Math 524: Linear Algebra

Notes $\#\alpha.\Omega$ — Intermission: Applications and Computational Linear Algebra

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Outline

1. Student Learning Targets, and Objectives
   - SLOs: ...
2. A Quick Summary of Some Key Results (so far)
3. Pondering $\mathbb{F}^m$, $\mathbb{F}^n$, and $\mathbb{F}^{m \times n}$
   - Practical Matrix Decompositions
   - Applications: Dynamic Pattern Formation; PCA

Student Learning Targets, and Objectives

Target Orthonormality

Objective Be able to express linear transformations and operators in terms of orthonormal basis/bases in order to leverage useful properties — *e.g.* upper triangularity, or diagonality of the matrix of a linear transformation / operator

This lecture serves as a bridge between what we have done and "the real world,"; in particular as it relates to our key take-away result for the semester: *The Singular Value Decomposition*

Introduction

Many of our results rest on one (or two) Orthonormal Basis (Bases).

Rewind (Existence of Orthonormal Basis [NOTES#6])

Every finite-dimensional inner product space has an orthonormal basis.

Rewind (Schur's Theorem [NOTES#6])

Suppose V is a finite-dimensional complex vector space and $T \in \mathcal{L}(V)$. Then T has an upper-triangular matrix with respect to some orthonormal basis of V.

Rewind (The Matrix of T^* [NOTES#7.1])

Let $T \in \mathcal{L}(V, W)$, and let $v_1, \dots, v_n$ be an orthonormal basis of V, and $w_1, \dots, w_m$ be an orthonormal basis of W. Then

$$\mathcal{M}(T^*, (w_1, \dots, w_m), (v_1, \dots, v_n)) = \mathcal{M}(T, (v_1, \dots, v_n), (w_1, \dots, w_m))^*$$

Key Results with Orthonormality

Rewind (Complex Spectral Theorem [NOTES#7.1])

Suppose $\mathbb{F} = \mathbb{C}$, and $T \in \mathcal{L}(V)$. Then the following are equivalent:

- T is normal ($TT^* = T^*T$)
- V has an orthonormal basis consisting of eigenvectors of T.
- T has a diagonal matrix wrt some orthonormal basis of V.

Rewind (Real Spectral Theorem [NOTES#7.1])

Suppose $\mathbb{F} = \mathbb{R}$, and $T \in \mathcal{L}(V)$. Then the following are equivalent:

(a) T is self-adjoint

(b) V has an orthonormal basis consisting of eigenvectors of T.

(c) T has a diagonal matrix wrt some orthonormal basis of V.

Key Results with Orthonormality

Rewind (Description of Isometries when $\mathbb{F} = \mathbb{C}$ [Notes#7.2])

Suppose V is a complex inner product space and $S \in \mathcal{L}(V)$. Then the following are equivalent:

(a) S is an isometry

(b) There is an orthonormal basis of V consisting of eigenvectors of S whose corresponding eigenvalues all have absolute value 1

Preview (Description of Isometries when $\mathbb{F} = \mathbb{R}$ [Axler::Chapter#9])

Suppose V is a real inner product space and $S \in \mathcal{L}(V)$. Then the following are equivalent:

(a) S is an isometry

(b) There is an orthonormal basis of V wrt which S has a block diagonal matrix such that each block on the diagonal is a 1×1 matrix containing ± 1, or is a 2×2 matrix of the form $\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$ with $\theta \in (0, \pi)$.

Key Results with Orthonormality

Rewind (Polar Decomposition [NOTES#7.2])

Suppose $T \in \mathcal{L}(V)$. Then there exists an isometry $S \in \mathcal{L}(V)$ such that

$$T = S\sqrt{T^*T}$$

$\exists$ orthonormal bases $\mathfrak{B}_1(V), \mathfrak{B}_2(V)$ so that both $\mathcal{M}(S; \mathfrak{B}_1(V))$ and $\mathcal{M}(\sqrt{T^*T}; \mathfrak{B}_2(V))$ are diagonal.

Rewind (Singular Value Decomposition [NOTES#7.2])

Suppose $T \in \mathcal{L}(V)$ has singular values $\sigma_1, \dots, \sigma_n$. Then there exists orthonormal bases $v_1, \dots, v_n$, and $u_1, \dots, u_n$ of V such that

$$T(w) = \sigma_1 \langle w,\ v_1 \rangle u_1 + \cdots + \sigma_n \langle w,\ v_n \rangle u_n$$

$\forall w \in V$.

Common Theme: $\exists\forall$

We can decompose EVERY operator using the [Polar Decomposition] or [Singular Value Decomposition]; and achieve some type of "diagonalization."
(2 ON-bases needed)

Likewise, we can diagonalize the ($\mathbb{C}$:normal/$\mathbb{R}$:self-adjoint) operators thanks to the [$\mathbb{C}/\mathbb{R}$ Spectral Theorems].
(1 ON-eigenbasis needed)

[Schur's Theorem] says that we can "upper triangularize" every operator.
(1 ON-basis needed)

Eigenvalue/Eigenvector Decomposition ∃ "for some"

Rewind (Sum of Eigenspaces is a Direct Sum [NOTES#5])

Suppose V is finite-dimensional and $T \in \mathcal{L}(V)$. Suppose also that $\lambda_1, \dots, \lambda_m$ are distinct eigenvalues of T. Then

$$E(\lambda_1, T) + \cdots + E(\lambda_m, T)$$

is a direct sum. Furthermore,

$$\dim\left(E(\lambda_1, T)\right) + \cdots + \dim\left(E(\lambda_m, T)\right) \leq \dim(V)$$

Rewind (Conditions Equivalent to Diagonalizability [NOTES#5])

Suppose V is finite-dimensional and $T \in \mathcal{L}(V)$. Let $\lambda_1, \dots, \lambda_m$ denote the distinct eigenvalues of T. Then the following are equivalent:

(a) T is diagonalizable.

(b) V has a basis consisting of eigenvectors of T

(c) $\exists$ 1-D subspaces $U_1, \dots, U_n$ of V, each invariant under T, such that $V = U_1 \oplus \cdots \oplus U_n$

(d) $V = E(\lambda_1, T) \oplus \cdots \oplus E(\lambda_n, T)$

(e) $\dim(V) = \dim(E(\lambda_1, T)) + \cdots + \dim(E(\lambda_n, T))$

Finding a "Wormhole" to $\mathbb{F}^m$, $\mathbb{F}^n$, and $\mathbb{F}^{m\times n}$

Rewind (Isomorphism, Isomorphic [NOTES#3.2])

- An **isomorphism** is an invertible linear map.
- Two vector spaces are called **isomorphic** if there is an isomorphism from one vector space onto the other one.

Rewind (Dimension shows whether vector spaces are isomorphic [NOTES#3.2])

Two finite-dimensional vector spaces over $\mathbb{F}$ are isomorphic if and only if they have the same dimension.

Bottom Line: Once appropriate inner products and ON-bases have been established, the matrices of the operators give us the connection to $\mathbb{F}^{m\times n}$, and all practical application-based "number crunching" is done on matrices ($\in \mathbb{F}^{m\times n}$) and vectors ($\in \mathbb{F}^m$ or $\in \mathbb{F}^n$).

At some point we have to think (hard) about matrices.

Practical Matrix Decompositions

There are many matrix decompositions, but the some of the most common (and useful) ones "shadow" what we have done for general operators:

Type	Form	Restrictions on A	Vectors
Diagonalization	$A = X\Lambda X^{-1}$	Non-defective	e.v
Unitary Diagonalization	$A = Q\Lambda Q^*$	Normal, $A^*A = AA^*$	e.v.
Schur Triangularization	$A = QTQ^*$	square	—
Polar	$A = SM$	square	—
Singular Value	$A = U\Sigma V^*$	none	s.v.

Notes: Λ: diagonal; Σ: diagonal/non-negative; X: columns are eigenvectors; Q, S, U, V: unitary (isometry); T triangular; M positive semi-definite

Practical Matrix Computations

We leave the many stories of HOW to compute the matrix factorizations (quickly, accurately) for [Math 543]; but note that the Singular Value Decomposition (in particular) is extremely useful for data analysis and compression.

The SVD shows up in many applications, often hiding behind some other name:

[MATH 543 (NOTES#4)] Hits on scholar.google.com

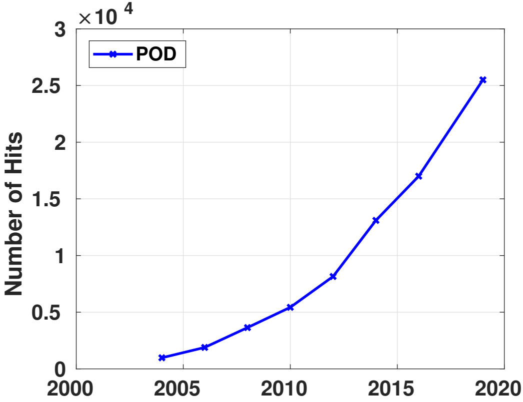

Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`"

Hits on scholar.google.com

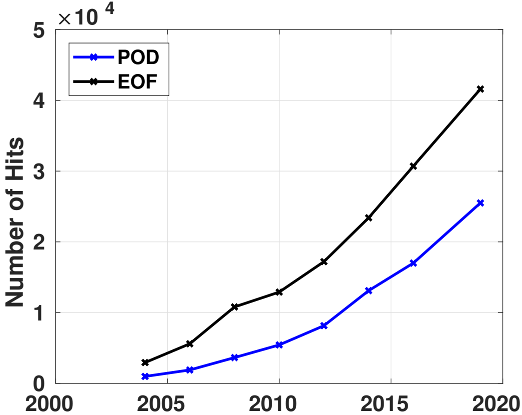

Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`"

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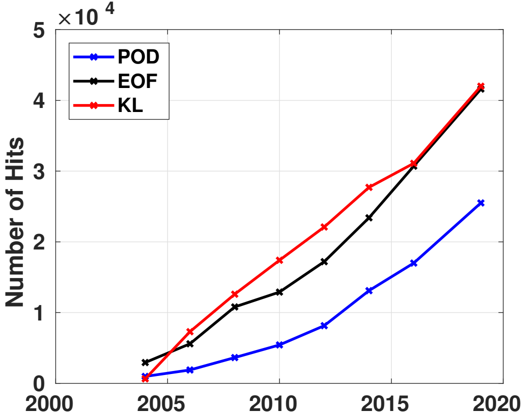

Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "Proper.Orthogonal.Decomposition", "Empirical.Orthogonal.(Function|Functions)", "Karhunen.Loeve"

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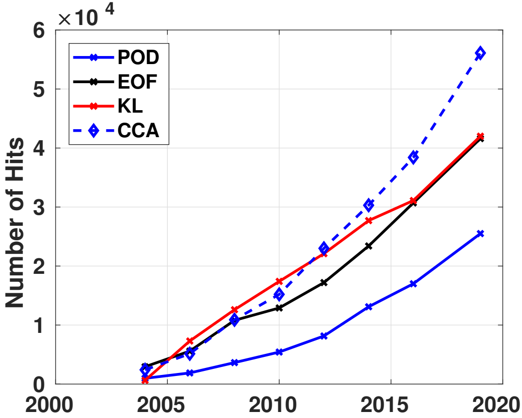

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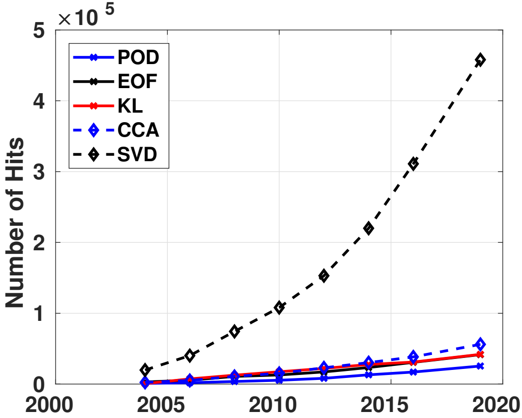

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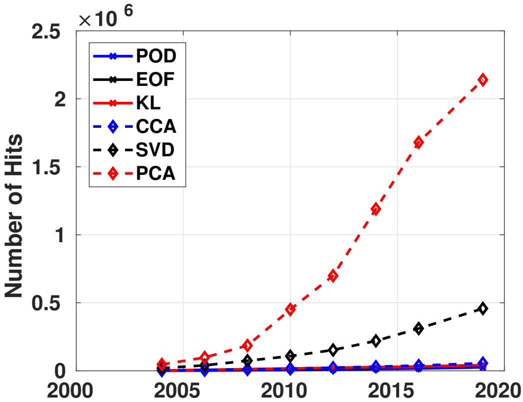

Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`", "`Karhunen.Loeve`", "`Canonical.Correlation.Analysis`", "`Singular.Value.Decomposition`", "`Principal.Component.Analysis`"

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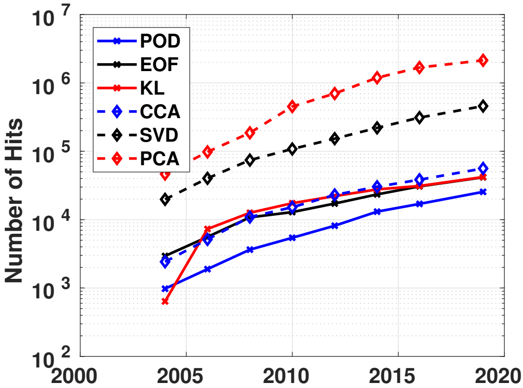

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Optimal Low-Rank Approximations

The "magic" property of the SVD is described by the following result:

Theorem (The SVD Provides the Optimal Low-Rank Approximations [Math 543 (Notes#5)])

For any ν with $0 \leq \nu < r$, define

$$A_\nu = \sum_{j=1}^{\nu} \sigma_j \vec{u}_j \vec{v}_j^*$$

if $\nu = p = \min(m,n)$, define $\sigma_{\nu+1} = 0$. Then

$$\|A - A_\nu\|_2 = \inf_{\substack{B \in \mathbb{C}^{m\times n} \\ \mathrm{rank}(B) \leq \nu}} \|A - B\|_2 = \sigma_{\nu+1}$$

Practically, is means that the first few $(\sigma_j, \vec{u}_j, \vec{v}_j)$-triples will optimally capture the "major modes" of whatever information is in the matrix A.

Application: Analysis of Dynamic Pattern Formation

The **Kuramoto-Sivashinsky** equation, here in polar coordinates

$$\begin{aligned} u_t \;=\; & -u_{rrrr} - \frac{1}{r^4}u_{\phi\phi\phi\phi} - \frac{2}{r^2}u_{rr\phi\phi} - \frac{2}{r}u_{rrr} + \frac{2}{r^3}u_{r\phi\phi} \\ & - \left[2 - \frac{1}{r^2}\right]u_{rr} - \left[\frac{4}{r^4} + \frac{2}{r^2}\right]u_{\phi\phi} - \left[\frac{1}{r^3} + \frac{2}{r}\right]u_r \\ & + \eta_1 u - \eta_2\left[u_r^2 + \frac{1}{r^2}u_\phi^2\right] - \eta_3 u^3, \end{aligned}$$

is a model for the behavior of cellular flames stabilized on a circular porous plug burner. For different simulation parameters $(\eta_1, \eta_2, \eta_3, R)$ it exhibits a wide array of complex flame patterns; — mimicking patterns observed in physical experiments.

$\exists$ Movies.

Integrating the Kuramoto-Sivashinsky Equation

- We defer all discussion on how to time-integrate the Kuramoto-Sivashinsky equation to [MATH 693B].
- We note that each time step (from t to $t+\delta t$, where δt is "small"), requires the solution of several non-Hermitian linear systems $A\vec{x} = \vec{b}$, where in our set-up $A \in \mathbb{R}^{m\times m}$, with $m = 2048$.
- In what follows, we keep the parameters $(\eta_1, \eta_2, \eta_3) = (0.32, 1.00, 0.017)$ constant, and vary **only** the radius of the circular burner.
- For the majority of radii, we get static (non-moving) patterns, which are quite easy to classify.
- However, for some fairly narrow parameter ranges we get time-dependent (dynamic) patters. We will use the SVD to analyze and classify these patterns.

Static Patterns Observed in the Kuramoto-Sivashinsky Simulations

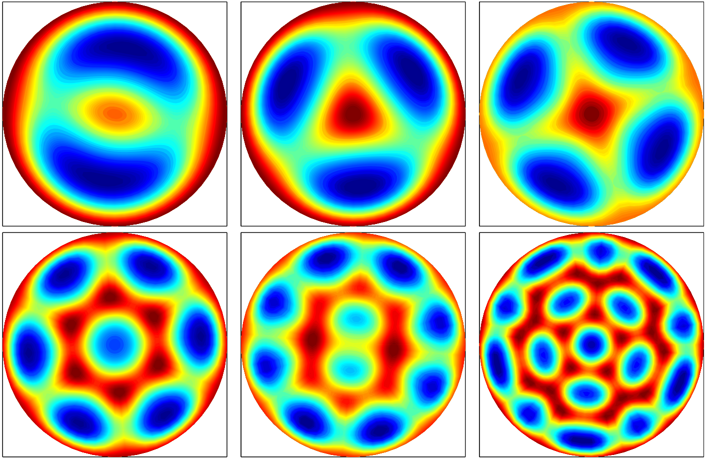
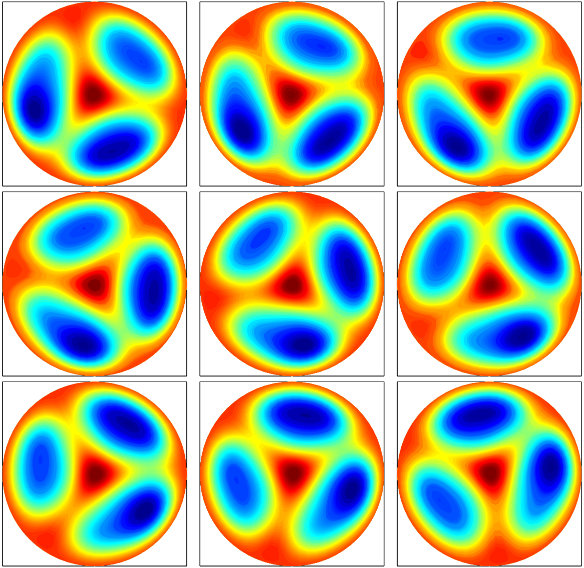
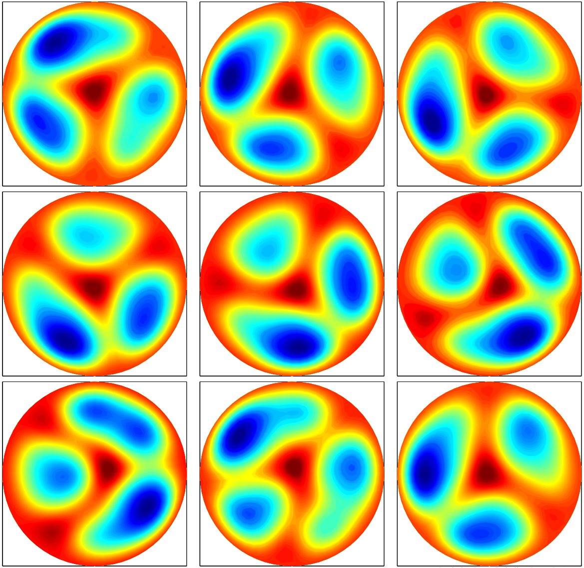


Figure: Some of the static patterns observed using the Kuramoto-Sivashinsky integration scheme. 2-cell pattern, $R = 5.0$; 3-cell pattern, $R = 6.0$; 4-cell pattern, $R = 8.0$; 6/1-cell pattern, $R = 10.0$; 8/2-cell pattern, $R = 12.0$; 10/5/1-cell pattern, $R = 14.5$; *Common simulation parameters:* $(\eta_1, \eta_2, \eta_3) = (0.32, 1.00, 0.017)$.

Dynamic Pattern #1: 3-Cell (Nearly) Rigid Rotation



Dynamic Pattern #2: 3-Cell “Hopping Pattern”



Dynamic Pattern #1–2: 3-Cell Dynamic States (Captions)

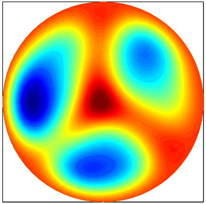
Figure (Slide 18): Snapshots of a three-cell nearly rigid rotation state from a simulation of the Kuramoto-Sivashinsky equation. The pattern is shown at times $t \in \{0, 15, 30, 45, 60, 75, 90, 105, 120\}$. The simulation parameter values are: $(\eta_1, \eta_2, \eta_3;\ R) = (0.32, 1.00, 0.017;\ 7.36)$. In this sequence we see how the patten stays the same, but rotates counter-clockwise.

Figure (Slide 19): Snapshots of a three-cell hopping state from a simulation of the Kuramoto-Sivashinsky equation. The pattern is shown at times $t \in \{0, 15, 30, 45, 60, 75, 90, 105, 120\}$. The simulation parameter values are: $(\eta_1, \eta_2, \eta_3;\ R) = (0.32, 1.00, 0.017;\ 7.7475)$. In this sequence we see how the "front-runner" of the two-cell formation bridges the gap to the solitary cell.

Analyzing the Dynamic Patterns — "The Method of Snapshots"

We use the SVD in order to analyze and classify these dynamic patters.

Each "frame", $u^{(i)}(r,\phi)$ with 32 radial, and 64 azimuthal points, of the sequence defines a 2048×1-vector $\tilde{f}_i$:



$$\rightarrow \quad \tilde{f}_i = \begin{bmatrix} u^{(i)}(r_1,\phi_1) \\ \vdots \\ u^{(i)}(r_1,\phi_{64}) \\ u^{(i)}(r_2,\phi_1) \\ \vdots \\ \vdots \\ u^{(i)}(r_{32},\phi_{64}) \end{bmatrix}$$

Analyzing the Dynamic Patterns: The Snapshot Matrices

For both the rigidly rotating, and the hopping pattern, we have computed 7200 frames, hence for each simulation we can build a 2048×7200 matrix of snapshots

$$\tilde{A} = \left[\begin{array}{cccc} \tilde{f}_1 & \tilde{f}_2 & \dots & \tilde{f}_{7200} \end{array} \right].$$

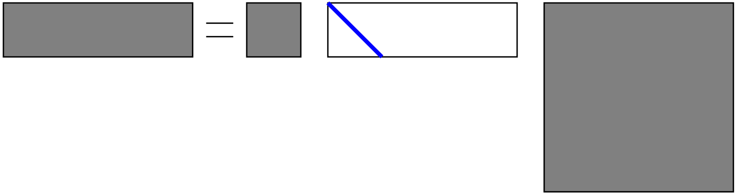
It turns out that for this application (and many others) it is advantageous to view each snapshot as a perturbation from the mean, so with $\vec{m}_f = \mathrm{mean}_{i=1,\dots,7200}(\tilde{f}_i)$, we define new vectors $\vec{f}_i = \tilde{f}_i - \vec{m}_f$, and a new "snapshot perturbation matrix"

$$A = \left[\begin{array}{cccc} \vec{f}_1 & \vec{f}_2 & \dots & \vec{f}_{7200} \end{array} \right].$$

Interpreting $U \Sigma V^* = A$

We now compute the SVD of the snapshot perturbation matrix, so that

$$A = U \Sigma V^*$$

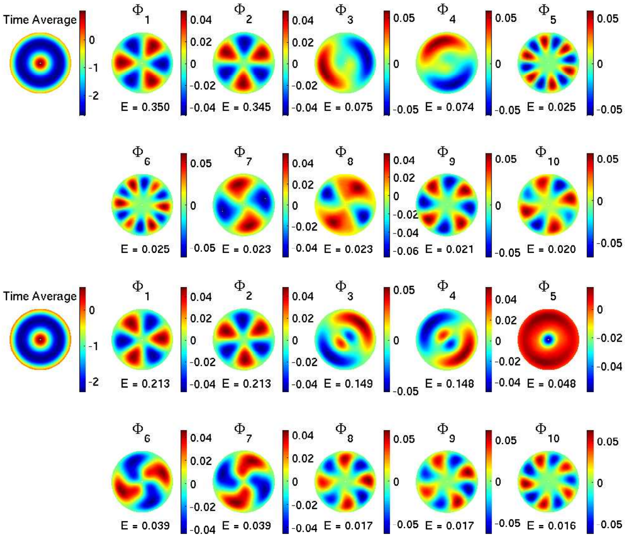


Restatement of the obvious: U is orthonormal, and has the same column space as A, *i.e.* it is an orthonormal basis for $\mathrm{range}(A)$.

The singular values σ_i tell us how "important" each column in U is, *i.e.* how much perturbation "energy" is controlled by the ith column of U.

In this application the left singular vectors (columns of U) are of interest.

$\vec{m}_f$ and $\vec{u}_1, \ldots, \vec{u}_{10}$ for Rigid Rotation and Hopping



Some Discussion...

For the **rigid rotation** we see that

$\sim$ 70% of the energy is controlled by $\vec{u}_1$-$\vec{u}_2$, which express rotations of 3-cell perturbations from the mean.

There is $\sim$ 15% of the energy in the $\vec{u}_3$-$\vec{u}_4$ pair (rotations of 1-cell perturbations), and

$\sim$ 5% of energy in 6-cell, and 2-cell perturbations;

the first 10 columns catch in excess of 98% of the energy, and hence provide an almost complete description of the motion.

Some Discussion...

For the **hopping motion**

we first notice that the rotations of 3-cell perturbations from the mean now only control $\sim 42\%$ of the motion, and

about 5 times as much energy ($\sim 10\%$) has "leaked" outside the first 10 columns.

— All of this is an indication that the motion is much more complex.

Further, the $\vec{u}_3$-$\vec{u}_4$ pair (of the rigid rotation) has formed a more complex $\vec{u}_3$-$\vec{u}_4$-$\vec{u}_5$ triple, and

the 2-, 4-, and 5-cell rotations have overtaken the importance of the 6-cell rotations (which is no longer in the "top 10.")

Expressing the Motion Using the Orthogonal Basis

Since U is an orthonormal basis, it is very straight-forward to write any frame as a linear combination of the basis vectors $\vec{u}_k$:

$$\vec{f}_i = \sum_{k=1}^{2048} a_{ik}\vec{u}_k, \quad \text{where} \quad a_{ik} = \vec{u}_k^* \vec{f}_i$$

Observation: Here the first 10 basis vectors control (98.1% rotation; 89.9% hopping) of the motion, therefore

$$\vec{f}_i \approx \sum_{k=1}^{\mathbf{10}} a_{ik}\vec{u}_k, \quad \text{where} \quad a_{ik} = \vec{u}_k^* \vec{f}_i$$

should be a good approximation.

$\rightsquigarrow$ **Compression:** By storing 10 (2048×1) basis vectors, 7200×10 coefficients, and the average vector (2048×1) $\vec{m}_f$ for a total of 94,528 values instead of the full $7200 \times 2048 = 14,745,600$-value dataset, we get a **compression ratio of $\frac{1}{156}$**.

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The Coefficients a_{ik}

The coefficients $a_{ik} = \vec{u}_k^* \vec{f}_i$ give us a lot of useful information.

If the rotation is completely rigid then when $\vec{u}_k$-$\vec{u}_{k+1}$ describe the rotation of some n-cell pattern, the points $(a_{i,k}, a_{i,k+1})$ should form a circle in $\mathbb{R}^2$, usually referred to as *phase space*...

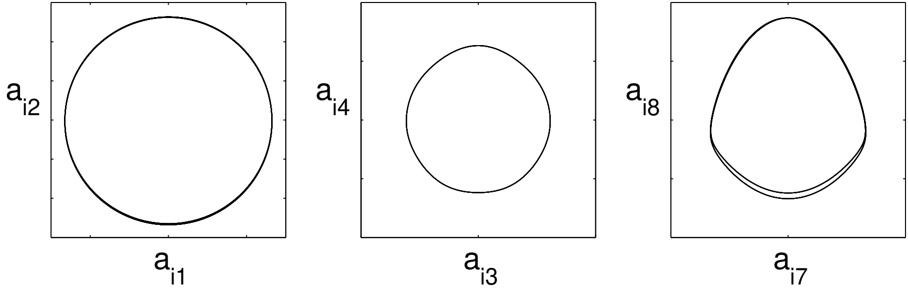

Figure: The phase plots for $\vec{u}_1$-$\vec{u}_2$, $\vec{u}_3$-$\vec{u}_4$, and $\vec{u}_7$-$\vec{u}_8$ corresponding to the nearly rigid rotation. We notice a very small deformation for the $\vec{u}_3$-$\vec{u}_4$ phase portrait, and see that the $\vec{u}_7$-$\vec{u}_8$ phase portrait (controlling $\sim 4.6\%$ energy) is quite egg-shaped and has period 2.

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The Coefficients a_{ik} — Hopping State

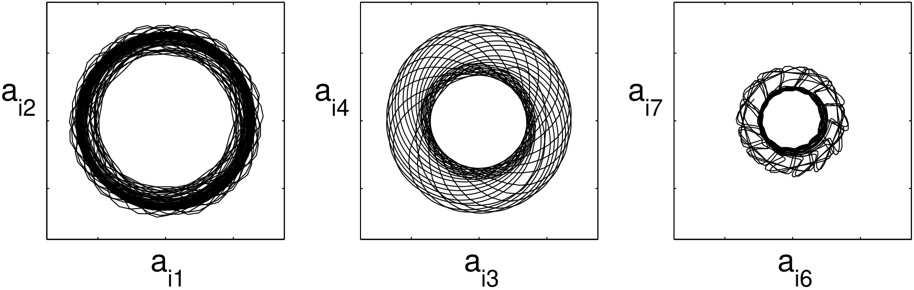

Figure: The phase plots for the hopping state looks very different. The three pairs: $\vec{u}_1$-$\vec{u}_2$, $\vec{u}_3$-$\vec{u}_4$, and $\vec{u}_7$-$\vec{u}_8$ all display quasi-periodic behavior.

The comparison of the phase-diagrams for the nearly rigid rotation and the hopping state is the most straight-forward way of classifying (and distinguishing) these dynamic patterns.

Looking at all the phase-diagrams for motions in the range $R \in [7.3600, 7.7475]$ may give us an insight into how the hopping state is "born."

Analyzing Other Types of Data

Clearly, the SVD does not care what kind of data we encode in the matrix A, we can think of many applications...

$\tilde{f}_i =$ Passport/DMV photographs (face recognition)

$\tilde{f}_i =$ Finger-prints

$\tilde{f}_i =$ DNA-(sub)sequence — GATTACA

$\tilde{f}_i =$ Multiple simultaneous temperature readings

$\tilde{f}_i =$ Demographic data

$\tilde{f}_i =$ Netflix data

$\tilde{f}_i =$ Purchase history

For time-dependent data, we can look that the phase-portraits; for other types of data, the k-tuple of coefficients $(a_{i1}, \ldots, a_{ik})$ defines a **"signature"** of $\vec{f}_i$ expressed in the orthogonal basis. The signature may be useful for identification purposes.

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Principal Component Analysis

Since Principal Component Analysis is the main(?) application area of the SVD, we should probably say something about it?

We borrow from [WIKIPEDIA]...

> *"Principal component analysis (PCA) is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables (entities each of which takes on various numerical values) into a set of values of linearly uncorrelated variables called principal components."*

Principal Component Analysis

> *"PCA can be done by eigenvalue decomposition of a data covariance (or correlation) matrix or singular value decomposition of a data matrix"*
>
> *"$X^T X$ itself can be recognized as proportional to the empirical sample covariance matrix of the dataset X."*

From our experience, conditioning strongly "suggests" we compute `svd`(A), where $\kappa(A) = \sigma_1/\sigma_n$, since the problem `eig`$(A^*A)$ suffers from $\kappa(A^*A) = (\sigma_1/\sigma_n)^2$.

We note (formally)

$$A^*A = X\Lambda X^{-1}, \quad A = U\Sigma V^* \Leftrightarrow A^*A = V\Sigma^2 V^*$$

which means that the right singular vectors (columns of V) contain the principal components.

Principal Component Analysis

Using $A = U\Sigma V^*$, the *Score Matrix* $T = U\Sigma$. (incidentally, U and Σ form a [Polar Decomposition (Notes#7.2)] of T).

"Full" Principal Component Analysis involves (among other things) making sure your data is properly organized and scaled. It is common to extract the mean values, and describe the variations from the mean in terms of z-scores.

Whereas the "core" computation is "just the SVD," the rest of the statistical explanations are best left to a statistician!