decomposition in the Presence of Symmetry Part I

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Abstract

The Karhunen-Loève decomposition is widely used to data which very often exhibits some symmetry, afforded by a group action. For a finite group we derive an algorithm using group representation theory to reduce the cost of determining the KL basis. We demonstrate the technique on a Lorenz-type ODE system. For a compact group such as tori or $SO(3,\mathbb{R})$ the method also applies, and we extend results to these cases. As a short example we consider the circle group S^1.

1 Introduction

The Karhunen-Loève (KL) Decomposition (or Principal Component Analysis) is a powerful tool for linear data compression [1]. This technique for analyzing a finite data set in a vector space V finds the optimal basis for the ambient space in the sense that the truncation errors are minimized for every desired compression dimension.

It is quite typical in data obtained from imaging or physical modeling that the underlying set of images or patterns enjoys some symmetry. In the image processing domain, bilateral symmetry is nearly ubiquitous (see for example [5]); more complicated image symmetry is evident in many atmospheric data imaging applications (where spherical symmetry is

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present) and imaging of wave phenomena (where circular or translational symmetry is often apparent). The model partial differential equations for many physical processes exhibit inherent symmetry, which is generally well reflected in both experimental data and simulation data. The concept of symmetry in data sets is always related to the action of a group G on V, which carries the data set onto itself.

Whenever a group acts linearly on a vector space, the space splits into irreducible subspaces for the action; for each irreducible representation ρ of the group G there are $\dim(\rho)$ corresponding projectors P_{ii}^{ρ} whose images are the "symmetry subspaces" V_i^{ρ}. There are natural isomorphisms P_{ij}^{ρ} between V_i^{ρ} and V_j^{ρ} when $i \neq j$. Therefore for data enjoying symmetry, we have two apparently competing decompositions of the ambient vector space, one coming from the KL basis and one coming from the group representations. In this paper we analyze the relationship between these two decompositions, and prove the following.

Theorem 1.1 *The KL basis for the full vector space V is obtained by projecting the data set (via the orthogonal projectors P_{11}^{ρ}) into the first symmetry subspaces V_1^{ρ} for each ρ, and computing a KL basis for the projected data set in V_1^{ρ}. These separate bases are then transfered (via the isomorphisms P_{j1}^{ρ}) to the other symmetry subspaces V_j^{ρ}, and concatenated to form the full KL basis for V.*

The KL basis for a data set in $\mathbb{R}^n$ is obtained by forming the n-by-n covariance matrix of the data and taking the eigenvectors. We show that the above process of passing to the symmetry subspaces reduces the full KL problem to a series of subproblems, each of smaller dimension. The total computational complexity is correspondingly reduced.

In Section 2 we introduce basic facts about the KL decomposition. In Section 3 we present the relevant facts concerning group representation theory which we require. Section 4 is the main part of the paper; there we combine the KL decomposition with the group theory to divide the problem into the sub-problems. We will not present proofs of the lemmas here, which are easy consequences of well-known results in group representation theory and quantum physics [10].

In Section 5 we present the analysis of the computational efficiency of the method for a finite group, and in Section 6 we present a simple example illustrating the technique. In Section 7 we remark on the application of these techniques to compact Lie groups, but will only present the example of the circle group S^1.

In this paper (Part I) we focus on the general theory, and develop it in detail for finite groups, giving an example in this case. In Part II, we will concentrate on compact Lie groups, and illustrate this theory by presenting the much more interesting and therefore complicated case of the special orthogonal group $SO(3)$.

The exploitation of symmetry in KL decomposition was first recognized by Sirovich in [7]; a recent preprint of Smaoui and Armbruster applies these methods to eigenfunction computations [8].

2 The Karhunen-Loève Decomposition

Let V be a complex vector space of dimension d containing a finite set U of N *pattern* vectors, say $U = \{u_i\}_{i=1}^N$. We assume that V is equipped with the standard Hermitian inner product defined by $(x, y) = \overline{x}^\top \cdot y$. The Karhunen-Loève decomposition of this set U of patterns provides an orthonormal basis for V which is optimal for arbitrary truncation errors, which we now explain.

Let $\mathcal{B} = \{v_1, \ldots, v_d\}$ be an ordered orthonormal basis for V. Then for any vector $u_i \in U$, we may write u_i uniquely as $u_i = \sum_j a_j v_j$, without error. The D-truncation of u_i with respect to this basis $\mathcal{B}$ is the vector $u_i^{(D)} = \sum_{j \le D} a_j v_j$, and the error vector of this truncation is $e_i^{(D)} = u_i - u_i^{(D)}$.

Given the set of pattern vectors U, and the basis $\mathcal{B}$, we define the *mean square error* of the D-truncation to be

$$e_{mse}^{(D)} = \frac{1}{|U|} \sum_i \|e_i^{(D)}\|^2.$$

The KL basis for V is that orthonormal basis for which the mean square errors $e_{mse}^{(D)}$ are minimized for every D between 1 and d.

The construction of the KL basis for V is well-known and given by the following theorem; recall that $u^* = \overline{u}^\top$.

Theorem 2.1 *The KL basis is given by the eigenvectors of the ensemble average covariance matrix* $C = (1/|U|)\sum_i u_i u_i^*$.

For a reference, see [1].

This covariance matrix C is positive definite Hermitian; thus, it has only non-negative real eigenvalues.

3 Basics from Group Representation Theory

In this section we collect the basic results of the representation theory of finite groups which we require. All of the results are completely standard and may be found in many texts, e.g. [4], [6], [9], [10].

Let G be a finite group with identity I and $|G|$ elements. Let V be a finite dimensional complex vector space. A *representation* of G on V is a homomorphism $\rho : G \to GL(V)$ of G to the group of linear automorphisms of V. Sometimes V is also called the representation of G. We will often write $g \cdot v$ or gv for $\rho(g)(v)$. The dimension of V is sometimes called the dimension, or degree, of ρ.

A subspace W of V is *invariant* under G if $gw \in W$ for all $g \in G$ and $w \in W$. A representation V is called *irreducible* if there is no proper nonzero invariant subspace of V. A finite group G admits only finitely many irreducible representations up to isomorphism; the number of irreducible representations of G is equal to the number c of conjugacy classes.

Suppose that W is a representation of G and $L : W \to W$ is a linear transformation which is G-equivariant, that is $L(gw) = gL(w)$ for every $g \in G$ and $w \in W$. If W is an irreducible representation, Schur's Lemma implies that every G-equivariant map is a multiple of the identity.

For each irreducible representation ρ we write $A^\rho(g)$ for the matrix $\rho(g)$; its entries are then $A^\rho_{ij}(g)$, for $1 \leq i, j \leq \dim(\rho)$. We have the following basic orthogonality relations for the entries of these A^ρ matrices:

$$\frac{1}{|G|}\sum_{g\in G} A^\rho_{ij}(hg)A^\tau_{k\ell}(g^{-1}) = \frac{1}{\dim(\rho)}A^\rho_{i\ell}(h)\delta_{jk}\delta_{\rho\tau} \tag{3.1}$$

(For a proof, see [3] or [6].) Define, for any representation V of G, the operator

$$P^\rho_{ij} = \frac{\dim(\rho)}{|G|}\sum_{g\in G} A^\rho_{ji}(g^{-1})g.$$

We define $V^\rho_i = \text{Image}(P^\rho_{ii})$ for $1 \leq i \leq \dim(\rho)$ and $V^\rho = \sum_{i=1}^{\dim(\rho)} V^\rho_i$.

The following now follows completely formally from the orthogonality relations:

Proposition 3.2 *These mappings $P^\rho_{ij} : V \to V$ have the following properties:*

(a) For ρ and τ irreducible representations of G, $P^\rho_{ij} \circ P^\tau_{kl} = P^\tau_{il}\delta_{\rho\tau}\delta_{jk}$

(b) The operators $\{P^\rho_{ii}\}$ are orthogonal projectors.

(c) The sum of these projectors is the identity on V: $\sum_\rho \sum_{i=1}^{\dim(\rho)} P^\rho_{ii} = I$.

(d) The space V splits as the direct sum $V = \bigoplus_\rho \bigoplus_{i=1}^{\dim(\rho)} V^\rho_i$.

(e) For $i \neq j$ the operator P^ρ_{ij} maps V^ρ_j isomorphically onto V^ρ_i, and is zero on V^τ_k if $\tau \neq \rho$ or $k \neq j$.

(f) For each ρ the sum $V^\rho = \sum_{i=1}^{\dim(\rho)} V^\rho_i$ is a direct sum, and is a G-invariant subspace of V, isomorphic to the irreducible representation ρ taken exactly $\dim(V^\rho_1)$ times.

We will say that a basis for V is *G-adapted* if it is formed by taking, for each ρ, a basis $\{v^\rho_{1,\alpha}\}$ for V^ρ_1, and applying the transfer operators P^ρ_{j1} for each j with $2 \leq j \leq \dim(\rho)$ to obtain bases $\{v^\rho_{j,\alpha} = P^\rho_{j1}(v^\rho_{1,\alpha})\}$ for V^ρ_j, and then concatenating these bases to obtain a basis $\{v^\rho_{j,\alpha}\}_{\rho,j,\alpha}$ for V.

We may take each irreducible representation to be unitary, so that $\rho^*(g)\rho(g) = I$ for every g; we will assume this in what follows. If we choose, in each subspace V_1^ρ, the basis $\{v_{1,\alpha}^\rho\}$ to be orthonormal, and the irreducible representations of G are all taken to be unitary, then an easy computation shows that the entire basis for V constructed in this way is orthonormal, so that $(v_{i,\alpha}^\rho)^* v_{j,\beta}^\tau = \delta_{\rho\tau}\delta_{ij}\delta_{\alpha\beta}$.

In this case we also have that $(P_{ij}^\rho(v))^* = v^* P_{ji}^\rho$, considering the operators as matrices.

4 KL Decomposition with Symmetry

Let V be a complex vector space and G a finite group of order $|G|$ acting on V. Moreover let us assume that the action is *unitary*, so that $g^*g = I$ for every $g \in G$. (We will usually suppress the notation for the mapping of G into $GL(V)$ and simply consider each $g \in G$ as a unitary matrix operator on V.)

Let V be the ambient space for a set of patterns $\mathcal{U}$; we think of $\mathcal{U}$ as the set of all possible patterns coming from the data being collected. The set $\mathcal{U}$ is typically a submanifold lying inside the vector space V.

Our symmetry hypothesis is that $\mathcal{U}$ is invariant under the action of G on V: for every $g \in G$ and $u \in \mathcal{U}$, the translate $g \cdot u$ is also in $\mathcal{U}$.

Note that this symmetry assumption is *not* that each pattern in $\mathcal{U}$ is G-invariant; only that a translate of a pattern is again a possible pattern.

Suppose we have a finite set of N patterns $U = \{u_i\}_{i=1}^N$ which lie in $\mathcal{U}$. We want to exploit the group action and the symmetry assumption to extract information about the KL basis for U.

This basis is given by the eigenvectors of the ensemble average covariance matrix $C = \frac{1}{N}\sum_{i=1}^N u_i u_i^*$.

Every pattern in U gives rise to $|G|$ other patterns by translating by the elements of the group; all of these patterns also will lie in the pattern space $\mathcal{U}$ by our symmetry assumption.

We "symmetrize" the data by collecting these $N|G|$ patterns in the set $\tilde{U}$:

$$\tilde{U} = \{g \cdot u \mid g \in G, u \in U\}.$$

A basis for the KL subspace based on this new set of patterns is given by the eigenvectors of the ensemble average covariance matrix $\tilde{C}$ which is defined using the enlarged set of patterns $\tilde{U}$:

$$\tilde{C} = \frac{1}{N|G|} \sum_{g \in G} \sum_{u \in U} (g \cdot u)(g \cdot u)^* = \frac{1}{N|G|} \sum_{g \in G} \sum_{u \in U} (guu^* g^*) = \frac{1}{|G|} \sum_{g \in G} gCg^*$$

The matrix $\tilde{C}$ is a $d \times d$ matrix, and as such can be viewed as an operator on the vector space V. It is easily seen to be G-equivariant. This G-equivariance immediately implies the following, which is a version of Wigner's Theorem:

Theorem 4.1

(a) The operator $\tilde{C}$ commutes with the projectors and transfer operators P^{ρ}_{ij}, and therefore each subspace V^{ρ}_i is $\tilde{C}$-invariant. Hence if we change to a G-adapted basis for V, the matrix $\tilde{C}$ will be in block form, with block B^{ρ}_i for the subspace V^{ρ}_i. In particular, the eigenvectors of $\tilde{C}$ can be taken to lie in the subspaces V^{ρ}_i.

(b) The blocks B^{ρ}_i are in fact independent of i: $B^{\rho}_i = B^{\rho}$ for each i. A vector $v \in V^{\rho}_j$ is an eigenvector for $\tilde{C}$ with eigenvalue λ if and only if the transfered vector $P^{\rho}_{ij}(v) \in V^{\rho}_i$ is an eigenvector for $\tilde{C}$ with eigenvalue λ.

(c) The eigenvalues of $\tilde{C}$ on $V^{\rho} = \sum_{i=1}^{\dim(\rho)} V^{\rho}_i$ each occur with multiplicity equal to a multiple of $\dim(\rho)$.

The $\alpha\beta$ entry of B^{ρ} is

$$(B^{\rho})_{\alpha\beta} = (v^{\rho}_{1\alpha})^* \tilde{C} v^{\rho}_{1\beta} = \frac{1}{|G||U|} \sum_{g,u} ((v^{\rho}_{1\alpha})^* gu)((v^{\rho}_{1\beta})^* gu)^*.$$

The numbers $(v^\rho_{1\alpha})^* gu$ are exactly the coordinates, in the G-adapted orthonormal basis, of the vectors gu, projected into V^ρ_1. Therefore, viewing P^ρ_{11} as a map from V to V^ρ_1, we have that

$$B^\rho = \frac{1}{|G||U|} \sum_{g,u} P^\rho_{11}(gu) P^\rho_{11}(gu)^* \tag{4.2}$$

and so B^ρ can be viewed as the covariance matrix of the projected symmetrized data. The following Lemma will be useful in the implementation of the reduction algorithm which will follow below.

Lemma 4.3 *Let ρ be an irreducible unitary representation of G, with matrices $A^\rho_{ij}(g)$ for $g \in G$.*

(a) For $v \in V$ and $g \in G$ we have $P^\rho_{ij}(gv) = \sum_k A^\rho_{jk}(g) P^\rho_{ik}(v)$.

(b) For $v \in V$ we have $\frac{1}{|G|} \sum_{g \in G} P^\rho_{11}(gv) P^\rho_{11}(gv)^* = \frac{1}{\dim(\rho)} \sum_k P^\rho_{1k}(v) P^\rho_{1k}(v)^*$.

Proof: To prove (a), we see that

$$\begin{aligned}
P^\rho_{ij}(gv) &= \frac{1}{|G|} \sum_{a \in G} A^\rho_{ji}(a^{-1}) agv = \frac{1}{|G|} \sum_{b \in G} A^\rho_{ji}(gb^{-1}) bv \quad (\text{setting } b = ag) \\
&= \frac{1}{|G|} \sum_{b \in G} \sum_k A^\rho_{jk}(g) A^\rho_{ki}(b^{-1}) bv \\
&= \sum_k A^\rho_{jk}(g) \frac{1}{|G|} \sum_{b \in G} A^\rho_{ki}(b^{-1}) bv = \sum_k A^\rho_{jk}(g) P^\rho_{ik}(v).
\end{aligned}$$

Now (b) follows since by (a) we have $P^\rho_{11}(gv) = \sum_k A^\rho_{1k}(g) P^\rho_{1k}(v)$ and so

$$\begin{aligned}
\frac{1}{|G|} \sum_{g \in G} P^\rho_{11}(gv) P^\rho_{11}(gv)^* &= \frac{1}{|G|} \sum_{g \in G} \sum_{k,\ell} A^\rho_{1k}(g) P^\rho_{1k}(v) P^\rho_{1\ell}(v)^* \overline{A^\rho_{1\ell}(g)} \\
&= \sum_{k,\ell} [\frac{1}{|G|} \sum_{g \in G} A^\rho_{1k}(g) A^\rho_{\ell 1}(g^{-1})] P^\rho_{1k}(v) P^\rho_{1\ell}(v)^* \\
&= \frac{1}{\dim(\rho)} \sum_k P^\rho_{1k}(v) P^\rho_{1k}(v)^*
\end{aligned}$$

since in the second line the bracketed expression equals $\frac{1}{\dim(\rho)} \delta_{k\ell}$ using (3.1). **Q.E.D.**

Combining 4.2 with the previous Lemma gives us that

$$B^\rho = \frac{1}{\dim(\rho)|U|} \sum_{u \in U} \sum_{k=1}^{\dim(\rho)} P_{1k}^\rho(u) P_{1k}^\rho(u)^* \tag{4.4}$$

We note that this formula for B^ρ is more efficient than the formula (4.2); the sum is over the dimension of the representation ρ instead of over the group elements. In order to use this to compute the entries of the matrix for B^ρ, we have the following lemma.

Lemma 4.5 *Let $\{v_{k\beta}^\rho\}$ be a G-adapted basis for V^ρ (so that $\{v_{1\beta}^\rho\}$ is an orthonormal basis for V_1^ρ). Then the entries $b_{\alpha\beta}^\rho$ of B^ρ in this basis are*

$$b_{\alpha\beta}^\rho = \frac{1}{\dim(\rho)|U|} \sum_{u} \sum_{k=1}^{\dim(\rho)} (v_{k\alpha}^\rho)^* u u^* v_{k\beta}^\rho.$$

Proof: Since $\{v_{1\beta}^\rho\}$ is an orthonormal basis for V_1^ρ, the $\alpha\beta$ entry of B^ρ is

$$b_{\alpha\beta}^\rho = (v_{1\alpha}^\rho)^* B^\rho v_{1\beta}^\rho = \frac{1}{\dim(\rho)|U|} \sum_{u} \sum_{k=1}^{\dim(\rho)} (v_{1\alpha}^\rho)^* P_{1k}^\rho(u) P_{1k}^\rho(u)^* v_{1\beta}^\rho \tag{4.6}$$

using (4.4). For any γ, we have

$$\begin{aligned}
(v_{1\gamma}^\rho)^* P_{1k}^\rho(u) &= \frac{\dim(\rho)}{|G|} \sum_{g \in G} A_{k1}^\rho(g^{-1}) (v_{1\gamma}^\rho)^* g u \\
&= \frac{\dim(\rho)}{|G|} \sum_{g \in G} \overline{A_{1k}^\rho(g)} (g^* v_{1\gamma}^\rho)^* u \\
&= \frac{\dim(\rho)}{|G|} \sum_{g \in G} \overline{A_{1k}^\rho(g) u^* (g^* v_{1\gamma}^\rho)} \\
&= \overline{u^*} \frac{\dim(\rho)}{|G|} \sum_{a \in G} \overline{A_{1k}^\rho(a^{-1}) a v_{1\gamma}^\rho} \quad \text{setting } a = g^* \\
&= \overline{u^*} \overline{P_{k1}^\rho(v_{1\gamma}^\rho)} \\
&= \overline{u^*} \overline{v_{k\gamma}^\rho} \text{ since the basis is } G\text{-adapted} \\
&= (v_{k\gamma}^\rho)^* u
\end{aligned}$$

so that $(v_{1\alpha}^\rho)^* P_{1k}^\rho(u) = (v_{k\alpha}^\rho)^* u$ and $P_{1k}^\rho(u)^* v_{1\beta}^\rho = u^* v_{k\beta}^\rho$. Plugging these into the equation (4.6) gives the result. **Q.E.D.**

The previous Lemma motivates the following notation. For each pattern u, define the column vector u_k^ρ (whose dimension is equal to $\dim V_1^\rho$) by setting the α coordinate equal to

$$(u_k^\rho)_\alpha = (v_{k\alpha}^\rho)^* u$$

where $\{v_{k\alpha}^\rho\}$ is the given G-adapted basis for V. Then Lemma 4.5 exactly says that

$$B^\rho = \frac{1}{\dim(\rho)|U|} \sum_u \sum_{k=1}^{\dim(\rho)} (u_k^\rho)(u_k^\rho)^*. \tag{4.7}$$

It is the above formuation which enables us now to give a precise algorithm for exploiting the symmetry assumption in determining a KL basis for V.

Algorithm for Exploiting Symmetry

in the KL basis computation:

Given: A complex vector space V of dimension d, a set of patterns U drawn from a pattern subset $\mathcal{U}$, and a unitary symmetry group G satisfying $g \cdot u \in \mathcal{U}$ for all $g \in G$ and $u \in U$.

1. Determine the irreducible unitary representations ρ of G, and a G-adapted basis $\{v^{\rho}_{k\alpha}\}$ for V. Let d_ρ be the dimension of V^{ρ}_{1}.

2. For each ρ, each $k = 1, \ldots, \dim(\rho)$, and each pattern $u \in U$, form the vector u^{ρ}_{k} of dimension d_ρ by $(u^{\rho}_{k})_\alpha = (v^{\rho}_{k\alpha})^* u$.

3. For each ρ, form the $d_\rho \times d_\rho$ matrix B^ρ of $\tilde{C}|_{V^{\rho}_{1}}$ by $B^\rho = \frac{1}{\dim(\rho)|U|} \sum_u \sum_{k=1}^{\dim(\rho)} (u^{\rho}_{k})(u^{\rho}_{k})^*$.

4. For each ρ, find the d_ρ eigenvalues λ^{ρ}_{α} and corresponding eigenvectors w^{ρ}_{α} (for $1 \leq \alpha \leq d_\rho$) of the matrix B^ρ. Write each eigenvector as $w^{\rho}_{\alpha} = (w^{\rho}_{\alpha 1} \cdots w^{\rho}_{\alpha d_\rho})^\top$.

5. Define

$$z^{\rho}_{k\alpha} = \sum_{\beta} w^{\rho}_{\alpha\beta} v^{\rho}_{k\beta}$$

for each ρ, each $k = 1, \ldots, \dim(\rho)$, and each $\alpha = 1, \ldots, d_\rho$. The KL basis for V consists of these vectors $z^{\rho}_{k\alpha}$, each with eigenvalue λ^{ρ}_{α} (independent of k).

We note that Step 1 is to be considered as the overhead of the method, which can be done once, and subsequently applied to many different KL problems in the space V. The power of the method is that it replaces the eigenvector computation for the large $d \times d$ matrix $\tilde{C}$ with several eigenvector computations of the smaller matrices B^ρ.

5 The Computational Efficiency

In order to calculate the efficiency of the proposed method, we assume that a general method such as QR is used to compute the eigenvectors and eigenvalues of symmetric (or Hermitian) matrices; for a $k \times k$ matrix, these methods are typically of order k^3, that is, the number of flops required to find the eigenvectors and eigenvalues is approximately ak^3 for some constant a (see [2] for example).

Therefore in our original problem, the cost of directly computing the KL basis is ad^3, since d is the dimension of the ambient space V.

The dimension of the symmetry subspaces V_k^ρ for each irreducible representation depends on the precise nature of the representation of the group G on the space V. However it is quite typical that this representation is a direct sum of several copies of the regular representation, or varies from this in a minor way often due to fixed points in a permutation representation. For the regular representation, which is of dimension $|G|$, the dimension of the first symmetry subspace V_1^ρ is $\dim(\rho)$. Therefore if V is approximately a direct sum of regular representations, then the dimension of V_1^ρ will be approximately $d_\rho = d \cdot \dim(\rho)/|G|$. Hence the cost of finding the eigenvectors in this symmetry subspace will be approximately $ad^3 \dim(\rho)^3/|G|^3$.

Solving this sub-problem for each ρ and summing, we see that the approximate ratio of the cost of solving the original problem to the cost of using the method outlined above is

$$\alpha(G) = \frac{ad^3}{ad^3 \sum_\rho \dim(\rho)^3/|G|^3} = \frac{|G|^3}{\sum_\rho \dim(\rho)^3}.$$

For a cyclic group C_m of order m, all irreducible representations ρ are one–dimensional, and there are m of them. Hence $\alpha(C_m) = m^2$.

For a dihedral group $D_{m/2}$ of order m (where m is even), all irreducible representations are either one– or two–dimensional; there are at most 4 representations of degree one and approximately $m/4$ representations of degree two, the precise numbers depending on the value of m modulo 4. Therefore $\alpha(D_{m/2}) \approx m^2/2$. For the group D_4 of symmetries of the square, the precise factor is $128/3 \approx 42$.

Finally we look at the group O of symmetries of the cube; it has order 48 and there are

4 irreducible representations of degree one, 2 of degree 2, and 4 of degree 3. Therefore

$$\alpha(O) = \frac{48^3}{4 \cdot 1^3 + 2 \cdot 2^3 + 4 \cdot 3^3} = 110592/128 = 864.$$

The other extreme situation is when each $d_\rho = 1$. In this case each submatrix B^ρ is simply a number, equal to the eigenvalue λ_1^ρ, and no eigenvector computations are required: the eigenvectors are exactly vectors $\{v_{k\alpha}^\rho\}$ of the G-adapted basis. This very special situation actually occurs more often than one might expect, especially for the compact Lie groups.

Finally we remark that this method is useful when the number of patterns N is much larger than the dimension of the ambient space V.

6 An Example

As noted in the Introduction, it is typical that data obtained from physical modeling enjoys some symmetry, because the underlying differential equations governing the evolution of the pattern data is equivariant under a group action. In particular, for an ODE system of the form $\dot{x} = F(x)$, if $F(\sigma x) = \sigma F(x)$ for all σ in a group G, then whenever $x(t)$ is a trajectory for the dynamical system, so will $\sigma x(t)$ be. Hence pattern data arising from time series of the evolution of trajectories will enjoy the symmetry of the group G.

In this section we present an example of this type using data generated by a 7-dimensional ODE system which exhibits S_3 symmetry. The ODE system we consider has variables x_i, y_i for $i = 1, 2, 3$ and p; the system is given by

$$\begin{aligned}
\dot{x}_i &= \sigma(y_i - x_i) \\
\dot{y}_i &= \tau x_i - y_i - p x_i \\
\dot{p} &= -bp + \frac{a}{3} \sum_{i=1}^{3} x_i y_i.
\end{aligned}$$

This system was kindly suggested to us by Gerhard Dangelmayr. We use as parameters $\sigma = 10$, $\tau = 28$, $b = \frac{8}{3}$, and $a = 1$, which gives a symmetry-adapted Lorenz-type system exhibiting a strange attractor with a chaotic trajectory. We hope that the chaotic nature of the trajectory produces data which "fills up" the attractor, allowing us to use one trajectory to produce a good approximation to the attractor.

The group S_3 acts simply by permuting the indices of the x_i's and y_i's; the variable p is fixed. It is clear that the ODE is preserved by this action, and therefore solutions to the ODE are carried into other solutions.

After choosing an initial condition randomly, a trajectory is generated for each time step t; this gives a 7-dimensional vector $\underline{x}(t)$ for each time step. A fourth-order Runge-Kutta scheme was used to generate 5000 time steps; the first 1000 were discarded, producing a data set U of 4000 vectors in the 7-dimensional space V.

S_3 has three irreducible representations: the one-dimensional trivial representation W_1, the one-dimensional alternating representation W_2, and the two-dimensional standard representation W_3. The alternating representation does not occur in our 7-dimensional representation V; the trivial representation occurs 3 times and the standard occurs twice. Hence there are three symmetry subspaces: V_1^1 is 3-dimensional, V_1^3 and V_2^3 are two-dimensional. G-adapted bases for these subspaces are:

$$
\begin{aligned}
V_1^1: \quad v_{11}^1 &= \frac{\sqrt{3}}{3}(1,1,1,0,0,0,0)^\top, v_{12}^1 = \frac{\sqrt{3}}{3}(0,0,0,1,1,1,0)^\top, v_{13}^1 = (0,0,0,0,0,0,1)^\top \\
V_1^3: \quad v_{11}^3 &= \frac{\sqrt{6}}{6}(2,-1,-1,0,0,0,0)^\top, v_{12}^3 = \frac{\sqrt{6}}{6}(0,0,0,2,-1,-1,0)^\top \\
V_2^3: \quad v_{21}^3 &= \frac{\sqrt{2}}{2}(0,1,-1,0,0,0,0)^\top, v_{22}^3 = \frac{\sqrt{2}}{2}(0,0,0,0,1,-1,0)^\top
\end{aligned}
$$

We find the 3×3 matrix $B^{(1)}$ and the 2×2 matrix $B^{(3)}$ for the two symmetry subspaces to be:

$$
B^{(1)} = \begin{pmatrix} 160.596 & 160.799 & 2.393 \\ 160.799 & 203.127 & 1.063 \\ 2.393 & 1.063 & 62.959 \end{pmatrix} \quad B^{(3)} = \begin{pmatrix} 4.868 & 4.874 \\ 4.874 & 6.15 \end{pmatrix}
$$

The eigenvalues and eigenvectors of $B^{(1)}$ are:

$$344.08 : w_1^1 = (.659, .752, .008)^\top$$
$$62.97 : w_2^1 = (-.0135, .023, -1)^\top$$
$$19.63 : w_3^1 = (.7519, -.6589, -.02537)^\top$$

The eigenvalues and eigenvectors of $B^{(3)}$ are:

$$10.42 : w_1^3 = (.6594, .7518)^\top$$
$$.59 : w_2^3 = (.7518, -.6594)^\top$$

We can now form the resulting set of eigenvectors of $\tilde{C}$ by using the eigenvectors in the last step together with the G-adapted basis for V. We list the eigenvalues with their eigenvectors.

$$\begin{aligned}
344.08 : z_{11}^1 &= w_{11}^1 v_{11}^1 + w_{12}^1 v_{12}^1 + w_{13}^1 v_{13}^1 = (.38, .38, .38, .434, .434, .434, .008)^\top \\
62.96 : z_{12}^1 &= w_{21}^1 v_{11}^1 + w_{22}^1 v_{12}^1 + w_{23}^1 v_{13}^1 = (-.0078, -.0078, -.0078, .013, .013, .013, -1)^\top \\
19.63 : z_{13}^1 &= w_{31}^1 v_{11}^1 + w_{32}^1 v_{12}^1 + w_{33}^1 v_{13}^1 = (.434, .434, .434, -.38, -.38, -.38, -.025)^\top \\
10.42 : z_{11}^3 &= w_{11}^3 v_{11}^3 + w_{12}^3 v_{12}^3 = (.538, -.269, -.269, .614, -.307, -.307, 0)^\top \\
z_{21}^3 &= w_{11}^3 v_{21}^3 + w_{12}^3 v_{22}^3 = (0, .466, -.466, 0, .532, -.532, 0)^\top \\
.59 : z_{12}^3 &= w_{21}^3 v_{11}^3 + w_{22}^3 v_{12}^3 = (.614, -.307, -.307, -.538, .269, .269, 0)^\top \\
z_{22}^3 &= w_{21}^3 v_{21}^3 + w_{22}^3 v_{22}^3 = (0, .532, -.532, 0, -.466, .466, 0)^\top
\end{aligned}$$

Finding this set of vectors was our goal because they provide the full KL-basis for the enlarged pattern set $\tilde{U}$ (consisting of 24000 vectors) and the 7×7 enlarged ensemble average covariance matrix $\tilde{C}$. For completelness, this matrix is presented below; all computations have been done with six digit precision, the results were then rounded to three decimal places of accuracy.

$$\tilde{C} = \begin{pmatrix} 56.778 & 51.909 & 51.909 & 56.849 & 51.975 & 51.975 & 1.382 \\ 51.909 & 56.778 & 51.909 & 51.975 & 56.849 & 51.975 & 1.382 \\ 51.909 & 51.909 & 56.777 & 51.975 & 51.975 & 56.849 & 1.382 \\ 56.849 & 51.975 & 51.975 & 71.809 & 65.659 & 65.659 & .614 \\ 51.975 & 56.849 & 51.975 & 65.659 & 71.809 & 65.659 & .614 \\ 51.975 & 51.975 & 56.849 & 65.658 & 65.658 & 71.809 & .614 \\ 1.382 & 1.382 & 1.382 & .614 & .614 & .614 & 62.96 \end{pmatrix}$$

We note that 95% of the energy of the data is concentrated in the eigenspaces of the three largest eigenvalues.

Let us now compare the eigenvalues and eigenvectors of C (which is the ensemble averaged coveriance matrix based on the small set of patterns U), and $\tilde{C}$. We have:

$$C = \begin{pmatrix} 26.172 & 37.429 & 48.691 & 26.205 & 37.476 & 48.752 & .966 \\ 37.429 & 53.528 & 69.633 & 37.476 & 53.595 & 69.721 & 1.382 \\ 48.691 & 69.633 & 90.584 & 48.752 & 69.721 & 90.699 & 1.797 \\ 26.205 & 37.476 & 48.752 & 33.103 & 47.341 & 61.585 & .429 \\ 37.476 & 53.595 & 69.721 & 47.341 & 67.703 & 88.074 & .614 \\ 48.752 & 69.721 & 90.699 & 61.585 & 88.074 & 114.573 & .799 \\ .966 & 1.382 & 1.797 & .429 & .614 & .799 & 62.96 \end{pmatrix}$$

The non zero eigenvalues and their eigenvectors of C are:

$$364.836 : y_1 = (.258, .37, .481, .295, .422, .548, .008)^\top$$

$$62.97 : y_2 = (.006, .008, .011, -.009, -.013, -.017, 1)^\top$$

$$20.817 : y_3 = (.295, .422, .548, -.258, -.369, -.48, -.027)^\top$$

This information tells us that all the generated patterns lie in the three dimensional subspace generated by the eigenvectors above. When we look at the enlarged pattern set, we would expect that the same thing is true, and we have indeed seen that the energy *is* concentrated in a 3-dimensional subspace. The final step is to compare these two 3-dimensional subspaces.

A comparison of the eigenvectors of these two matrices show that they span essentially the same three dimensional subspace of $\mathbb{R}^7$. Taking the dot-product of the eigenvectors makes this clear.

$$(y_i \cdot x_j) = \begin{pmatrix} .971 & .0001 & 0 & -.207 & -.119 & 0 & 0 \\ .001 & -1 & .001 & .002 & .001 & -.006 & -.003 \\ 0 & .002 & .971 & 0 & 0 & -.206 & -.119 \end{pmatrix}$$

In a perfect system, the above 7×3 matrix would have a 3×3 identity block at the left, and zeroes elsewhere. That this is not the case may be due to several factors: the particular trajectory used may not fill up the attractor as well as desired, and the Runga-Kutta scheme to compute the trajectory will introduce some errors also. However, the agreement between the two 3-spaces is convincingly close.

7 Compact Lie Groups

In this section we extend the above theory, which was developed for finite groups, to the case of compact Lie groups.

Let G be a compact Lie group with identity I; recall that there is a unique normalized Haar measure dg on G. The representation theory of G is in many ways similar to that of a finite group; the main difference is that averages over the finite group are replaced with integrals in the Haar measure, and that there are in general infinitely many finite-dimensional irreducible unitary continuous representations up to isomorphism. In particular Schur's Lemma still holds: every G-equivariant map on an irreducible representation is a multiple of the identity.

For each finite-dimensional continuous irreducible representation ρ we again write $A^\rho(g)$ for the matrix $\rho(g)$, with entries $A^\rho_{ij}(g)$. The basic orthogonality relations (3.1) hold in this context also:

$$\int_G A^\rho_{ij}(hg) A^\tau_{k\ell}(g^{-1}) dg = \frac{1}{\dim(\rho)} A^\rho_{i\ell}(h) \delta_{jk} \delta_{\rho\tau} \tag{7.1}$$

We again define, for any finite-dimensional continuous representation V of G, the operator

$$P^\rho_{ij}(v) = \dim(\rho) \int_G A^\rho_{ji}(g^{-1}) g \cdot v \;\; dg.$$

We set $V^\rho_i = \mathrm{Image}(P^\rho_{ii})$ for $1 \leq i \leq \dim(\rho)$ and $V^\rho = \sum_{i=1}^{\dim(\rho)} V^\rho_i$.

The analogue of Proposition 3.2 holds without any changes in this situation. In fact if V is not finite-dimensional, the operators P_{ij}^{ρ} are still defined, and parts (a), (b), and (e) still hold; moreover (f) also holds if each symmetry subspace V^{ρ} is finite-dimensional. We have the identical definition for an orthonormal G-adapted basis for V.

The typical application of the theory occurs when the Lie group G acts on a compact manifold M, and therefore acts on the space of continuous $\mathbb{C}^n$-valued functions $\mathcal{F}^n(M)$, via the formula $(g \cdot f)(m) = f(g^{-1}m)$. The standard Hermitian metric on $\mathcal{F}^n(M)$ is

$$(f_1, f_2) = \frac{1}{\mathrm{vol}(M)} \int_M f_1(m)^* f_2(m)\, dm.$$

Suppose that $U \subset \mathcal{F}^n(M)$ is a submanifold of data. Under the assumption that the symmetry subspaces of $\mathcal{F}^n(M)$ are all finite-dimensional, we have the identical theory applying in order to compute the KL basis for $\mathcal{F}^n(M)$ with respect to the data set U. Since U may be a submanifold of data, we have that sums over U are replaced by integrals; and with this mild change the algorithm holds almost without change:

Algorithm for Exploiting Symmetry

in the KL basis computation

in the Compact Lie Group case

Given: A manifold M, a submanifold of patterns U drawn from the space of functions $\mathcal{F}^n(M)$, and a compact Lie group G acting on M preserving the set U. We assume that each symmetry subspace is finite-dimensional.

1. Determine the irreducible unitary representations ρ of G, and a G-adapted basis $\{v_{k\alpha}^{\rho}\}$ for $\mathcal{F}^n(M)$. Let d_ρ be the dimension of V_1^{ρ}.

2. For each ρ, each $k = 1, \ldots, \dim(\rho)$, consider the function $\gamma_{k\alpha}^{\rho} : U \to \mathbb{C}$ defined by

$$\gamma_{k\alpha}^{\rho}(u) = (v_{k\alpha}^{\rho}, u) = \frac{1}{\mathrm{vol}(M)} \int_M v_{k\alpha}^{\rho}(m)^* u(m)\, dm.$$

3. For each ρ, form the $d_\rho \times d_\rho$ matrix B^ρ by

$$(B^\rho)_{ij} = \frac{1}{\dim(\rho)\,\mathrm{vol}(U)} \sum_{k=1}^{\dim(\rho)} \int_U \gamma^\rho_{ki}(u)\overline{\gamma^\rho_{kj}(u)}\; du.$$

4. For each ρ, find the d_ρ eigenvalues λ^ρ_α and corresponding eigenvectors w^ρ_α (for $1 \leq \alpha \leq d_\rho$) of the matrix B^ρ. Write each eigenvector as $w^\rho_\alpha = (w^\rho_{\alpha 1} \cdots w^\rho_{\alpha d_\rho})^\top$.

5. Define

$$z^\rho_{k\alpha} = \sum_\beta w^\rho_{\alpha\beta} v^\rho_{k\beta}$$

for each ρ, each $k = 1, \ldots, \dim(\rho)$, and each $\alpha = 1, \ldots, d_\rho$. The KL basis for $\mathcal{F}^n(M)$ consists of these vectors $z^\rho_{k\alpha}$, each with eigenvalue λ^ρ_α (independent of k).

Note that since G has in general infinitely many irreducible representations, the method actually is useful for finding that part of the KL basis which resides in any particular symmetry subspace, i.e., for fixed ρ.

8 Example: The circle group S^1

Consider the compact Lie group $G = S^1$. G acts on $M = G$ by translation, and we consider the space $\mathcal{F}$ of continuous functions on M, which of course correspond to continuous periodic functions on the line.

The irreducible representations of G are all one-dimensional, indexed by integers n; $\rho_n(\theta) = \exp(2\pi i n\theta)$. For each n, the symmetry space is also one-dimensional, and $v^n_{11}(x) = \exp(-2\pi i n x)$; $d_\rho = d_n = 1$ for every n. Since all dimensions are one, we will drop the subscripts; the G-adapted basis is $v^n(x) = \exp(-2\pi i n x)$. The functionals γ^n on $\mathcal{F}$ are

$$\gamma^n(u) = (v^n, u) = \frac{1}{2\pi}\int_0^{2\pi} \exp(2\pi i n\theta)u(\theta)\; d\theta.$$

For any pattern set U, the KL basis consists of these v^n's, and the only unknowns are the eigenvalues. Each matrix $B^\rho = B^n$ is 1×1, with entry the eigenvalue λ_n; by the above, it is

$$\lambda_n = \frac{1}{\mathrm{vol}(U)} \int_U \gamma^n(u)\overline{\gamma^n(u)}\; du.$$

This theory then simply reproduces the Fourier Analysis for the set U; the KL basis consists of exactly the Fourier modes $v^n(x) = \exp(-2\pi inx)$, with the eigenvalues given above.

9 Summary and look ahead

In this paper we have derived an algorithm which allows us to considerably reduce the cost of the KL analysis of symmetric data using group representation theory. We started by exhibiting the results in the case of finite groups and extended the results to compact Lie groups. Examples for both cases were given.

We will exhibit an example of data with $SO(3)$ symmetry in Part II which will follow shortly. This example is far more interesting but also far more complicated than any of those given here.

It is also worth noticing that the given algorithm does not only reduce the computational cost of the KL analysis, but also gives more insight into the structure of the decomposition.

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