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Principle Component Analysis and Model Reduction for Dynamical Systems with Symmetry Constraints

Mili Shah and Danny C. Sorensen

Abstract— **Dimension reduction in molecular dynamics simulation is often realized through a principle component analysis based upon a singular value decomposition (SVD) of the trajectory. The left singular vectors of a truncated SVD provide the reduced basis. In many biological molecules, such as HIV1 protease, reflective or rotational symmetry should be present in the molecular configuration. Determining this symmetry allows one to provide SVD major modes of motion that best describe the symmetric movements of the protein. We present a method to compute the plane of reflective symmetry or the axis of rotational symmetry of a large set of points. Moreover, we develop an SVD that best approximates the given set while respecting the symmetry.**

Interesting subproblems arise in the presence of noisy data or in situations where most, but not all of the structure is symmetric. An important part of the determination of the axis of rotational symmetry or the plane of reflection symmetry is an iterative re-weighting scheme. This scheme is rapidly convergent in practice and seems to be very effective in ignoring outliers (points that do not respect the symmetry).

I. Introduction

Determining symmetry within a collection of spatially oriented points is a problem that occurs in many fields including molecular biology, chemistry, and image processing. In these applications, large amounts of data are generally collected and knowing information about symmetry leads better modeling of physical processes as well as more efficient storage and computational schemes.

Given a dynamical system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0$, there are well known techniques for dimension reduction based upon the Gramian of the trajectory $\{\mathbf{x}(t), t \geq 0\}$. The technique is known as Proper Orthogonal Decomposition (POD) in computational fluid dynamics and as Principle Component Analysis (PCA) in molecular dynamics. For a system with n-dimensional state vectors, the Gramian

$$\mathcal{P} = \int_o^\infty \mathbf{x}(\tau)\mathbf{x}(\tau)^T d\tau$$

is an $n \times n$ symmetric positive (semi-)definite matrix (assuming it exists). The eigensystem of $\mathcal{P}$

$$\mathcal{P} = \mathbf{U}\mathbf{S}^2\mathbf{U}^T$$

provides an orthogonal basis via the columns of $\mathbf{V}$ and in this basis we have the representation

$$\mathbf{x}(t) = \mathbf{U}\mathbf{S}\mathbf{v}(t)$$

with the components of $\mathbf{w}(t)$ being mutually orthogonal $\mathcal{L}_2(0,\infty)$ functions. If the the diagonal elements of positive semidefinite diagonal matrix $\mathbf{S}$ decay rapidly (assuming they are in decreasing order) then a reduced basis representation of the trajectory may be obtained by discarding the trailing terms and considering the approximation $\mathbf{x}_k = \mathbf{U}_k\mathbf{S}_k\mathbf{v}_k(t)$ where the subscript k denotes the leading k columns and/or components.

This is usually approximated using snapshots consisting of values $\mathbf{x}(t_j)$ of the trajectory at discrete time points and forming the $n \times m$ matrix

$$\mathbf{X} = [\mathbf{x}(t_1), \mathbf{x}(t_2), \ldots, \mathbf{x}(t_m)].$$

The singular value decomposition (SVD) of $\mathbf{X}$ provides

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T \approx \mathbf{U}_k\mathbf{S}_k\mathbf{V}_k^T$$

where

$$\mathbf{U}^T\mathbf{U} = \mathbf{V}^T\mathbf{V} = \mathbf{I}_n \quad \mathbf{S} = diag(\sigma_1, \sigma_2, \cdots, \sigma_n)$$

with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. This is a direct approximation to the continuous derivation if we consider

$$\mathcal{P} \approx \frac{1}{m}\mathbf{X}\mathbf{X}^T = \frac{1}{m}\sum_j \mathbf{x}(t_j)\mathbf{x}(t_j)^T.$$

with the approximation to $\mathcal{P}$ given by a quadrature rule. Here we are concerned with introducing symmetry constraints into this approximation when appropriate. In molecular dynamics, there is often a known spatial structural symmetry for the state variables and the purpose of the constrained SVD approximation developed here is to impose such symmetry constraints on the approximate trajectory through a symmetry preserving SVD.

We shall concentrate on determining two types of symmetry: Rotational and Reflective. Computationally, this requires construction of certain symmetric transformations in general $I\!R^n$ space - reflection and rotation. For reflective symmetry, we will look for the normal $\mathbf{w}$ to a hyperplane $\mathcal{H}$ for which $\mathcal{S}$ can be split into two mirror image sets. While for rotational symmetry, the axis $\mathbf{q}$ about which $\mathcal{S}$ can be rotated $2\pi/k$ degrees and return to the same set will be determined. For practical application, we must also consider noisy data sets and construct a respective normal vector $\mathbf{w}$ or axis of rotation $\mathbf{q}$ that diminishes the anomalies of the system. This requires

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M. Shah is a graduate student in the Department of Computational and Applied Mathematics, Rice University, 6100 Main St., Houston, TX 77005-1892, USA, mili@caam.rice.edu

D.C. Sorensen is a professor in the Department of Computational and Applied Mathematics, Rice University, 6100 Main St., Houston, TX 77005-1892, USA, sorensen@rice.edu

an iterative re-weighting scheme that minimizes deviation from symmetry in a weighted Frobenius norm. Finally, for either type of symmetry, once the normal vector or axis of rotation has been determined we provide a means to directly compute the SVD of the best approximation to the given data set that will also respect the prescribed symmetry. From this symmetry preserving SVD, the best low rank symmetry preserving approximation can be created. We also provide a means to compute just the dominant portion (leading k terms) of the symmetry preserving SVD that is well suited to large scale computation. This computation only requires matrix-vector products involving the point set (represented as a matrix).

The ARPACK software [1] can be used in the large scale case. The computation is no more expensive, than that of finding the leading terms of the SVD of the full trajectory without the symmetry constraint. Computational examples involving the backbone of the HIV-1 protease molecule are presented here. These examples provide trajectories that result in matrices of dimension 9,000 by 10,000. The computations were performed on a parallel cluster using the parallel P_ARPACK version of ARPACK.

There has been considerable research in the area of symmetry detection within other applications. Atallah [2] constructs an order $(n \log n)$ algorithm that determines the line of reflective symmetry of a planar object by reducing the system to a combinatorial questions on words. Optimizing a coefficient of symmetry is employed by Marola to determine an axis of symmetry for planar images [3]. Zabrodsky, *et. al* [4] employ a continuous symmetry measure and apply it to finding 2D reflective and rotational symmetries in chemistry. Kazhdan extends this idea to 3D objects by creating a continuous 2D function that measures the invariance of an object with respect to reflective symmetry about each plane that goes through the object's center of mass.

Many papers use the following fundamental properties of symmetry, which can be found in [5], [6], to determine reflective and rotational symmetry. In this literature, the term principle axis (or principal components) refer to the eigen vectors of the correlation matrix of the set of points (the right singular vectors). The observation is that:

- Any plane of symmetry of a body is perpendicular to a principal axis.
- Any axis of symmetry of a body is a principal axis.

The principal axes are the eigenvectors of the covariance matrix. Minovic, *et. al.* start with this idea and build an octree representation to find symmetries of a 3D object. Sun and Sherrah begin by looking at the extended Gaussian image of an object. Then, they search along the principal axes for the strongest symmetry measure. Colliot *et. al* [7] determine the axes of reflective symmetry by starting with the principal axes and optimizing a symmetry measure by using the Nelder-Mead downhill simplex method. They apply this method to object recognition and brain scan algorithms.

This paper is organized as follows. Section 2 defines perfect reflective and rotational symmetry. Finding an optimal hyperplane of reflective symmetry for noisy data is analyzed in section 3; while choosing the axes of rotational symmetry for impure data is discussed in section 4. Finally, section 5 develops a symmetry preserving SVD that best approximates the given data set and provides an algorithm for directly computing the best low rank symmetry preserving approximation in a way that is suitable for large scale computation. Computational results are presented in section 6.

Throughout the discussion, $\|\cdot\|$ shall denote the 2-norm and $\|\cdot\|_F$ shall denote the Frobenius norm. All lemmas and theorems are presented here without proof. The complete details are available in our technical report [8].

II. Perfect Symmetry

A. Reflective Symmetry

Recall that a hyperplane $\mathcal{H}$ is specified by a constant γ and a vector $\mathbf{w}$ via $\mathcal{H} := \{\mathbf{x} : \gamma + \mathbf{w}^T\mathbf{x} = 0\}$. The vector $\mathbf{w}$ is called the normal to the plane. A set of points $\mathcal{S} \in I\!R^n$ is said to be *reflectively symmetric with respect to the hyperplane* $\mathcal{H}$ if for every point $\mathbf{s} \in \mathcal{S}$, there exists a point $\hat{\mathbf{s}} \in \mathcal{S}$ such that $\hat{s} = s + \tau\mathbf{w}$ for some scalar τ with $\mathbf{s} + \frac{\tau}{2}\mathbf{w} \in \mathcal{H}$. We shall assume that $\gamma = 0$ throughout this discussion so the plane of symmetry, specifically the center $\mathbf{c}$ (defined below), passes through the origin. This can always be attained in general by a simple uniform translation of all the points of $\mathcal{S}$ and $\mathcal{H}$ by a fixed multiple of $\mathbf{w}$. For simplicity, we shall also assume that no points of $\mathcal{S}$ lie in the plane of symmetry.

Lemma 2.1: A set $\mathcal{S}$ is reflectively symmetric with respect to a hyperplane $\mathcal{H}$ with unit normal $\mathbf{w}$ if and only if

$$\mathcal{S} = (\mathbf{I} - 2\mathbf{w}\mathbf{w}^T)\mathcal{S}.$$

Lemma 2.2: If $\mathcal{S}$ is reflectively symmetric about $\mathcal{H}$, then the center $\mathbf{c} \in \mathcal{H}$ where

$$\mathbf{c} = \frac{1}{N}\sum_{\mathbf{s}\in\mathcal{S}} \mathbf{s},$$

and N is the number of elements of $\mathcal{S}$.

If $\mathcal{S}$ is reflectively symmetric about $\mathcal{H}$, we can arrange the points of $\mathcal{S}$ into two sets represented as matrices $\mathbf{X}_0$ and $\mathbf{X}_1$ such that

$$\mathbf{X}_0 = (\mathbf{I} - 2\mathbf{w}\mathbf{w}^T)\mathbf{X}_1.$$

Moreover, it is easily arranged that $\mathbf{w}^T\mathbf{X}_0 > 0$ and that $\mathbf{w}^T\mathbf{X}_1 < 0$.

B. Rotational Symmetry

A set of points $\mathcal{S} \in I\!R^n \bigcap \mathbf{q}^\perp$ is said to be *k-fold rotationally symmetric about an axis* $\mathbf{q} \in I\!R^n$ if there exist $\mathbf{R}(\mathbf{q})$ such that for every point $\mathbf{s} \in \mathcal{S}$, there exists $k-1$ distinct points $\mathbf{s}_1, \mathbf{s}_2, ..., \mathbf{s}_{k-1} \in \mathcal{S}$ such that $\mathbf{R}(\mathbf{q})^i\mathbf{s} = \mathbf{s}_i$ for $i = 1, 2, ...k-1$. We call $\mathbf{q}$ the rotational axis of symmetry and $\mathbf{R}(\mathbf{q})$ the rotation matrix.

Lemma 2.3: A set $\mathcal{S}$ is k-fold rotationally symmetric with respect to a rotational axis $\mathbf{q}$ if and only if for $i = 1, 2, ..., k-1$

$$\mathcal{S} = \mathbf{R}(\mathbf{q})^i\mathcal{S} = (\mathbf{I} - \mathbf{Q}\mathbf{G}\mathbf{Q}^T)^i\mathcal{S}.$$

where $[\mathbf{q}\ \mathbf{Q}] \in I\!R^{n\times(n)}$ is an orthogonal matrix, and $\mathbf{I}-\mathbf{G} \in I\!R^{(n-1)\times(n-1)}$ rotates any $\mathbf{X} \in I\!R^{(n-1)\times(n-1)}$ by $\theta = 2\pi/k$ degrees.
Note, $(\mathbf{R}(\mathbf{q}))^k = (\mathbf{I} - \mathbf{Q}\mathbf{G}\mathbf{Q}^T)^k = \mathbf{I}$.

If $\mathcal{S}$ is k-fold rotationally symmetric about $\mathbf{q}$, we can arrange the points of $\mathcal{S}$ into k sets represented as matrices $\mathbf{X}_0, \mathbf{X}_1, ..., \mathbf{X}_{k-1}$ such that

$$\mathbf{X}_i = (\mathbf{I} - \mathbf{Q}\mathbf{G}\mathbf{Q}^T)^i\mathbf{X}_0$$

for $i = 1, 2, ..., k-1$. Again, we will assume that the center $\mathbf{c}$ of the data is at the origin. This can always be attained in general by a simple uniform translation of all the points of $\mathcal{S}$.

III. Optimal Value of Reflective Normal $\mathbf{w}$

Generally, in practice, the given set $\mathcal{S}$ is not exactly symmetric with respect to any particular plane. However, we may think of calculating a $\mathbf{w}$ that does the best possible job of specifying a plane that separates $\mathcal{S}$ into two sets $\mathbf{X}_0$ and $\mathbf{X}_1$ (again posed as matrices) that are "nearly" symmetric with respect to the plane.

It is possible to find an initial separation of $\mathcal{S}$ into $\mathbf{X}_0$ and $\mathbf{X}_1$ that are paired to be nearly symmetric with respect to a plane determined by a calculated $\mathbf{w}$. Methods for this are discussed in [5] However, for this discussion, we shall assume that a partitioning of $\mathcal{S}$ into $\mathbf{X}_0$ and $\mathbf{X}_1$, is given such that the columns of the two matrices are correctly paired with respect to the desired reflective symmetry.

The specification of $\mathbf{w}$ may be expressed as an optimization problem

$$\min_{\|\mathbf{w}\|=1} \{\|(\mathbf{X}_0 - \mathbf{W}\mathbf{X}_1)\mathbf{D}\|_F : \mathbf{W} = \mathbf{I} - 2\mathbf{w}\mathbf{w}^T\}, \qquad (1)$$

where $\mathbf{D}$ is a diagonal weighting matrix. The weighting $\mathbf{D}$ is introduced to provide a means to de-emphasize anomalies and outliers in the supposed symmetry relation. If $\mathbf{D}$ is given, then the minimization can be solved.

Lemma 3.1: The solution $\mathbf{w}$ of to the minimization problem (1) is the unit eigenvector corresponding to the smallest eigenvalue of the symmetric indefinite matrix

$$\mathbf{M} = \mathbf{X}_0\mathbf{D}^2\mathbf{X}_1^T + \mathbf{X}_1\mathbf{D}^2\mathbf{X}_0^T. \qquad (2)$$

We have devised an optimization method based upon pattern search that enables the iterative construction of such weights that do ultimately diminish the influence of outliers in the final symmetric SVD approximation. The basic idea is to weight the i-th column of $\mathbf{X}_0 - \mathbf{W}\mathbf{X}_1$, i.e. $\mathbf{x}_i^{(0)} - (\mathbf{I} - 2\mathbf{w}\mathbf{w}^T)\mathbf{x}_i^{(1)}$, by the norm of the reciprocal of $\mathbf{x}_i^{(0)} - (\mathbf{I} - 2\mathbf{z}\mathbf{z}^T)\mathbf{x}_i^{(1)}$, where $\mathbf{z}$ is a unit vector. Therefore,

$$\min_{\|\mathbf{w}\|=1} \|(\mathbf{X}_0 - \mathbf{W}\mathbf{X}_1)\mathbf{D}(\mathbf{z})\|_F^2 = \sum_{j=1}^{N}\left(\frac{f_j(\mathbf{w})}{f_j(\mathbf{z})}\right)^2 = F(\mathbf{z},\mathbf{w}) \qquad (3)$$

where $f_j(\mathbf{z}) = \|\mathbf{x}_j^{(0)} - (\mathbf{I} - 2\mathbf{z}\mathbf{z}^T)\mathbf{x}_j^{(1)}\|$ and $\mathbf{D}(\mathbf{z}) = diag\left\{f_j(\mathbf{z})^{-1}\right\}$. This allows points that are 'more' symmetric with respect to $\mathbf{z}$ to have higher weights than those that are not. To find the optimal normal to this weighting, we choose $\mathbf{w}$ as the point that minimizes $\|(\mathbf{X}_0 - \mathbf{W}\mathbf{X}_1)\mathbf{D}(\mathbf{z})\|$, as described in Lemma 3.2. Therefore, the $\mathbf{z}$ which eliminates the most anomalies is the solution to the following max-min problem:

$$\max_{\|\mathbf{z}\|=1}\left\{\min_{\|\mathbf{w}\|=1} F(\mathbf{z},\mathbf{w})\right\}. \qquad (4)$$

It turns out that whenever $\mathbf{w} = \mathbf{z}$ solves $\min_{\|\mathbf{w}\|=1} F(\mathbf{z},\mathbf{w})$ then this provides a solution to the *max-min* problem and provides the desired weighting $\mathbf{D}$. Formally, this is expressed in the following lemma.

Lemma 3.2: If $\mathbf{w} = \mathbf{z}$ is a fixed point of (3), then $\mathbf{w}$ is a solution to (4) and $F(\mathbf{z},\mathbf{w}) = F(\mathbf{z},\mathbf{z}) = N$.
The existence of a fixed point is in [8].

We can find the fixed point of (3) numerically by using a modified pattern search method [9] on an equivalent optimization problem:

$$\min_{\|\mathbf{z}\|=1} \phi(\mathbf{z}) = \|\mathbf{z} - \mathbf{w}\| \qquad (5)$$

where, as before, $\mathbf{w}$ is the eigenvector associated to with the smallest eigenvalue of (2) with $\mathbf{D} = diag(f_j(\mathbf{z})^{-1})$.

IV. Optimal Value of Rotational Axis $\mathbf{q}$

Recall for a perfectly rotationally symmetric set

$$\mathbf{X}_i = (\mathbf{I} - \mathbf{Q}\mathbf{G}\mathbf{Q}^T)^i\mathbf{X}_0$$

where $[\mathbf{q}\ \mathbf{Q}]$ is an orthogonal matrix. Therefore, we see that

$$\mathbf{q}^T\mathbf{X}_i = \mathbf{q}^T(\mathbf{I} - \mathbf{Q}\mathbf{G}\mathbf{Q}^T)^i\mathbf{X}_0 = \mathbf{q}^T\mathbf{X}_0$$

for all $i = 1, 2, ..., k$. However, in general we are not given a perfectly symmetric data set $\mathcal{S}$. Therefore, we need to calculate a rotational axis $\mathbf{q}$ that best fits the data.

We shall assume a partitioning of $\mathcal{S}$ into $\mathbf{X}_0, \mathbf{X}_1, ..., \mathbf{X}_k$ such that the columns of the matrices are correctly paired. Therefore, we can now form an optimization problem

$$\min_{\|\mathbf{q}\|=1} \{\|\mathbf{q}^T[(k-1)\mathbf{X}_0 - \sum_{i=1}^{k-1}\mathbf{X}_i]\|\} \qquad (6)$$

to find our rotational axis of symmetry $\mathbf{q}$. It should be noted that Minovic *et. al* [5], [6] suggest looking at the principal axis of the inertia matrix associated with the distinct eigenvalue for an initial guess to the rotational axis of symmetry (perfect symmetry requires one distinct and two equal eigenvalues in 3-D). However, this technique may fail in the presence of noise, since a single distinct eigenvalue may not exist.

Lemma 4.1: The solution $\mathbf{q}$ to the minimization problem (6) is the unit eigenvector corresponding to the smallest eigenvalue of $\mathbf{M}\mathbf{M}^T$, where

$$\mathbf{M} = (k-1)\mathbf{X}_0 - \sum_{i=1}^{k-1}\mathbf{X}_i. \qquad (7)$$

As in the reflective symmetry, we can introduce a weighting scheme that minimizes the influence of outliers in the supposed rotational symmetry relation.

$$\min_{\|\mathbf{q}\|=1} \{\|\mathbf{q}^T[(k-1)\mathbf{X}_0 - \sum_{i=1}^{k-1}\mathbf{X}_i]\mathbf{D}\|\} \qquad (8)$$

where $\mathbf{D}$ is a diagonal weighting matrix.

Lemma 4.2: The solution to (8) is the unit eigenvector $\mathbf{q}$ corresponding to the smallest eigenvalue of $\mathbf{MD}^2\mathbf{M}^T$, where $\mathbf{M}$ is defined as in (7).

We created a search that diminishes the influence of outliers in the final SVD approximation by weighting the i-th column of $\mathbf{M}$ by $g_i(\mathbf{z})^{-1}$, where $g_i(\mathbf{z}) = \|\mathbf{z}^T\left[(k-1)\mathbf{x}_i^{(0)} - \sum_{j=1}^{k}\mathbf{x}_i^{(j)}\right]\|$ and $\mathbf{z}$ is a unit vector. Therefore,

$$\min_{\|\mathbf{q}\|=1}\{\|\mathbf{q}^T[(k-1)\mathbf{X}_0 - \sum_{i=1}^{k-1}\mathbf{X}_i]\mathbf{D}(\mathbf{z})\|^2\}$$

$$= \sum_{i=1}^{N}\left(\frac{g_i(\mathbf{q})}{g_i(\mathbf{z})}\right)^2 = G(\mathbf{z},\mathbf{q}), \tag{9}$$

which puts greater weight on points that are more symmetric with respect to $\mathbf{z}$ than points that are not. Then, $\mathbf{w}$ is picked to have the best normal with respect to the weighting as described in Lemma 4.2. Hence, the optimal $\mathbf{z}$ is the solution to the following max-min problem:

$$\max_{\|\mathbf{z}\|=1}\left\{\min_{\|\mathbf{q}\|=1} G(\mathbf{z},\mathbf{q})\right\}. \tag{10}$$

Again, a fixed point will provide a solution.

Lemma 4.3: If $\mathbf{q} = \mathbf{z}$ is a fixed point of (9), then $\mathbf{q}$ is a solution to (10) and $G(\mathbf{z},\mathbf{q}) = G(\mathbf{z},\mathbf{z}) = N$.

By using the modified compass search method on the equivalent optimization problem:

$$\min_{\|\mathbf{z}\|=1}\phi(\mathbf{z}) = \|\mathbf{z}-\mathbf{q}\| \tag{11}$$

where $\mathbf{q}$ is the eigenvector associated with the smallest eigenvalue of (8) with $\mathbf{D} = diag(g_j(\mathbf{z})^{-1})$, we can numerically find the fixed point to (9). The procedure for the modified search is also used to solve this problem.

V. Best Symmetric Approximation to a Set

To find the best reflective or rotational symmetric approximation to a set we can take advantage of the following theorem. For reflective symmetry $\mathbf{R} = \mathbf{W}$ and $\mathbf{W}^2 = \mathbf{I}$, and in the case of rotational symmetry $\mathbf{R} = \mathbf{R}(\mathbf{q})$ and $\mathbf{R}(\mathbf{q})^k = \mathbf{I}$.

Theorem 5.1: If

$$\mathbf{X} = [\mathbf{X}_0;\mathbf{X}_1;...;\mathbf{X}_{k-1}]$$

where

$$\mathbf{R}^{k-i}\mathbf{X}_i = \mathbf{X}_0 + \mathbf{E}_i,$$

and $\mathbf{R}^k = \mathbf{I}$, then

$$\min_{\hat{\mathbf{X}}_{j+1}=\mathbf{R}\hat{\mathbf{X}}_j}\|\begin{pmatrix}\mathbf{X}_0\\ :\\ \mathbf{X}_{k-1}\end{pmatrix} - \begin{pmatrix}\hat{\mathbf{X}}_0\\ :\\ \hat{\mathbf{X}}_{k-1}\end{pmatrix}\|^2$$

$$= \frac{1}{k}\sum_{i=0}^{k-1}\|\mathbf{E}_i\|^2,$$

and the SVD of this optimal solution is given by

$$\begin{pmatrix}\hat{\mathbf{X}}_0\\ :\\ \hat{\mathbf{X}}_{k-1}\end{pmatrix} = \mathbf{USV}^T,$$

where

$$\begin{aligned}\mathbf{U} &= \frac{1}{\sqrt{k}}\begin{pmatrix}\mathbf{U}_0\\ :\\ \mathbf{U}_{k-1}\end{pmatrix}\\ \mathbf{S} &= \sqrt{k}\mathbf{S}_0\\ \mathbf{V} &= \mathbf{V}_0\end{aligned}$$

and for $i = 0,1,2,...,k-1$,

$$\mathbf{U}_i = \mathbf{R}^i\mathbf{U}_0,$$

with

$$\mathbf{U}_0\mathbf{S}_0\mathbf{V}_0^T = \frac{1}{k}(\mathbf{X}_0 + \mathbf{R}^{k-1}\mathbf{X}_1 + \mathbf{R}^{k-2}\mathbf{X}_2 + ... + \mathbf{R}\mathbf{X}_{k-1}).$$

The proof of the theorem relies upon the following two lemmas.

Lemma 5.2: Suppose that the set is perfectly symmetric so that $\mathbf{E}_i = 0$ for all $i = 0,1,2,...,k-1$ and let

$$\begin{pmatrix}\mathbf{X}_0\\ \mathbf{X}_1\\ :\\ \mathbf{X}_{k-1}\end{pmatrix} = \begin{pmatrix}\mathbf{U}_0\\ \mathbf{U}_1\\ :\\ \mathbf{U}_{k-1}\end{pmatrix}\mathbf{SV}^T$$

be the short form SVD of $\mathbf{X}$. Then

$$\mathbf{U}_i = \mathbf{R}^i\mathbf{U}_0$$

where $i = 0,1,...,k-1$.

Lemma 5.3: Let $\mathbf{Z}_0 = \frac{1}{k}(\mathbf{X}_0 + \hat{\mathbf{X}}_1 + ... + \hat{\mathbf{X}}_{k-1})$. Then $\mathbf{Z} = \mathbf{Z}_0$ solves

$$\min_{\mathbf{Z}}\|\begin{pmatrix}\mathbf{X}_0\\ :\\ \hat{\mathbf{X}}_{k-1}\end{pmatrix} - \begin{pmatrix}\mathbf{Z}\\ :\\ \mathbf{Z}\end{pmatrix}\|_F^2$$

It is now possible to specify the best low rank approximation that preserves symmetry. If $\mathbf{X}$ is a noisy set, then

$$\min_{\hat{\mathbf{X}}_0}\|\begin{pmatrix}\mathbf{X}_0\\ \mathbf{R}^{k-1}\mathbf{X}_1\\ :\\ \mathbf{R}\mathbf{X}_{k-1}\end{pmatrix} - \begin{pmatrix}\hat{\mathbf{X}}_0\\ \hat{\mathbf{X}}_0\\ :\\ \hat{\mathbf{X}}_0\end{pmatrix}\|_F^2$$

$$= \frac{1}{k}\sum_{i=0}^{k-1}\|\mathbf{E}_i\|_F^2,$$

where $\mathbf{R}^{k-i}\mathbf{X}_i = \mathbf{X}_0 + \mathbf{E}_i$ and $\hat{\mathbf{X}}_0 = \frac{1}{k}\sum_{i=0}^{k-1}\mathbf{R}^{k-i}\mathbf{X}_i$.

Now, since

$$\begin{pmatrix}\mathbf{I} & & & \\ & \mathbf{R} & & \\ & & \ddots & \\ & & & \mathbf{R}^{k-1}\end{pmatrix}$$

is unitary, we have

$$\min_{\hat{\mathbf{X}}_j=\mathbf{R}^j\hat{\mathbf{X}}_0} \| \begin{pmatrix} \mathbf{X}_0 \\ : \\ \mathbf{X}_{k-1} \end{pmatrix} - \begin{pmatrix} \hat{\mathbf{X}}_0 \\ : \\ \hat{\mathbf{X}}_{k-1} \end{pmatrix} \|^2 = \frac{1}{k}\sum_{i=0}^{k-1} \|\mathbf{E}_i\|^2.$$

VI. Algorithms and Computational Results

The algorithmic structure for both the reflective and rotationally symmetric SVD approximation is the same. It consists of two major steps

1) Determine the normal $\mathbf{w}$ or the axis $\mathbf{q}$ for reflective or rotational symmetry respectively.
2) Compute the standard SVD

$$\mathbf{U}_0\mathbf{S}_0\mathbf{V}_0^T = \frac{1}{k}(\mathbf{X}_0 + \mathbf{R}^{k-1}\mathbf{X}_1 + \mathbf{R}^{k-2}\mathbf{X}_2 + ... + \mathbf{R}\mathbf{X}_{k-1})$$

where $\mathbf{R}$ is a reflector determined by $\mathbf{w}$ or a rotation about the axis determined by $\mathbf{q}$.

We seek the dominant (largest) singular values and this can be done in a straightforward manner using the ARPACK software on a serial computer or P_ARPACK on a parallel system. Only the leading k terms (singular values) are required. It is not necessary to compute all of the singular values just to discard them. One may either specify k or utilize a restarting scheme to adjust k until $\sigma_k \geq tol * \sigma_1 > \sigma_{k+1}$. The important computational point is the the only requirement is to compute matrix-vector products of the form

$$\mathbf{u} = \frac{1}{k}(\mathbf{X}_0 + \mathbf{R}^{k-1}\mathbf{X}_1 + \mathbf{R}^{k-2}\mathbf{X}_2 + ... + \mathbf{R}\mathbf{X}_{k-1})\mathbf{v}$$

and this is essentially the same work one would require to compute the corresponding standard SVD of $\mathbf{X}$ without the symmetry constraint.

This method has been implemented using P_ARPACK on a Linux cluster with 6 dual-processor nodes consisting of 1600MHz AMD Athlon processors with 1GB RAM per node and a 1GB/s Ethernet connection. The method was applied to compute the leading 10 symmetric major modes for a HIV-1 protease molecule. The molecule consists of 3120 atoms and hence the state has 9360 degrees of freedom. The molecular dynamics trajectory consisted of 10000 time steps (snapshots). This resulted in

1) The first 10 symmetric singular vectors took 131 secs. This includes axis of rotation determination.
2) The first 10 standard singular vectors took 88 secs.

These computations were done for both reflective and rotational symmetry with essentially the same computational time. The computation of the reflective normal or the axis of rotation was included in both symmetry preserving SVD's. As this axis determination is quite demanding, these computations indicate that obtaining the leading terms of the SVD is comparable for both the symmetry preserving and standard SVD cases. Moreover, both are well suited to the large scale setting when P_ARPACK is used.

It turns out that HIV-1 protease has a 2-fold rotational symmetry and this aspect is preserved while providing good approximations to the full trajectory. Visualizations are available at the web site http://www.caam.rice.edu/ sorensen/ under "recent talks".

VII. Conclusion

This paper has described a mathematical formulation of a symmetry preserving SVD which has led to practical (parallel) algorithms suitable for large scale computation. Criteria and methods were given for the calculation of reflective and rotational axis of symmetry of objects in $\mathbb{R}^n$ that are able to overcome problems with noisy data and outliers. The resulting technique is able to compute the best low rank symmetry preserving approximation to a given set.

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