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MODEL REDUCTION BY PROPER ORTHOGONAL DECOMPOSITION COUPLED WITH CENTROIDAL VORONOI TESSELLATIONS

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ABSTRACT

Proper orthogonal decompositions (POD) have been used to define reduced bases for low-dimensional approximations of complex systems, including turbulent flows. Centroidal Voronoi tessellations (CVT) have been used in a variety of data compression and clustering settings. We review both strategies in the context of model reduction for complex systems and propose combining the ideas of CVT and POD into a hybrid method that inherets favorable characteristics from both its parents. The usefulness of such an approach and various practical implementation strategies are discussed.

INTRODUCTION

Model reduction plays an important role in the approximation of turbulent and chaotic systems and in the real-time feedback control of complex systems. In the former case, there is a need to identify highly persistent spatio-temporal structures using simple approaches. In the latter case, low-dimensional state models are needed so that actuation can be determined quickly from sensed data. Furthermore, typical strategies for approximating solutions of optimal flow control problems require multiple solutions of the state system, i.e., of the fluid equations. This renders such strategies too costly for routine use, and, in fact, makes them near impossible to implement for most practical three-dimensional flow control problems. As a result, there have been many studies devoted to the development, testing, and use of reduced-order models for complex dynamical systems such as unsteady fluid flows.

A popular technique for model reduction is based on *proper orthogonal decomposition* (POD) which is also known as Karhunen-Loève analysis or the method of empirical orthogonal eigenfunctions. POD has become popular due to its potential for extracting empirical information from experimental data or from data obtained from high-fidelity numerical simulations. For model reduction in the context of partial differential equations, approximation is effected by solving partial differential equations for long time periods or for various parameter values, then performing the POD analysis on snapshots of the solution, and then using the Galerkin method to project the partial differential equation model onto the reduced POD basis. The many studies devoted to the use of POD for obtaining low-dimensional dynamical system approximations include, among others, references (Aubry, et al., 1993)–(Volkwein, 1999). The use of POD analysis in control problems for partial differential equations has been considered in references (Arian, et al., 2002)–(Volkwein, 2002).

Centroidal Voronoi tessellation (CVT) is a clustering technique which for discrete data sets is also known as k-means clustering. It is a widely used method for data compression and for determining the similarities or dissimilarities of members of data sets. Here, we propose the use of CVTs of snapshot sets as an alternative to POD analyses for reduced order modeling. In addition, CVT and POD may be combined to define a generalization of POD. There are several reasons related to costs and benefits that make the CVT and POD+CVT approaches promising in the

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context of model reduction. The purpose of the paper is to explore these alternatives to POD and to discuss their potential advantages.

PROPER ORTHOGONAL DECOMPOSITION

In the proper orthogonal decompositions (POD) technique, dominant features from experimental or numerical data are extracted through a set of orthogonal functions which are related to the eigenfunctions of the correlation matrix of the data.

For n snapshots $\widetilde{\mathbf{u}}_j \in \mathbb{R}^N$, $j = 1,\ldots,n$, let $\widetilde{\mu} = \frac{1}{n}\sum_{j=1}^{n}\widetilde{\mathbf{u}}_j$. Then, $\mathbf{u}_j = \widetilde{\mathbf{u}}_j - \widetilde{\mu}$ for $j = 1\ldots,n$ define the set of modified snapshots. Let $d \le n$. Then, the POD basis $\{\phi_i\}_{i=1}^{d}$ of cardinality d is found by successively solving, for $i = 1,\ldots,d$, $\lambda_i = \max_{|\phi_i|=1}\frac{1}{n}\sum_{j=1}^{n}|\phi_i^T\mathbf{u}_j|^2$ and $\phi_i^T\phi_\ell = 0$ for $\ell \le i-1$. If $n \ge N$, this decomposition is known as the *direct* method; if $n < N$, then it is known as the *snapshot* method. For the latter case, $\phi_i = \frac{1}{\sqrt{n\lambda_i}}A\chi_i$, where χ_i with $|\chi_i| = 1$ denotes the eigenvector corresponding to the i-th largest eigenvalue λ_i of the $n\times n$ correlation matrix $K = (K_{j\ell})$, where $K_{j\ell} = \frac{1}{n}\mathbf{u}_j^T\mathbf{u}_\ell$. From now on, we will only consider the case $n < N$.

The POD basis is optimal in the following sense (Holmes, et. al, 1996). Let $\{\psi_i\}_{i=1}^{n}$ denote an arbitrary orthonormal basis for the span of the modified snapshot set $\{\mathbf{u}_j\}_{j=1}^{n}$. Let $P_{\psi,d}\mathbf{u}_j$ be the projection of $\mathbf{u}_j$ in the subspace spanned by $\{\psi_i\}_{i=1}^{d}$ and let the *error* be defined by $\mathcal{E} = \sum_{j=1}^{n}|\mathbf{u}_j - P_{\psi,d}\mathbf{u}_j|^2$. Then, the minimum error is obtained when $\psi_i = \phi_i$ for $i = 1,\ldots,d$, i.e., when the ψ_i's are the POD basis vectors. If one wishes for the relative error to be less than a prescribed tolerance ε, i.e., if one wants $\mathcal{E} \le \delta\Sigma_{j=1}^{n}|\mathbf{u}_j|^2$, one should choose d to be the smallest integer such that $\left(\sum_{j=1}^{d}\lambda_j/\sum_{j=1}^{n}\lambda_j\right) \ge \gamma = 1-\varepsilon$.

CENTROIDAL VORONOI TESSELLATIONS

A centroidal Voronoi tessellation (CVT) is a Voronoi tessellation of a given set such that the associated generating points are centroids, i.e., the centers of mass with respect to a given density function, of the corresponding Voronoi regions. In the current context, we will use the set $\{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ of modified, normalized snapshots, where $\widehat{\mathbf{u}}_j = \mathbf{u}_j/|\mathbf{u}_j|$.

Given the *discrete* set of modified, normalized snapshots $W = \{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ belonging to $\mathbb{R}^N$, a set $\{V_i\}_{i=1}^{k}$ is a *tessellation* of W if $V_i \subset W$ for $i = 1,\ldots,k$, $V_i \cap V_j = \emptyset$ for $i \ne j$, and $\cup_{i=1}^{k}V_i = W$. Given a set of points $\{\mathbf{z}_i\}_{i=1}^{k}$ belonging to $\mathbb{R}^N$ (but not necessarily to W), the *Voronoi set* corresponding to the point $\mathbf{z}_i$ is defined by $\widehat{V}_i = \{\mathbf{u} \in W \ \mid\ |\mathbf{u}-\mathbf{z}_i| \le |\mathbf{u}-\mathbf{z}_j| \text{ for } j = 1,\ldots,k,\ j \ne i\}$, where equality holds only for $i < j$. The set $\{\widehat{V}_i\}_{i=1}^{k}$ is called a *Voronoi tessellation* or *Voronoi diagram* of W.

Given a density function $\rho(\mathbf{y}) \ge 0$, defined for $\mathbf{y} \in W$, the mass centroid $\mathbf{z}^*$ of any subset $V \subset W$ is defined by $\mathbf{z}^* = \sum_{\mathbf{y}\in V}\rho(\mathbf{y})\mathbf{y}\Big/\sum_{\mathbf{y}\in V}\rho(\mathbf{y})$. Note that, in general, $\mathbf{z}^* \notin W$. (One can constrain the center of mass to belong to the set W by generalizing the definition of the center of mass.) The density function can be used to assign weights to the snapshots, e.g., to allow for some snapshots to have greater influence than others. This flexibility in the definition of CVTs may be useful in model reduction applications.

If $\mathbf{z}_i = \mathbf{z}_i^*$ for $i = 1,\ldots,k$, where $\{\mathbf{z}_i\}_{i=1}^{k}$ is the set of generating points for the Voronoi tessellation $\{\widehat{V}_i\}_{i=1}^{k}$ and $\{\mathbf{z}_i^*\}_{i=1}^{k}$ are the set of mass centroids of the Voronoi regions, we refer to the Voronoi tessellation as a *centroidal Voronoi tessellation.* CVT's of discrete sets are closely related to optimal *k-means clusters* and Voronoi regions and centroids are referred to as *clusters* and *cluster centers*, respectively. The concept of CVT's can be extended to more general sets, including regions in Euclidean spaces, and more general metrics. They have a variety of applications including data compression, optimal allocations of resources, cell division, territorial behavior of animals, optimal sensor and actuator location, and numerical analysis including both grid-based and meshfree algorithms for interpolation, multi-dimensional integration, and partial differential equations; see references (Du, et al., 1999)–(Okabe, et al., 2000).

Given the discrete set of points $W = \{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ belonging to $\mathbb{R}^N$, we define the error with respect to a tessellation $\{V_i\}_{i=1}^{k}$ of W and a set of points $\{\mathbf{z}_i\}_{i=1}^{k}$ belonging to W or, more generally, belonging to $\mathbb{R}^N$ by $\mathcal{F}\left((\mathbf{z}_i,V_i), i = 1,\ldots,k\right) = \sum_{i=1}^{k}\sum_{\mathbf{y}\in V_i}\rho(\mathbf{y})|\mathbf{y}-\mathbf{z}_i|^2$. It can be shown that a necessary condition for the error $\mathcal{F}$ to be minimized is that the pair $\{\mathbf{z}_i,V_i\}_{i=1}^{k}$ form a CVT of W. We note that the error $\mathcal{F}$ is also often referred to as the *variance, cost, distortion error,* or *mean square error*.

Algorithms for constructing CVT's

There are several algorithms known for constructing centroidal Voronoi tessellations of a given set; see references (Du, et al., 1999; Ju, et al., 2002; Lloyd, 1982; MacQueen, 1967). One representative is *MacQueen's method* (MacQueen, 1967) (see also (Du, et al., 1999; Ju, et al., 2002)), a very elegant probabilistic algorithm which divides sampling points into k sets or clusters by taking means of clusters. A second representative is a deterministic algorithm known in some circles as *Lloyd's method* (Lloyd, 1982) (see also (Du, et al., 1999)) and which is the obvious iteration between computing Voronoi diagrams and mass centroids, i.e., a given set of generators are replaced in an iterative process by the mass centroids of the Voronoi regions corresponding to those generators. A new probabilistic method, given in (Ju, et al., 2002), may be viewed as a generalization of both the MacQueen and Lloyd methods and is amenable to efficient parallelization.

CVT BASED POD

As was already mentioned, the concept of centroidal Voronoi tessellations can be extended to more general notions of distance. This allows for combining POD and CVT to take advantage of the best features of both approaches. To effect the generalization, we need new definitions for the concepts of distance and center of mass.

First, the distance $\delta(\mathbf{u}, \mathcal{Z})$ from a vector $\mathbf{u}$ to a d-dimensional subspace $\mathcal{Z}$ is given by $\delta^2(\mathbf{u}, \mathcal{Z}) = 1 - (\sum_{i=1}^{d}(\mathbf{u}^T\theta_i)^2)/|\mathbf{u}|^2$, where $\{\theta_i\}_{i=1}^{d}$ forms an orthonormal basis for $\mathcal{Z}$. Then, given a set of vectors (e.g., normalized, modified snapshots) $W = \{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ and a set of d-dimensional subspaces $\{\mathcal{Z}_i\}_{i=1}^{k}$ (which are called the generators), we define the generalized Voronoi tessellation of W by $\mathcal{V}_i = \{\widehat{\mathbf{u}}_j \in W \mid \delta^2(\widehat{\mathbf{u}}_j, \mathcal{Z}_i) \le \delta^2(\widehat{\mathbf{u}}_j, \mathcal{Z}_\ell)\ \forall \ell \ne i\}$ for $i = 1, \ldots, k$. A tie-breaking rule may be applied to insure that in the case equality holds in the above definition, each normalized, modified snapshot only belongs to one generalized Voronoi region.

Second, given a set of vectors $\mathcal{V} = \{\widehat{\mathbf{u}}_j\}$ that span an m-dimensional subspace of $\mathbb{R}^N$ (e.g., again, for us these are a subset of cardinality m of the modified snapshots), the concept of d-generalized centroid ($d \le m$) of $\mathcal{V}$ may be defined by an orthonormal basis $\{\phi_i\}_{i=1}^{d}$ which minimizes $\mathcal{D} = \sum_{\mathbf{u}_j \in \mathcal{V}} |\mathbf{u}_j - P\mathbf{u}_j|^2$, where P denotes the projection operator into the d-dimensional subspace spanned by $\{\phi_i\}_{i=1}^{d}$. For simplicity, we call such a centroid or basis the *d-g centroid of $\mathcal{V}$*. Note that the optimal basis $\{\phi_i\}_{i=1}^{d}$ is the d-dimensional POD basis for the set $\mathcal{V}$.

We are now ready to define CVT based POD. We note that the generators $\{\mathcal{Z}_j\}$ in general may not be required to have the same dimension. Thus, if k denotes the number of generators, we may use a multi-index $\mathbf{d} = \{d_i\}_{i=1}^{k}$ to replace the scalar index d.

Definition 1. *A set of finite subspaces $\{\mathcal{Z}_j\}_{i=1}^{k}$ with dimensions $\mathbf{d} = \{d_i\}_{i=1}^{k}$, respectively, along with the corresponding generalized Voronoi tessellation $\{\mathcal{V}_j\}_{i=1}^{k}$ is called a d-g* CVT *if and only if the $\mathcal{Z}_i$'s are themselves the d-g centroids of the $\mathcal{V}_i$'s.*

Definition 2. *The union of basis vectors corresponding to a d-g CVT is called a* CVT based POD *or a* centroidal Voronoi orthogonal decomposition (CVOD).

To recapitulate, CVOD can be viewed as a generalization of CVT for which the set W of normalized, modified snapshots is divided into k clusters or generalized Voronoi regions $\{\mathcal{V}_i\}_{i=1}^{k}$ and for which the generators are d_i-dimensional spaces each of which is spanned by the d_i-dimensional POD basis for the cluster. CVOD can also be viewed as a generalization of POD for which the set of modified snapshots is divided into k clusters and then a POD basis is separately determined for each cluster. In fact, if $d_i = 1$ for $i = 1, \ldots, k$, then CVT based POD reduces to the standard CVT. On the other hand, if $k = 1$, then CVT based POD reduces to the standard POD.

Algebraically, one may also interpret CVOD as follows. First, the original correlation matrix for the whole set of normalized, modified snapshots W is replaced by a block diagonal matrix with diagonal blocks being the correlation matrices for the snapshots in individual Voronoi sets $\{V_i\}$; then, the POD analysis is separately performed on each of the blocks. These Voronoi sets form a generalized centroidal Voronoi tessellation of W in the sense given in Definition 1. Thus, the role of CVT within CVOD may be viewed as providing, in some sense, an optimal clustering of the modified snapshots; the role of POD is then to provide an optimal reduced basis for each cluster.

There are cases where certain snapshots need to be weighted more heavily; thus, weighted POD's have been defined (Christensen, et al., 2000). In light of the fact that a nonuniform density function can be used in the standard CVT construction, we may also define the weighted CVOD with a prescribed *discrete density* or a set of weights, i.e., we may minimize $\sum_{\widehat{\mathbf{u}}_j \in \mathcal{V}} \rho(\widehat{\mathbf{u}}_j)\delta^2(\widehat{\mathbf{u}}_j, \mathcal{Z}_i)$ over a d_i-dimensional subspace of $\mathcal{V}$ for a given density function ρ.

Optimization properties of CVT based POD

Similar to the original CVT, the d-g CVT minimizes the error functional

$$\mathcal{G}\Big((\mathcal{Z}_i, \mathcal{V}_i), i = 1 \ldots, k\Big) = \sum_{i=1}^{k} \sum_{\widehat{\mathbf{u}}_j \in \mathcal{V}_i} \rho_j \delta^2(\widehat{\mathbf{u}}_j, \mathcal{Z}_i).$$

over all possible subdivisions of the set $\{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ of normalized, modified snapshots into k clusters $\{\mathcal{V}_i\}_{i=1}^{k}$ and all possible d_i-dimensional spaces $\mathcal{Z}_i$, $i = 1, \ldots, k$, where $\{\rho_j\}_{j=1}^{n}$ the values of denotes a density function. This optimization property is one of the key properties of CVT based POD that may make it very useful in practice.

The functional $\mathcal{G}$ also provides a natural error tolerance measure in the sense that

$$\mathcal{G}\Big((\mathcal{Z}_i, \mathcal{V}_i), i = 1 \ldots, k\Big) = \sum_{i=1}^{k} |\mathcal{V}_i| \sum_{j=d_i+1}^{|\mathcal{V}_i|} \lambda_{i_j},$$

where $|\mathcal{V}_i|$ denotes the cardinality of the Voronoi set or cluster $\mathcal{V}_i$ and the λ_{i_j}'s are the eigenvalues (in decreasing order) of the (weighted) local correlation matrix of the snapshots in the cluster. In addition, for k large, it has been conjectured (Du, et al., 1999) that CVT's enjoys the equi-partition of error property; it is natural to extend such a conjecture to CVT based POD. Such an error equi-partition property leads naturally to adaptive strategies to refine the CVOD analysis. Intuitively, one may compare the relative *local error*

$$|\mathcal{V}_i| \sum_{j=d_i+1}^{|\mathcal{V}_i|} \lambda_{i_j} \Big/ \mathcal{G}\Big((\mathcal{Z}_i, \mathcal{V}_i), i = 1 \ldots, k\Big)$$

with a given tolerance. One possible strategy is to enlarge the index d_i if the local error for the corresponding cluster (Voronoi set) $\mathcal{V}_i$ is much bigger than the errors for other clusters. On the other hand, if the error for one cluster is much smaller, then the index may be reduced. If the overall local errors are all very big, then besides enlarging d_i's, a larger value of k may also be desirable, i.e., more clusters may be used. While enlarging d_i may reduce the global error more efficiently, it also increases the computational cost in solving the eigenvalue problem. Thus, a balance needs to be maintained between enlarging k and increasing the d_i's.

Lloyd's method for CVT based POD

A natural extension of the Lloyd method for computing standard CVT's is readily available. Let us begin with a given set of d_i-dimensional subspaces $\{\mathcal{Z}_i\}_{i=1}^k$. One may then construct the generalized Voronoi tessellation of the set of modified snapshots and then compute the *d-g* centroid of each generalized Voronoi set; these new centroids replace $\{\mathcal{Z}_i\}_{i=1}^k$ for the next iteration. More precisely, we have the following algorithm.

Algorithm 1. *Generalized Lloyd's method* (a deterministic iteration)

> *Given a set of normalized, modified snapshots* $\{\widehat{\mathbf{u}}_j\}_{j=1}^n$ *and a discrete density function* $\{\rho_j\}_{j=1}^n$*, a positive integer k, and a multi-index* $\mathbf{d} = \{d_i\}_1^k$*;*
>
> 0. *choose an initial set of k subspaces* $\{\mathcal{Z}_i\}_1^k$ *with dimensions* $\mathbf{d} = \{d_i\}_1^k$*;*
> 1. *determine the generalized Voronoi tessellation* $\mathcal{V}_i = \{\widehat{\mathbf{u}}_j \in W \mid \delta^2(\widehat{\mathbf{u}}_j, \mathcal{Z}_i) \le \delta^2(\mathbf{u}_j, \mathcal{Z}_\ell) \quad \forall \ell \neq i\ \}$ *for* $i = 1, \ldots, k$*, along with a tie-breaking rule;*
> 2. *find the d-g centroids* $\{\mathcal{Z}_i^*\}_{i=1}^k$ *of* $\{\mathcal{V}_i\}_{i=1}^k$*;*
> 3. *set* $\{\mathcal{Z}_i = \mathcal{Z}_i^*\}_{i=1}^k$ *as the new set of generators;*
> 4. *if the new generators meet some convergence criterion, terminate; otherwise, return to step* 1.

Note that the determination of the *d-g* centroids in Step 2 is equivalent to conducting a POD analysis of each of the Voronoi regions. Thus, one may also view Lloyd's method as an iterative procedure that decomposes the whole process of finding a *d-g* CVT into a sequence of POD analyses in sets with a smaller number of modified snapshots. Since the computational complexity of the POD analysis for n snapshots is related to that of solving the eigenproblem for an $n \times n$ matrix, it is very demanding computationally when n is large. The POD analysis of the smaller set of snapshots in Step 2, on the one hand, reduces the dimension of the matrix eigenproblem and thus requires less memory and computation time; on the other hand, it can also be done concurrently for each generalized Voronoi region, thus leaving much room for improvements in efficiency through parallelization.

The above algorithm has the desirable feature that the *d-g* CVT error functional $\mathcal{G}\Big((\mathcal{Z}_i, \mathcal{V}_i),\ i = 1 \ldots, k\Big)$ decreases during the iteration. Moreover, as in the case of the original Lloyd iteration for the standard CVT (Du and Wang, 2002), it can be shown that if the local minimizers of $\mathcal{G}$ share the same functional value, then the iteration is globally convergent. For the more general case, we also expect the iteration to converge to local minimizers based on earlier computational experiences, though no rigorous theory is yet available.

Constrained CVT based POD

Sometimes, the physical system and thus the modified snapshots inherit certain symmetry properties, such as rotational symmetry, which are to be preserved by the selected representations (Aubry, et al., 1993). In other situations, constraints needs to be enforced such as the vectors need to be divergence free or are constrained to a hypersurface, etc. (Christensen, et al., 2000). For CVT, it is easy to modify the basic definition to allow additional constraints to be placed on the centroids; see (Du, et al., 1999) and (Du, et al., 2002). Thus, we can introduce the notion of *constrained CVOD* by extending the definition of generalized mass centroids from Euclidean spaces to other manifolds or more general constrained sets.

ADAPTIVE CVOD VIA A PENALIZED FUNCTIONAL

The standard CVOD is defined with a given number of generators k and a multi-index $\{d_i\}_{i=1}^k$. Determining the number k and the associated dimensions d_i of local POD bases can be an interesting problem in itself. In fact, in many applications, this is perhaps more important than constructing the bases. Thus, it is critical that a practical implementation of the CVOD analysis to allow for adapatively choosing k and $\{d_i\}_{i=1}^k$. There are certainly many choices and the decision rule is not unique. For instance, one possible route to systematic adaptivity is to consider minimizing the energy functional

$$\tilde{cg} = \sum_{i=1}^k \sum_{\mathbf{u}_j \in \mathcal{V}_i} \rho_j \delta^2(\mathbf{u}_j, \mathcal{Z}_i) + \alpha \sum_{i=1}^k \beta(d_i)$$

among all feasible sets $\{k, \{d_i\}_{i=1}^k, \{\mathcal{V}_i\}_{i=1}^k, \{\mathcal{Z}_i\}_{i=1}^k\}$. Here, α may be viewed as a positive penalization constant. β can be any increasing, convex function satisfying $\beta(0) = 0$, though it may be of a problem-specific form that reflects the decay properties of the variance (error) within the a clustered set of snapshots as the dimension of the generating vectors increases.

The two terms in the energy represent different properties of the CVOD: the first term measures the quality of the representation by the CVOD while the second term measures the dimensions of the reduced model. The convexity of the function β would imply that for a given sum, $\sum_{i=1}^{k} d_i$, and given the same value in the first term, it is optimal to evenly distribute the indices $\{d_i\}_{i=1}^{k}$ in order to reduce the second term.

Obviously, for a given α, taking $\sum_{i=1}^{k} d_i$ to be the same as the number of snapshots would minimize the first term of the energy. However, since no reduction of the model is made, the second term would be large. On the other hand, taking smaller k and smaller $\{d_i\}_{i=1}^{k}$ would mean a reduction in the second term, but the value of the first term would become larger. Thus, α plays a natural role of balancing the two terms. The larger α is, the smaller the dimension of the CVOD one would get, resulting in a more efficient representation; the smaller α is, the larger dimension one would get for the CVOD which also gives a representation of higher quality.

Currently, we are developing deterministic and probablistic algorithms for adaptively computing the CVOD that minimizes the above functional.

MODEL REDUCTION

We mentioned previously that CVT's have been used in data compression; one particular application was to image reconstruction; see (Du, et al., 1999). Therefore, it is natural to examine CVT's and CVOD's in another data compression setting, namely model reduction. A reduced basis, be it POD or CVT or CVOD, can be used to define a low-order model in the usual manner. The partial differential equations governing the dynamics of the system are projected over the subspace spanned by a particular basis and a system of ordinary differential equations for the temporal modes is obtained. The projection is effected through the standard Galerkin method.

In the CVT case, the idea, just as it was in the POD setting, is to extract, from a given set of normalized, modified snapshots $\{\widehat{\mathbf{u}}_j\}_{j=1}^{n}$ of vectors in $\mathbb{R}^N$, a smaller set of vectors also belonging to $\mathbb{R}^N$. In the POD setting, the reduced set was the d-dimensional set of vectors $\{\phi_j\}_{i=1}^{d}$. In the CVT setting, the reduced set is the k-dimensional set of vectors $\{\mathbf{z}_k\}_{i=1}^{k}$ that are the generators of a centroidal Voronoi tessellation of the set of normalized, modified snapshots. Just as POD produced an optimal reduced basis in the sense that the error $\mathcal{E}$ is minimized, CVT produces an optimal reduced basis in the sense that the error $\mathcal{F}$ is minimized.

We provide a little more detail in the CVOD setting. Let $F(t,x,u(x,t)) = 0$ be a system of partial differential equations with suitable boundary and/or initial conditions for the unknown function u. Here, t could be the time variable or some system parameter. Then, the CVOD based model reduction is performed as follows.

Algorithm 2. *CVOD based model reduction procedure*

1. *Construct a set of normalized, modified snapshots* $\{u_j\}_1^n$ *by solving (most probably approximately) the system of differential equations for different values of* t.
2. *Calculate the CVOD for the set* $\{u_j\}_1^n$ *for some integer* k *and multi-index* $\{d_j\}_{j=1}^{k}$ *to obtain a set of basis vectors* $\{\phi_m\}_{m=1}^{|\mathbf{d}|}$.
3. *Solve the reduced system:*

$$\left\langle \phi_m, F(t,X,\sum_{l=1}^{|\mathbf{d}|}\beta_l\phi_l)\right\rangle = 0 \quad \text{for } m = 1,2,\ldots,|\mathbf{d}|\,.$$

Why should one use CVOD instead of POD? Although the advantages of CVOD still have to be substantiated through numerical experiments, one can make some arguments.

CVOD naturally introduces the concept of clustering into the decomposition. By imposing a clustering, each sub-CVOD basis for a specific cluster can be used to capture the dynamics of that cluster. As we have already mentioned, CVOD also reduces the amount of work relative to the full POD analysis. POD involves the solution of an $n \times n$ eigenproblem, where n is the number of snapshots; CVOD instead requires the solution of several smaller eigenproblems. CVT itself requires no eigenproblem solution. Another interesting feature of CVOD which has been observed in other contexts, e.g., image processing (Du, et al., 1999), is that it avoids the over-crowding of the reduced basis into a few dominant modes which is a possible drawback of POD.

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