A Tutorial on Principal Component Analysis

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Principal component analysis (PCA) is a mainstay of modern data analysis - a black box that is widely used but poorly understood. The goal of this paper is to dispel the magic behind this black box. This tutorial focuses on building a solid intuition for how and why principal component analysis works; furthermore, it crystallizes this knowledge by deriving from simple intuitions, the mathematics behind *PCA* . This tutorial does not shy away from explaining the ideas informally, nor does it shy away from the mathematics. The hope is that by addressing both aspects, readers of all levels will be able to gain a better understanding of *PCA* as well as the when, the how and the why of applying this technique.

I. INTRODUCTION

Principal component analysis (*PCA*) has been called one of the most valuable results from applied linear algebra. *PCA* is used abundantly in all forms of analysis - from neuroscience to computer graphics - because it is a simple, non-parametric method of extracting relevant information from confusing data sets. With minimal additional effort *PCA* provides a roadmap for how to reduce a complex data set to a lower dimension to reveal the sometimes hidden, simplified structure that often underlie it.

The goal of this tutorial is to provide both an intuitive feel for *PCA*, and a thorough discussion of this topic. We will begin with a simple example and provide an intuitive explanation of the goal of *PCA*. We will continue by adding mathematical rigor to place it within the framework of linear algebra to provide an explicit solution. We will see how and why *PCA* is intimately related to the mathematical technique of singular value decomposition (*SVD*). This understanding will lead us to a prescription for how to apply *PCA* in the real world. We will discuss both the assumptions behind this technique as well as possible extensions to overcome these limitations.

The discussion and explanations in this paper are informal in the spirit of a tutorial. The goal of this paper is to *educate*. Occasionally, rigorous mathematical proofs are necessary although relegated to the Appendix. Although not as vital to the tutorial, the proofs are presented for the adventurous reader who desires a more complete understanding of the math. The only assumption is that the reader has a working knowledge of linear algebra. Please feel free to contact me with any suggestions, corrections or comments.

II. MOTIVATION: A TOY EXAMPLE

Here is the perspective: we are an experimenter. We are trying to understand some phenomenon by measuring various quantities (e.g. spectra, voltages, velocities, etc.) in our system. Unfortunately, we can not figure out what is happening because the data appears clouded, unclear and even redundant. This is not a trivial problem, but rather a fundamental obstacle in empirical science. Examples abound from complex systems such as neuroscience, photometry, meteorology and oceanography - the number of variables to measure can be unwieldy and at times even *deceptive*, because the underlying relationships can often be quite simple.

Take for example a simple toy problem from physics diagrammed in Figure 1. Pretend we are studying the motion of the physicist's ideal spring. This system consists of a ball of mass m attached to a *massless, frictionless* spring. The ball is released a small distance away from equilibrium (i.e. the spring is stretched). Because the spring is "ideal," it oscillates indefinitely along the x-axis about its equilibrium at a set frequency.

This is a standard problem in physics in which the motion along the x direction is solved by an explicit function of time. In other words, the underlying dynamics can be expressed as a function of a single variable x.

However, being ignorant experimenters we do not know any of this. We do not know which, let alone how many, axes and dimensions are important to measure. Thus, we decide to measure the ball's position in a three-dimensional space (since we live in a three dimensional world). Specifically, we place three movie cameras around our system of interest. At 200 Hz each movie camera records an image indicating a two dimensional position of the ball (a projection). Unfortunately, because of our ignorance, we do not even know what are the *real* "x", "y" and "z" axes, so we choose three camera axes $\{\vec{\mathbf{a}}, \vec{\mathbf{b}}, \vec{\mathbf{c}}\}$ at some arbitrary angles with respect to the system. The angles between our measurements

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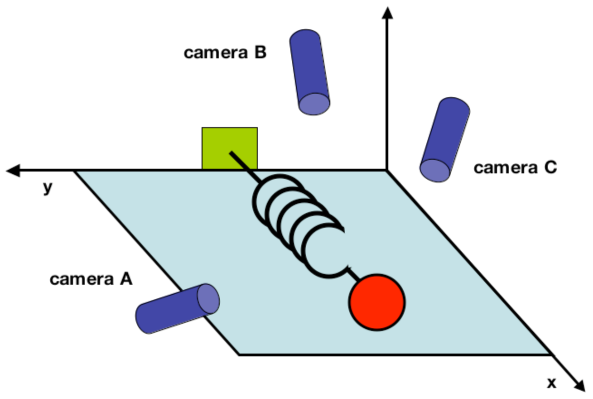


FIG. 1 A diagram of the toy example.

might not even be 90^o! Now, we record with the cameras for several minutes. The big question remains: *how do we get from this data set to a simple equation of x?*

We know a-priori that if we were smart experimenters, we would have just measured the position along the x-axis with one camera. But this is not what happens in the real world. We often do not know which measurements best reflect the dynamics of our system in question. Furthermore, we sometimes record more dimensions than we actually need!

Also, we have to deal with that pesky, real-world problem of *noise*. In the toy example this means that we need to deal with air, imperfect cameras or even friction in a less-than-ideal spring. Noise contaminates our data set only serving to obfuscate the dynamics further. *This toy example is the challenge experimenters face everyday.* We will refer to this example as we delve further into abstract concepts. Hopefully, by the end of this paper we will have a good understanding of how to systematically extract x using principal component analysis.

III. FRAMEWORK: CHANGE OF BASIS

The goal of principal component analysis is to compute the most meaningful *basis* to re-express a noisy data set. The hope is that this new basis will filter out the noise and reveal hidden structure. In the example of the spring, the explicit goal of *PCA* is to determine: “the dynamics are along the x-axis.” In other words, the goal of *PCA* is to determine that $\hat{\mathbf{x}}$ - the unit basis vector along the x-axis - is the important dimension. Determining this fact allows an experimenter to discern which dynamics are important, which are just redundant and which are just noise.

A. A Naive Basis

With a more precise definition of our goal, we need a more precise definition of our data as well. We treat every time sample (or experimental trial) as an individual sample in our data set. At each time sample we record a set of data consisting of multiple measurements (e.g. voltage, position, etc.). In our data set, at one point in time, camera A records a corresponding ball position (x_A, y_A). One sample or trial can then be expressed as a 6 dimensional column vector

$$\vec{X} = \begin{bmatrix} x_A \\ y_A \\ x_B \\ y_B \\ x_C \\ y_C \end{bmatrix}$$

where each camera contributes a 2-dimensional projection of the ball’s position to the entire vector $\vec{X}$. If we record the ball’s position for 10 minutes at 120 Hz, then we have recorded $10 \times 60 \times 120 = 72000$ of these vectors.

With this concrete example, let us recast this problem in abstract terms. Each sample $\vec{X}$ is an m-dimensional vector, where m is the number of measurement types. Equivalently, every sample is a vector that lies in an m-dimensional *vector space* spanned by some orthonormal basis. From linear algebra we know that all measurement vectors form a linear combination of this set of unit length basis vectors. What is this orthonormal basis?

This question is usually a tacit assumption often overlooked. Pretend we gathered our toy example data above, but only looked at camera A. What is an orthonormal basis for (x_A, y_A)? A naive choice would be $\{(1,0),(0,1)\}$, but why select this basis over $\{(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}),(\frac{-\sqrt{2}}{2},\frac{-\sqrt{2}}{2})\}$ or any other arbitrary rotation? The reason is that the *naive basis reflects the method we gathered the data.* Pretend we record the position $(2,2)$. We did **not** record $2\sqrt{2}$ in the $(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2})$ direction and 0 in the perpindicular direction. Rather, we recorded the position $(2,2)$ on our camera meaning 2 units **up** and 2 units to the **left** in our camera window. Thus our naive basis reflects the method we measured our data.

How do we express this naive basis in linear algebra? In the two dimensional case, $\{(1,0),(0,1)\}$ can be recast as individual row vectors. A matrix constructed out of these row vectors is the 2×2 identity matrix I. We can generalize this to the m-dimensional case by constructing an $m \times m$ identity matrix

$$\mathbf{B} = \begin{bmatrix} \mathbf{b_1} \\ \mathbf{b_2} \\ \vdots \\ \mathbf{b_m} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = \mathbf{I}$$

where each *row* is an orthornormal basis vector $\mathbf{b}_i$ with m components. We can consider our naive basis as the effective starting point. All of our data has been recorded in this basis and thus it can be trivially expressed as a linear combination of $\{\mathbf{b}_i\}$.

B. Change of Basis

With this rigor we may now state more precisely what *PCA* asks: *Is there another basis, which is a linear combination of the original basis, that best re-expresses our data set?*

A close reader might have noticed the conspicuous addition of the word *linear*. Indeed, *PCA* makes one stringent but powerful assumption: *linearity*. Linearity vastly simplifies the problem by (1) restricting the set of potential bases, and (2) formalizing the implicit assumption of continuity in a data set.[1]

With this assumption *PCA* is now limited to re-expressing the data as a *linear combination* of its basis vectors. Let $\mathbf{X}$ be the original data set, where each *column* is a single sample (or moment in time) of our data set (i.e. $\vec{X}$). In the toy example $\mathbf{X}$ is an $m \times n$ matrix where $m = 6$ and $n = 72000$. Let $\mathbf{Y}$ be another $m \times n$ matrix related by a linear transformation $\mathbf{P}$. $\mathbf{X}$ is the original recorded data set and $\mathbf{Y}$ is a re-representation of that data set.

$$\mathbf{PX} = \mathbf{Y} \tag{1}$$

Also let us define the following quantities.[2]

- $\mathbf{p_i}$ are the *rows* of $\mathbf{P}$
- $\mathbf{x_i}$ are the *columns* of $\mathbf{X}$ (or individual $\vec{X}$).
- $\mathbf{y_i}$ are the *columns* of $\mathbf{Y}$.

Equation 1 represents a *change of basis* and thus can have many interpretations.

1. $\mathbf{P}$ is a matrix that transforms $\mathbf{X}$ into $\mathbf{Y}$.
2. Geometrically, $\mathbf{P}$ is a rotation and a stretch which again transforms $\mathbf{X}$ into $\mathbf{Y}$.
3. The rows of $\mathbf{P}$, $\{\mathbf{p_1}, \ldots, \mathbf{p_m}\}$, are a set of new basis vectors for expressing the *columns* of $\mathbf{X}$.

The latter interpretation is not obvious but can be seen by writing out the explicit dot products of $\mathbf{PX}$.

$$\begin{aligned}\mathbf{PX} &= \begin{bmatrix}\mathbf{p_1} \\ \vdots \\ \mathbf{p_m}\end{bmatrix}\begin{bmatrix}\mathbf{x_1} & \cdots & \mathbf{x_n}\end{bmatrix} \\ \mathbf{Y} &= \begin{bmatrix}\mathbf{p_1}\cdot\mathbf{x_1} & \cdots & \mathbf{p_1}\cdot\mathbf{x_n} \\ \vdots & \ddots & \vdots \\ \mathbf{p_m}\cdot\mathbf{x_1} & \cdots & \mathbf{p_m}\cdot\mathbf{x_n}\end{bmatrix}\end{aligned}$$

We can note the form of each column of $\mathbf{Y}$.

$$\mathbf{y}_i = \begin{bmatrix}\mathbf{p_1}\cdot\mathbf{x_i} \\ \vdots \\ \mathbf{p_m}\cdot\mathbf{x_i}\end{bmatrix}$$

We recognize that each coefficient of $\mathbf{y_i}$ is a dot-product of $\mathbf{x_i}$ with the corresponding row in $\mathbf{P}$. In other words, the j^{th} coefficient of $\mathbf{y_i}$ is a projection on to the j^{th} row of $\mathbf{P}$. This is in fact the very form of an equation where $\mathbf{y_i}$ is a projection on to the basis of $\{\mathbf{p_1}, \ldots, \mathbf{p_m}\}$. Therefore, the *rows* of $\mathbf{P}$ are indeed a new set of basis vectors for representing of *columns* of $\mathbf{X}$.

C. Questions Remaining

By assuming linearity the problem reduces to finding the appropriate *change of basis*. The row vectors $\{\mathbf{p_1}, \ldots, \mathbf{p_m}\}$ in this transformation will become the *principal components* of $\mathbf{X}$. Several questions now arise.

- What is the best way to "re-express" $\mathbf{X}$?
- What is a good choice of basis $\mathbf{P}$?

These questions must be answered by next asking ourselves what features we would like $\mathbf{Y}$ *to exhibit.* Evidently, additional assumptions beyond *linearity* are required to arrive at a reasonable result. The selection of these assumptions is the subject of the next section.

IV. VARIANCE AND THE GOAL

Now comes the most important question: *what does "best express" the data mean?* This section will build up an intuitive answer to this question and along the way tack on additional assumptions. The end of this section will conclude with a mathematical goal for deciphering "garbled" data.

In a linear system "garbled" can refer to only three potential confounds: *noise, rotation* and *redundancy.* Let us deal with each situation individually.

A. Noise and Rotation

Measurement noise in any data set must be low or else, no matter the analysis technique, no information about a system can be extracted. There exists no absolute scale for noise but rather all noise is measured relative to the measurement. A common measure is the *signal-to-noise ratio* (*SNR*), or a ratio of variances σ^2,

$$SNR = \frac{\sigma^2_{signal}}{\sigma^2_{noise}}. \tag{2}$$

A high *SNR* ($\gg 1$) indicates high precision data, while a low *SNR* indicates noise contaminated data.

[1] A subtle point it is, but we have already assumed linearity by implicitly stating that the data set even characterizes the dynamics of the system. In other words, we are already relying on the superposition principal of linearity to believe that the data provides an ability to interpolate between individual data points

[2] In this section $\mathbf{x_i}$ and $\mathbf{y_i}$ are *column* vectors, but be forewarned. In all other sections $\mathbf{x_i}$ and $\mathbf{y_i}$ are *row* vectors.

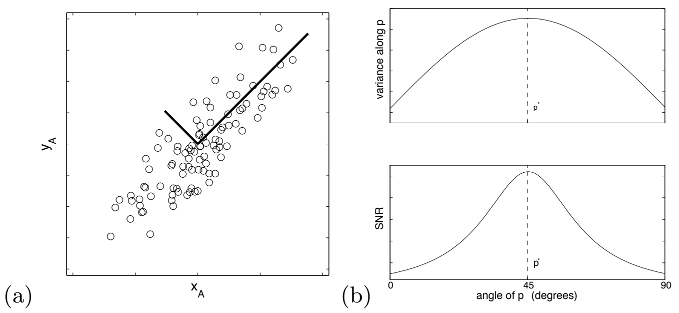


FIG. 2 (a) Simulated data of (x_A, y_A) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. (b) Rotating these axes finds an optimal p^* where the variance and *SNR* are maximized. The *SNR* is defined as the ratio of the variance along p^* and the variance in the perpindicular direction.

Pretend we plotted all data from camera A from the spring in Figure 2a. Remembering that the spring travels in a straight line, every individual camera should record motion in a straight line as well. Therefore, any spread deviating from straight-line motion must be noise. The variance due to the signal and noise are indicated by each line in the diagram. The ratio of the two lengths, the *SNR*, thus measures how "fat" the cloud is - a range of possiblities include a thin line ($SNR \gg 1$), a perfect circle ($SNR = 1$) or even worse. By positing reasonably good measurements, quantitatively we *assume* that directions with largest variances in our measurement vector space contain the dynamics of interest. In Figure 2 the direction with the largest variance is not $\hat{x}_A = (1, 0)$ nor $\hat{y}_A = (0, 1)$, but the direction along the long axis of the cloud. Thus, by assumption the dynamics of interest exist along directions with largest variance and presumably highest *SNR* .

Our assumption suggests that the basis for which we are searching is not the naive basis $(\hat{x}_A, \hat{y}_A)$ because these directions do not correspond to the directions of largest variance. Maximizing the variance (and by assumption the *SNR*) corresponds to finding the appropriate rotation of the naive basis. This intuition corresponds to finding the direction p^* in Figure 2b. How do we find p^*? In the 2-dimensional case of Figure 2a, p^* falls along the direction of the best-fit line for the data cloud. Thus, rotating the naive basis to lie parallel to p^* would reveal the direction of motion of the spring for the 2-D case. How do we generalize this notion to an arbitrary number of dimensions? Before we approach this question we need to examine this issue from a second perspective.

B. Redundancy

Figure 2 hints at an additional confounding factor in our data - redundancy. This issue is particularly evident in the example of the spring. In this case multiple sensors record the same dynamic information. Reconsider Figure 2 and ask whether it was really necessary to record 2 variables? Figure 3 might reflect a range of possibile plots between two arbitrary measurement types r_1 and r_2. Panel (a) depicts two recordings with no apparent relationship. In other words, r_1 is entirely uncorrelated with r_2. Because one can not predict r_1 from r_2, one says that r_1 and r_2 are statistcally independent. This situation could occur by plotting two variables such as $(x_A, humidity)$.

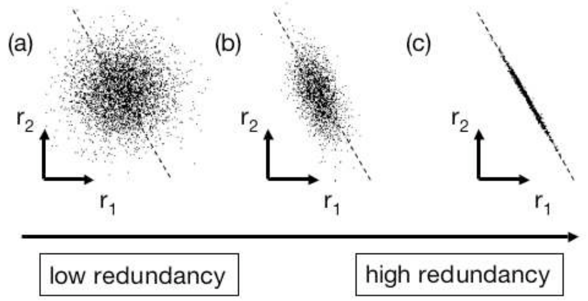


FIG. 3 A spectrum of possible redundancies in data from the two separate recordings r_1 and r_2 (e.g. x_A, y_B). The best-fit line $r_2 = kr_1$ is indicated by the dashed line.

On the other extreme, Figure 3c depicts highly correlated recordings. This extremity might be achieved by several means:

- A plot of (x_A, x_B) if cameras A and B are very nearby.
- A plot of $(x_A, \tilde{x}_A)$ where x_A is in meters and $\tilde{x}_A$ is in inches.

Clearly in panel (c) it would be more meaningful to just have recorded a single variable, not both. Why? Because one can calculate r_1 from r_2 (or vice versa) using the best-fit line. Recording solely one response would express the data more concisely and reduce the number of sensor recordings ($2 \rightarrow 1$ variables). Indeed, this is the very idea behind dimensional reduction.

C. Covariance Matrix

In a 2 variable case it is simple to identify redundant cases by finding the slope of the best-fit line and judging the quality of the fit. How do we quantify and generalize these notions to arbitrariliy higher dimensions? Consider two sets of measurements with zero means [3]

$$A = \{a_1, a_2, \ldots, a_n\} \ , \ B = \{b_1, b_2, \ldots, b_n\}$$

[3] These data sets are in *mean deviation form* because the means have been subtracted off or are zero.

where the subscript denotes the sample number. The variance of A and B are individually defined as,

$$\sigma_A^2 = \langle a_i a_i \rangle_i \ , \ \sigma_B^2 = \langle b_i b_i \rangle_i$$

where the expectation[4] is the average over n variables. The *covariance* between A and B is a straight-forward generalization.

$$covariance\ of\ A\ and\ B \equiv \sigma_{AB}^2 = \langle a_i b_i \rangle_i$$

The covariance measures the degree of the linear relationship between two variables. A large (small) value indicates high (low) redundancy. In the case of Figures 2a and 3c, the covariances are quite large. Some additional facts about the covariance.

- $\sigma_{AB}^2 \geq 0$ (non-negative). σ_{AB} is zero if and only if A and B are entirely uncorrelated.
- $\sigma_{AB}^2 = \sigma_A^2$ if $A = B$.

We can equivalently convert A and B into corresponding row vectors.

$$\begin{aligned} \mathbf{a} &= [a_1\ a_2\ \ldots\ a_n] \\ \mathbf{b} &= [b_1\ b_2\ \ldots\ b_n] \end{aligned}$$

so that we may now express the covariance as a dot product matrix computation.

$$\sigma_{\mathbf{ab}}^2 \equiv \frac{1}{n-1}\mathbf{a}\mathbf{b}^T \qquad (3)$$

where $\frac{1}{n-1}$ is a constant for normalization.[5]

Finally, we can generalize from two vectors to an arbitrary number. We can rename the row vectors $\mathbf{x_1} \equiv \mathbf{a}$, $\mathbf{x_2} \equiv \mathbf{b}$ and consider additional indexed row vectors $\mathbf{x_3}, \ldots, \mathbf{x_m}$. Now we can define a new $m \times n$ matrix $\mathbf{X}$.

$$\mathbf{X} = \begin{bmatrix} \mathbf{x_1} \\ \vdots \\ \mathbf{x_m} \end{bmatrix} \qquad (4)$$

One interpretation of $\mathbf{X}$ is the following. Each *row* of $\mathbf{X}$ corresponds to all measurements of a particular type ($\mathbf{x_i}$). Each *column* of $\mathbf{X}$ corresponds to a set of measurements from one particular trial (this is $\vec{X}$ from section 3.1). We now arrive at a definition for the *covariance matrix* $\mathbf{C_X}$.

$$\mathbf{C_X} \equiv \frac{1}{n-1}\mathbf{X}\mathbf{X}^T. \qquad (5)$$

[4] $\langle \cdot \rangle_i$ denotes the average over values indexed by i.

[5] The most straight-forward normalization is $\frac{1}{n}$. However, this provides a biased estimation of variance particularly for small n. It is beyond the scope of this paper to show that the proper normalization for an unbiased estimator is $\frac{1}{n-1}$.

Consider how the matrix form $\mathbf{X}\mathbf{X}^T$, in that order, computes the desired value for the ij^{th} element of $\mathbf{C_X}$. Specifically, the ij^{th} element of $\mathbf{C_X}$ is the dot product between the vector of the i^{th} measurement type with the vector of the j^{th} measurement type (or substituting $\mathbf{x_i}$ and $\mathbf{x_j}$ for $\mathbf{a}$ and $\mathbf{b}$ into Equation 3). We can summarize several properties of $\mathbf{C_X}$:

- $\mathbf{C_X}$ is a square symmetric $m \times m$ matrix.
- The diagonal terms of $\mathbf{C_X}$ are the *variance* of particular measurement types.
- The off-diagonal terms of $\mathbf{C_X}$ are the *covariance* between measurement types.

$\mathbf{C_X}$ captures the correlations between all possible pairs of measurements. The correlation values reflect the noise and redundancy in our measurements.

- In the diagonal terms, by assumption, large (small) values correspond to interesting dynamics (or noise).
- In the off-diagonal terms large (small) values correspond to high (low) redundancy.

Pretend we have the option of manipulating $\mathbf{C_X}$. We will suggestively define our manipulated covariance matrix $\mathbf{C_Y}$. What features do we want to optimize in $\mathbf{C_Y}$?

D. Diagonalize the Covariance Matrix

We can summarize the last two sections by stating that our goals are (1) to minimize redundancy, measured by covariance, and (2) maximize the signal, measured by variance. By definition covariances must be non-negative, thus the minimal covariance is zero. What would the optimized covariance matrix $\mathbf{C_Y}$ look like? Evidently, in an "optimized" matrix all off-diagonal terms in $\mathbf{C_Y}$ are zero. Thus, $\mathbf{C_Y}$ must be diagonal.

There are many methods for diagonalizing $\mathbf{C_Y}$. It is curious to note that *PCA* arguably selects the easiest method, perhaps accounting for its widespread application.

PCA assumes that all basis vectors $\{\mathbf{p_1}, \ldots, \mathbf{p_m}\}$ are orthonormal (i.e. $\mathbf{p_i} \cdot \mathbf{p_j} = \delta_{ij}$). In the language of linear algebra, *PCA* assumes $\mathbf{P}$ is an orthonormal matrix. Secondly *PCA* assumes the directions with the largest variances the signals and the most "important." In other words, they are the most *principal*. Why are these assumptions easiest?

Envision how *PCA* works. In our simple example in Figure 2b, P acts as a generalized rotation to align a basis with the maximally variant axis. In multiple dimensions this could be performed by a simple algorithm:

1. Select a normalized direction in m-dimensional space along which the variance in $\mathbf{X}$ is maximized. Save this vector as $\mathbf{p_1}$.

2. Find another direction along which variance is maximized, however, because of the orthonormality condition, restrict the search to all directions perpindicular to all previous selected directions. Save this vector as p_i

3. Repeat this procedure until m vectors are selected.

The resulting ordered set of $\mathbf{p}$'s are the *principal components*.

In principle this simple algorithm works, however that would bely the true reason why the orthonormality assumption is particularly judicious. Namely, the true benefit to this assumption is that *it makes the solution amenable to linear algebra*. There exist decompositions that can provide efficient, explicit algebraic solutions.

Notice what we also gained with the second assumption. We have a method for judging the "importance" of the each prinicipal direction. Namely, the variances associated with each direction $\mathbf{p_i}$ quantify how "principal" each direction is. We could thus rank-order each basis vector $\mathbf{p_i}$ according to the corresponding variances.We will now pause to review the implications of all the assumptions made to arrive at this mathematical goal.

E. Summary of Assumptions and Limits

This section provides an important context for understanding when *PCA* might perform poorly as well as a road map for understanding new extensions to *PCA*. The Discussion returns to this issue and provides a more lengthy discussion.

I. *Linearity*
Linearity frames the problem as a change of basis. Several areas of research have explored how applying a nonlinearity prior to performing *PCA* could extend this algorithm - this has been termed *kernel PCA*.

II. *Mean and variance are sufficient statistics.*
The formalism of *sufficient statistics* captures the notion that the mean and the variance entirely describe a probability distribution. The only class of probability distributions that are fully described by the first two moments are exponential distributions (e.g. Gaussian, Exponential, etc).

In order for this assumption to hold, the probability distribution of $\mathbf{x_i}$ must be exponentially distributed. Deviations from this could invalidate this assumption.[6] On the flip side, this assumption formally guarantees that the *SNR* and the covariance matrix fully characterize the noise and redundancies.

III. *Large variances have important dynamics.*
This assumption also encompasses the belief that the data has a high *SNR*. Hence, principal components with larger associated variances represent interesting dynamics, while those with lower variances represent noise.

IV. *The principal components are orthogonal.*
This assumption provides an intuitive simplification that makes *PCA* soluble with linear algebra decomposition techniques. These techniques are highlighted in the two following sections.

We have discussed all aspects of deriving *PCA* - what remain are the linear algebra solutions. The first solution is somewhat straightforward while the second solution involves understanding an important algebraic decomposition.

V. SOLVING PCA: EIGENVECTORS OF COVARIANCE

We derive our first algebraic solution to *PCA* using linear algebra. This solution is based on an important property of eigenvector decomposition. Once again, the data set is $\mathbf{X}$, an $m \times n$ matrix, where m is the number of measurement types and n is the number of samples. The goal is summarized as follows.

> Find some orthonormal matrix $\mathbf{P}$ where $\mathbf{Y} = \mathbf{PX}$ such that $\mathbf{C_Y} \equiv \frac{1}{n-1}\mathbf{YY}^T$ is diagonalized. The rows of $\mathbf{P}$ are the *principal components* of $\mathbf{X}$.

[6] **A sidebar question:** What if $\mathbf{x}_i$ are not Gaussian distributed? Diagonalizing a covariance matrix might not produce satisfactory results. The most rigorous form of removing redundancy is statistical independence.

$$P(\mathbf{y}_1, \mathbf{y}_2) = P(\mathbf{y}_1)P(\mathbf{y}_2)$$

where $P(\cdot)$ denotes the probability density. The class of algorithms that attempt to find the $\mathbf{y_1}, \ldots, \mathbf{y}_m$ that satisfy this statistical constraint are termed independent component analysis (*ICA*). In practice though, quite a lot of real world data are Gaussian distributed - thanks to the Central Limit Theorem - and *PCA* is usually a robust solution to slight deviations from this assumption.

We begin by rewriting $\mathbf{C_Y}$ in terms of our variable of choice $\mathbf{P}$.

$$\begin{aligned}\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{YY}^T \\ &= \frac{1}{n-1}(\mathbf{PX})(\mathbf{PX})^T \\ &= \frac{1}{n-1}\mathbf{PXX}^T\mathbf{P}^T \\ &= \frac{1}{n-1}\mathbf{P}(\mathbf{XX}^T)\mathbf{P}^T \\ \mathbf{C_Y} &= \frac{1}{n-1}\mathbf{PAP}^T\end{aligned}$$

Note that we defined a new matrix $\mathbf{A} \equiv \mathbf{XX}^T$, where $\mathbf{A}$ is *symmetric* (by Theorem 2 of Appendix A).

Our roadmap is to recognize that a symmetric matrix ($\mathbf{A}$) is diagonalized by an orthogonal matrix of its eigenvectors (by Theorems 3 and 4 from Appendix A). For a symmetric matrix $\mathbf{A}$ Theorem 4 provides:

$$\mathbf{A} = \mathbf{EDE}^T \qquad (6)$$

where $\mathbf{D}$ is a diagonal matrix and $\mathbf{E}$ is a matrix of eigenvectors of $\mathbf{A}$ arranged as columns.

The matrix $\mathbf{A}$ has $r \leq m$ orthonormal eigenvectors where r is the rank of the matrix. The rank of $\mathbf{A}$ is less than m when $\mathbf{A}$ is *degenerate* or all data occupy a subspace of dimension $r \leq m$. Maintaining the constraint of orthogonality, we can remedy this situation by selecting $(m - r)$ additional orthonormal vectors to "fill up" the matrix $\mathbf{E}$. These additional vectors do not effect the final solution because the variances associated with these directions are zero.

Now comes the trick. *We select the matrix* $\mathbf{P}$ *to be a matrix where each row* $\mathbf{p_i}$ *is an eigenvector of* $\mathbf{XX}^T$. By this selection, $\mathbf{P} \equiv \mathbf{E^T}$. Substituting into Equation 6, we find $\mathbf{A} = \mathbf{P}^T\mathbf{DP}$. With this relation and Theorem 1 of Appendix A ($\mathbf{P}^{-1} = \mathbf{P}^T$) we can finish evaluating $\mathbf{C_Y}$.

$$\begin{aligned}\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{PAP}^T \\ &= \frac{1}{n-1}\mathbf{P}(\mathbf{P}^T\mathbf{DP})\mathbf{P}^T \\ &= \frac{1}{n-1}(\mathbf{PP}^T)\mathbf{D}(\mathbf{PP}^T) \\ &= \frac{1}{n-1}(\mathbf{PP}^{-1})\mathbf{D}(\mathbf{PP}^{-1}) \\ \mathbf{C_Y} &= \frac{1}{n-1}\mathbf{D}\end{aligned}$$

It is evident that the choice of $\mathbf{P}$ diagonalizes $\mathbf{C_Y}$. This was the goal for *PCA*. We can summarize the results of *PCA* in the matrices $\mathbf{P}$ and $\mathbf{C_Y}$.

- The principal components of $\mathbf{X}$ are the eigenvectors of $\mathbf{XX}^T$; or the rows of $\mathbf{P}$.
- The i^{th} diagonal value of $\mathbf{C_Y}$ is the variance of $\mathbf{X}$ along $\mathbf{p_i}$.

In practice computing *PCA* of a data set $\mathbf{X}$ entails (1) subtracting off the mean of each measurement type and (2) computing the eigenvectors of $\mathbf{XX}^T$. This solution is encapsulated in demonstration Matlab code included in Appendix B.

VI. A MORE GENERAL SOLUTION: SVD

This section is the most mathematically involved and can be skipped without much loss of continuity. It is presented solely for completeness. We derive another algebraic solution for *PCA* and in the process, find that *PCA* is closely related to singular value decomposition (*SVD*). In fact, the two are so intimately related that the names are often used interchangeably. What we will see though is that *SVD* is a more general method of understanding *change of basis*.

We begin by quickly deriving the decomposition. In the following section we interpret the decomposition and in the last section we relate these results to *PCA*.

A. Singular Value Decomposition

Let $\mathbf{X}$ be an arbitrary $n \times m$ matrix[7] and $\mathbf{X}^T\mathbf{X}$ be a rank r, square, symmetric $n \times n$ matrix. In a seemingly unmotivated fashion, let us define all of the quantities of interest.

- $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \ldots, \hat{\mathbf{v}}_r\}$ is the set of *orthonormal* $m \times 1$ eigenvectors with associated eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_r\}$ for the symmetric matrix $\mathbf{X}^T\mathbf{X}$.

$$(\mathbf{X}^T\mathbf{X})\hat{\mathbf{v}}_i = \lambda_i\hat{\mathbf{v}}_i$$

- $\sigma_i \equiv \sqrt{\lambda_i}$ are positive real and termed the *singular values.*
- $\{\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \ldots, \hat{\mathbf{u}}_r\}$ is the set of *orthonormal* $n \times 1$ vectors defined by $\hat{\mathbf{u}}_\mathbf{i} \equiv \frac{\mathbf{1}}{\sigma_\mathbf{i}}\mathbf{X}\hat{\mathbf{v}}_\mathbf{i}$.

We obtain the final definition by referring to Theorem 5 of Appendix A. The final definition includes two new and unexpected properties.

- $\hat{\mathbf{u}}_\mathbf{i} \cdot \hat{\mathbf{u}}_\mathbf{j} = \delta_{ij}$
- $\|\mathbf{X}\hat{\mathbf{v}}_\mathbf{i}\| = \sigma_i$

These properties are both proven in Theorem 5. We now have all of the pieces to construct the decomposition. The

[7] Notice that in this section only we are reversing convention from $m \times n$ to $n \times m$. The reason for this derivation will become clear in section 6.3.

"value" version of singular value decomposition is just a restatement of the third definition.

$$\mathbf{X}\hat{\mathbf{v}}_i = \sigma_i \hat{\mathbf{u}}_i \tag{7}$$

This result says a quite a bit. $\mathbf{X}$ multiplied by an eigenvector of $\mathbf{X}^T\mathbf{X}$ is equal to a scalar times another vector. The set of eigenvectors $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \ldots, \hat{\mathbf{v}}_r\}$ and the set of vectors $\{\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \ldots, \hat{\mathbf{u}}_r\}$ are both orthonormal sets or bases in r-dimensional space.

We can summarize this result for all vectors in one matrix multiplication by following the prescribed construction in Figure 4. We start by constructing a new diagonal matrix $\mathbf{\Sigma}$.

$$\mathbf{\Sigma} \equiv \begin{bmatrix} \sigma_{\tilde{1}} & & & & & \\ & \ddots & & & \Large 0 & \\ & & \sigma_{\tilde{r}} & & & \\ & & & 0 & & \\ & \Large 0 & & & \ddots & \\ & & & & & 0 \end{bmatrix}$$

where $\sigma_{\tilde{1}} \geq \sigma_{\tilde{2}} \geq \ldots \geq \sigma_{\tilde{r}}$ are the rank-ordered set of singular values. Likewise we construct accompanying orthogonal matrices $\mathbf{V}$ and $\mathbf{U}$.

$$\begin{aligned} \mathbf{V} &= [\hat{\mathbf{v}}_{\tilde{\mathbf{1}}}\ \hat{\mathbf{v}}_{\tilde{\mathbf{2}}}\ \ldots\ \hat{\mathbf{v}}_{\tilde{\mathbf{m}}}] \\ \mathbf{U} &= [\hat{\mathbf{u}}_{\tilde{\mathbf{1}}}\ \hat{\mathbf{u}}_{\tilde{\mathbf{2}}}\ \ldots\ \hat{\mathbf{u}}_{\tilde{\mathbf{n}}}] \end{aligned}$$

where we have appended an additional $(m-r)$ and $(n-r)$ orthonormal vectors to "fill up" the matrices for $\mathbf{V}$ and $\mathbf{U}$ respectively[8]. Figure 4 provides a graphical representation of how all of the pieces fit together to form the matrix version of *SVD*.

$$\mathbf{XV} = \mathbf{U\Sigma} \tag{8}$$

where each column of $\mathbf{V}$ and $\mathbf{U}$ perform the "value" version of the decomposition (Equation 7). Because $\mathbf{V}$ is orthogonal, we can multiply both sides by $\mathbf{V}^{-1} = \mathbf{V}^T$ to arrive at the final form of the decomposition.

$$\mathbf{X} = \mathbf{U\Sigma V}^T \tag{9}$$

Although it was derived without motivation, this decomposition is quite powerful. Equation 9 states that *any* arbitrary matrix $\mathbf{X}$ can be converted to an orthogonal matrix, a diagonal matrix and another orthogonal matrix (or a rotation, a stretch and a second rotation). Making sense of Equation 9 is the subject of the next section.

[8] This is the same procedure used to fix the degeneracy in the previous section.

B. Interpreting SVD

The final form of *SVD* (Equation 9) is a concise but thick statement to understand. Let us instead reinterpret Equation 7.

$$\mathbf{Xa} = k\mathbf{b}$$

where $\mathbf{a}$ and $\mathbf{b}$ are column vectors and k is a scalar constant. The set $\{\hat{\mathbf{v}}_\mathbf{1}, \hat{\mathbf{v}}_\mathbf{2}, \ldots, \hat{\mathbf{v}}_\mathbf{m}\}$ is analogous to $\mathbf{a}$ and the set $\{\hat{\mathbf{u}}_\mathbf{1}, \hat{\mathbf{u}}_\mathbf{2}, \ldots, \hat{\mathbf{u}}_\mathbf{n}\}$ is analogous to $\mathbf{b}$. What is unique though is that $\{\hat{\mathbf{v}}_\mathbf{1}, \hat{\mathbf{v}}_\mathbf{2}, \ldots, \hat{\mathbf{v}}_\mathbf{m}\}$ and $\{\hat{\mathbf{u}}_\mathbf{1}, \hat{\mathbf{u}}_\mathbf{2}, \ldots, \hat{\mathbf{u}}_\mathbf{n}\}$ are orthonormal sets of vectors which *span* an m or n dimensional space, respectively. In particular, loosely speaking these sets appear to span all possible "inputs" ($\mathbf{a}$) and "outputs" ($\mathbf{b}$). Can we formalize the view that $\{\hat{\mathbf{v}}_\mathbf{1}, \hat{\mathbf{v}}_\mathbf{2}, \ldots, \hat{\mathbf{v}}_\mathbf{n}\}$ and $\{\hat{\mathbf{u}}_\mathbf{1}, \hat{\mathbf{u}}_\mathbf{2}, \ldots, \hat{\mathbf{u}}_\mathbf{n}\}$ span all possible "inputs" and "outputs"?

We can manipulate Equation 9 to make this fuzzy hypothesis more precise.

$$\begin{aligned} \mathbf{X} &= \mathbf{U\Sigma V}^T \\ \mathbf{U}^T\mathbf{X} &= \mathbf{\Sigma V}^T \\ \mathbf{U}^T\mathbf{X} &= \mathbf{Z} \end{aligned}$$

where we have defined $\mathbf{Z} \equiv \mathbf{\Sigma V}^T$. Note that the previous columns $\{\hat{\mathbf{u}}_\mathbf{1}, \hat{\mathbf{u}}_\mathbf{2}, \ldots, \hat{\mathbf{u}}_\mathbf{n}\}$ are now rows in $\mathbf{U}^T$. Comparing this equation to Equation 1, $\{\hat{\mathbf{u}}_\mathbf{1}, \hat{\mathbf{u}}_\mathbf{2}, \ldots, \hat{\mathbf{u}}_\mathbf{n}\}$ perform the same role as $\{\hat{\mathbf{p}}_\mathbf{1}, \hat{\mathbf{p}}_\mathbf{2}, \ldots, \hat{\mathbf{p}}_\mathbf{m}\}$. Hence, $\mathbf{U}^T$ is a *change of basis* from $\mathbf{X}$ to $\mathbf{Z}$. Just as before, we were transforming column vectors, we can again infer that we are transforming column vectors. The fact that the orthonormal basis $\mathbf{U}^T$ (or $\mathbf{P}$) transforms column vectors means that $\mathbf{U}^T$ is a basis that spans the columns of $\mathbf{X}$. Bases that span the columns are termed the *column space* of $\mathbf{X}$. The column space formalizes the notion of what are the possible "outputs" of any matrix.

There is a funny symmetry to *SVD* such that we can define a similar quantity - the *row space.*

$$\begin{aligned} \mathbf{XV} &= \mathbf{\Sigma U} \\ (\mathbf{XV})^T &= (\mathbf{\Sigma U})^T \\ \mathbf{V}^T\mathbf{X}^T &= \mathbf{U}^T\mathbf{\Sigma} \\ \mathbf{V}^T\mathbf{X}^T &= \mathbf{Z} \end{aligned}$$

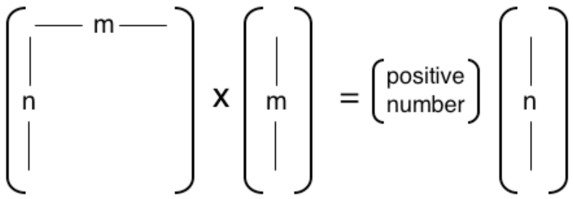
where we have defined $\mathbf{Z} \equiv \mathbf{U^T\Sigma}$. Again the rows of $\mathbf{V}^T$ (or the columns of $\mathbf{V}$) are an orthonormal basis for transforming $\mathbf{X}^T$ into $\mathbf{Z}$. Because of the transpose on $\mathbf{X}$, it follows that $\mathbf{V}$ is an orthonormal basis spanning the *row space* of $\mathbf{X}$. The row space likewise formalizes the notion of what are possible "inputs" into an arbitrary matrix.

We are only scratching the surface for understanding the full implications of *SVD*. For the purposes of this tutorial though, we have enough information to understand how *PCA* will fall within this framework.

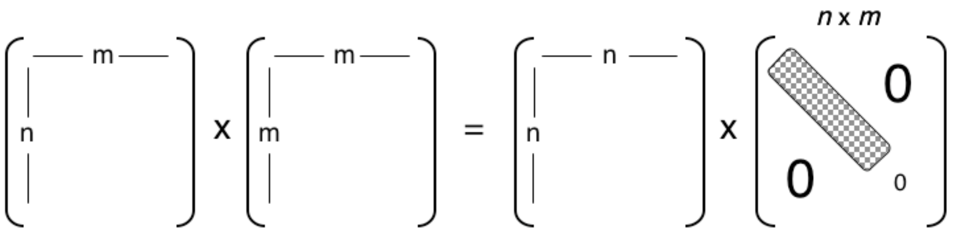
The "value" form of SVD is expressed in equation 7.

$$\mathbf{X}\hat{\mathbf{v}}_i = \sigma_i \hat{\mathbf{u}}_i$$

The mathematical intuition behind the construction of the matrix form is that we want to express all n "value" equations in just one equation. It is easiest to understand this process graphically. Drawing the matrices of equation 7 looks likes the following.



We can construct three new matrices $\mathbf{V}$, $\mathbf{U}$ and $\mathbf{\Sigma}$. All singular values are first rank-ordered $\sigma_{\tilde{1}} \geq \sigma_{\tilde{2}} \geq \ldots \geq \sigma_{\tilde{r}}$, and the corresponding vectors are indexed in the same rank order. Each pair of associated vectors $\hat{\mathbf{v}}_\mathbf{i}$ and $\hat{\mathbf{u}}_\mathbf{i}$ is stacked in the i^{th} column along their respective matrices. The corresponding singular value σ_i is placed along the diagonal (the ii^{th} position) of $\mathbf{\Sigma}$. This generates the equation $\mathbf{XV} = \mathbf{U\Sigma}$, which looks like the following.



The matrices $\mathbf{V}$ and $\mathbf{U}$ are $m \times m$ and $n \times n$ matrices respectively and $\mathbf{\Sigma}$ is a diagonal matrix with a few non-zero values (represented by the checkerboard) along its diagonal. Solving this single matrix equation solves all n "value" form equations.

FIG. 4 How to construct the matrix form of SVD from the "value" form.

C. SVD and PCA

With similar computations it is evident that the two methods are intimately related. Let us return to the original $m \times n$ data matrix $\mathbf{X}$. We can define a new matrix $\mathbf{Y}$ as an $n \times m$ matrix[9].

$$\mathbf{Y} \equiv \frac{1}{\sqrt{n-1}} \mathbf{X}^T$$

where each *column* of $\mathbf{Y}$ has zero mean. The definition of $\mathbf{Y}$ becomes clear by analyzing $\mathbf{Y}^T\mathbf{Y}$.

$$\begin{aligned} \mathbf{Y}^T\mathbf{Y} &= \left(\frac{1}{\sqrt{n-1}}\mathbf{X}^T\right)^T \left(\frac{1}{\sqrt{n-1}}\mathbf{X}^T\right) \\ &= \frac{1}{n-1}\mathbf{X}^{TT}\mathbf{X}^T \\ &= \frac{1}{n-1}\mathbf{X}\mathbf{X}^T \\ \mathbf{Y}^T\mathbf{Y} &= \mathbf{C}_\mathbf{X} \end{aligned}$$

By construction $\mathbf{Y}^T\mathbf{Y}$ equals the covariance matrix of $\mathbf{X}$. From section 5 we know that the principal components of $\mathbf{X}$ are the eigenvectors of $\mathbf{C}_\mathbf{X}$. If we calculate the *SVD* of $\mathbf{Y}$, the columns of matrix $\mathbf{V}$ contain the eigenvectors of $\mathbf{Y}^T\mathbf{Y} = \mathbf{C}_\mathbf{X}$. *Therefore, the columns of* $\mathbf{V}$ *are the principal components of* $\mathbf{X}$. This second algorithm is encapsulated in Matlab code included in Appendix B.

What does this mean? $\mathbf{V}$ spans the row space of $\mathbf{Y} \equiv \frac{1}{\sqrt{n-1}}\mathbf{X}^T$. Therefore, $\mathbf{V}$ must also span the column space of $\frac{1}{\sqrt{n-1}}\mathbf{X}$. We can conclude that finding the principal components[10] amounts to finding an orthonormal basis that spans the *column space* of $\mathbf{X}$.

[9] $\mathbf{Y}$ is of the appropriate $n \times m$ dimensions laid out in the derivation of section 6.1. This is the reason for the "flipping" of dimensions in 6.1 and Figure 4.

[10] If the final goal is to find an orthonormal basis for the coulmn space of $\mathbf{X}$ then we can calculate it directly without constructing $\mathbf{Y}$. By symmetry the columns of $\mathbf{U}$ produced by the *SVD* of $\frac{1}{\sqrt{n-1}}\mathbf{X}$ must also be the principal components.

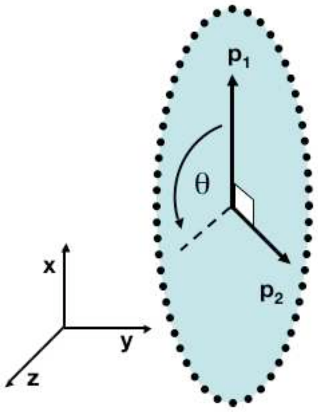


FIG. 5 Data points (black dots) tracking a person on a ferris wheel. The extracted principal components are $(\mathbf{p_1}, \mathbf{p_2})$ and the phase is $\hat{\theta}$.

VII. DISCUSSION AND CONCLUSIONS

A. Quick Summary

Performing *PCA* is quite simple in practice.

1. Organize a data set as an $m \times n$ matrix, where m is the number of measurement types and n is the number of trials.

2. Subtract off the mean for each measurement type or row $\mathbf{x_i}$.

3. Calculate the *SVD* or the eigenvectors of the covariance.

In several fields of literature, many authors refer to the individual measurement types $\mathbf{x_i}$ as the *sources*. The data projected into the principal components $\mathbf{Y} = \mathbf{PX}$ are termed the *signals*, because the projected data presumably represent the underlying items of interest.

B. Dimensional Reduction

One benefit of *PCA* is that we can examine the variances $\mathbf{C_Y}$ associated with the principle components. Often one finds that large variances associated with the first $k < m$ principal components, and then a precipitous drop-off. One can conclude that most interesting dynamics occur only in the first k dimensions.

In the example of the spring, $k = 1$. This process of throwing out the less important axes can help reveal hidden, simplified dynamics in high dimensional data. This process is aptly named *dimensional reduction*.

C. Limits and Extensions of PCA

Both the strength and weakness of *PCA* is that it is a *non-parametric* analysis. One only needs to make the assumptions outlined in section 4.5 and then calculate the corresponding answer. There are no parameters to tweak and no coefficients to adjust based on user experience - the answer is unique[11] and independent of the user.

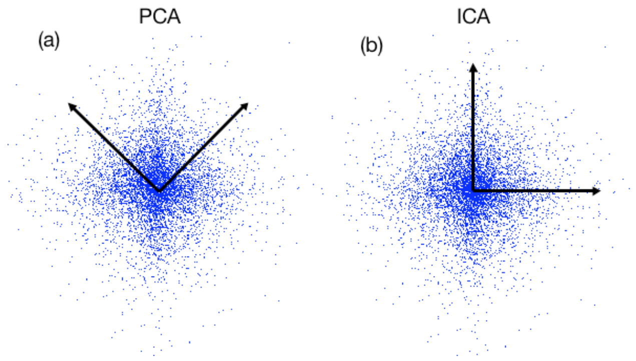


FIG. 6 Non-Gaussian distributed data causes *PCA* to fail. In exponentially distributed data the axes with the largest variance do not correspond to the underlying basis.

This same strength can also be viewed as a weakness. If one knows a-priori some features of the structure of a system, then it makes sense to incorporate these assumptions into a *parametric* algorithm - or an algorithm with selected parameters.

Consider the recorded positions of a person on a ferris wheel over time in Figure 5. The probability distributions along the axes are approximately Gaussian and thus *PCA* finds $(\mathbf{p_1}, \mathbf{p_2})$, however this answer might not be optimal. The most concise form of dimensional reduction is to recognize that the phase (or angle along the ferris wheel) contains all dynamic information. Thus, the appropriate parametric algorithm is to first convert the data to the appropriately centered polar coordinates and then compute *PCA*.

This prior *non-linear* transformation is sometimes termed a *kernel transformation* and the entire parametric algorithm is termed *kernel PCA*. Other common kernel transformations include Fourier and Gaussian transformations. This procedure is parametric because the user must incorporate prior knowledge of the structure in the selection of the kernel but it is also more optimal in the sense that the structure is more concisely described.

Sometimes though the assumptions themselves are too stringent. One might envision situations where the principal components need not be orthogonal. Furthermore, the distributions along each dimension $(\mathbf{x_i})$ need not be

[11] To be absolutely precise, the principal components are **not** uniquely defined; only the sub-space is unique. One can always flip the direction of the principal components by multiplying by -1. In addition, eigenvectors beyond the rank of a matrix (i.e. $\sigma_i = 0$ for $i > rank$) can be selected almost at whim. However, these degrees of freedom do not effect the qualitative features of the solution nor a dimensional reduction.

Gaussian. For instance, Figure 6 contains a 2-D exponentially distributed data set. The largest variances do not correspond to the meaningful axes; thus *PCA* fails.

This less constrained set of problems is not trivial and only recently has been solved adequately via *Independent Component Analysis (ICA)*. The formulation is equivalent.

> Find a matrix $\mathbf{P}$ where $\mathbf{Y} = \mathbf{PX}$ such that $\mathbf{C_Y}$ is diagonalized.

however it abandons all assumptions except linearity, and attempts to find axes that satisfy the most formal form of redundancy reduction - *statistical independence*. Mathematically *ICA* finds a basis such that the joint probability distribution can be factorized[12].

$$P(\mathbf{y_i}, \mathbf{y_j}) = P(\mathbf{y_i})P(\mathbf{y_j})$$

for all i and j, $i \neq j$. The downside of *ICA* is that it is a form of nonlinear optimizaiton, making the solution difficult to calculate in practice and potentially not unique. However *ICA* has been shown a very practical and powerful algorithm for solving a whole new class of problems.

Writing this paper has been an extremely instructional experience for me. I hope that this paper helps to demystify the motivation and results of *PCA*, and the underlying assumptions behind this important analysis technique. Please send me a note if this has been useful to you as it inspires me to keep writing!

APPENDIX A: Linear Algebra

This section proves a few unapparent theorems in linear algebra, which are crucial to this paper.

1. The inverse of an orthogonal matrix is its transpose.

The goal of this proof is to show that if $\mathbf{A}$ is an orthogonal matrix, then $\mathbf{A}^{-1} = \mathbf{A}^T$.

Let $\mathbf{A}$ be an $m \times n$ matrix.

$$\mathbf{A} = [\mathbf{a_1}\ \mathbf{a_2}\ \ldots\ \mathbf{a_n}]$$

where $\mathbf{a_i}$ is the i^{th} *column* vector. We now show that $\mathbf{A}^T\mathbf{A} = \mathbf{I}$ where $\mathbf{I}$ is the identity matrix.

Let us examine the ij^{th} element of the matrix $\mathbf{A}^T\mathbf{A}$. The ij^{th} element of $\mathbf{A}^T\mathbf{A}$ is $(\mathbf{A}^T\mathbf{A})_{ij} = \mathbf{a_i}^T\mathbf{a_j}$.

Remember that the columns of an orthonormal matrix are orthonormal to each other. In other words, the dot product of any two columns is zero. The only exception is a dot product of one particular column with itself, which equals one.

$$(\mathbf{A}^T\mathbf{A})_{ij} = \mathbf{a_i}^T\mathbf{a_j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$\mathbf{A}^T\mathbf{A}$ is the exact description of the identity matrix. The definition of $\mathbf{A}^{-1}$ is $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$. Therefore, because $\mathbf{A}^T\mathbf{A} = \mathbf{I}$, it follows that $\mathbf{A}^{-1} = \mathbf{A}^T$.

2. If A is any matrix, the matrices $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}\mathbf{A}^T$ are both symmetric.

Let's examine the transpose of each in turn.

$$\begin{aligned}(\mathbf{A}\mathbf{A}^T)^T &= \mathbf{A}^{TT}\mathbf{A}^T = \mathbf{A}\mathbf{A}^T \\ (\mathbf{A}^T\mathbf{A})^T &= \mathbf{A}^T\mathbf{A}^{TT} = \mathbf{A}^T\mathbf{A}\end{aligned}$$

The equality of the quantity with its transpose completes this proof.

3. A matrix is symmetric if and only if it is orthogonally diagonalizable.

Because this statement is bi-directional, it requires a two-part "if-and-only-if" proof. One needs to prove the forward and the backwards "if-then" cases.

Let us start with the forward case. If $\mathbf{A}$ is orthogonally diagonalizable, then $\mathbf{A}$ is a symmetric matrix. By hypothesis, orthogonally diagonalizable means that there exists some $\mathbf{E}$ such that $\mathbf{A} = \mathbf{EDE}^T$, where $\mathbf{D}$ is a diagonal matrix and $\mathbf{E}$ is some special matrix which diagonalizes $\mathbf{A}$. Let us compute $\mathbf{A}^T$.

$$\mathbf{A}^T = (\mathbf{EDE}^T)^T = \mathbf{E}^{TT}\mathbf{D}^T\mathbf{E}^T = \mathbf{EDE}^T = \mathbf{A}$$

Evidently, if $\mathbf{A}$ is orthogonally diagonalizable, it must also be symmetric.

The reverse case is more involved and less clean so it will be left to the reader. In lieu of this, hopefully the "forward" case is suggestive if not somewhat convincing.

4. A symmetric matrix is diagonalized by a matrix of its orthonormal eigenvectors.

Restated in math, let $\mathbf{A}$ be a square $n \times n$ symmetric matrix with associated eigenvectors $\{\mathbf{e_1}, \mathbf{e_2}, \ldots, \mathbf{e_n}\}$. Let $\mathbf{E} = [\mathbf{e_1}\ \mathbf{e_2}\ \ldots\ \mathbf{e_n}]$ where the i^{th} column of $\mathbf{E}$ is the eigenvector $\mathbf{e_i}$. This theorem asserts that there exists a diagonal matrix D where $\mathbf{A} = \mathbf{EDE}^T$.

This theorem is an extension of the previous theorem 3. It provides a prescription for how to find the matrix $\mathbf{E}$, the "diagonalizer" for a symmetric matrix. It says that the special diagonalizer is in fact a matrix of the original matrix's eigenvectors.

This proof is in two parts. In the first part, we see that the any matrix can be orthogonally diagonalized if and only if it that matrix's eigenvectors are all linearly independent. In the second part of the proof, we see that

[12] Equivalently, in the language of *information theory* the goal is to find a basis $\mathbf{P}$ such that the mutual information $I(\mathbf{y_i}, \mathbf{y_j}) = 0$ for $i \neq j$.

a symmetric matrix has the special property that all of its eigenvectors are not just linearly independent but also orthogonal, thus completing our proof.

In the first part of the proof, let $\mathbf{A}$ be just some matrix, not necessarily symmetric, and let it have independent eigenvectors (i.e. no degeneracy). Furthermore, let $\mathbf{E} = [\mathbf{e_1}\ \mathbf{e_2}\ \ldots\ \mathbf{e_n}]$ be the matrix of eigenvectors placed in the columns. Let $\mathbf{D}$ be a diagonal matrix where the i^{th} eigenvalue is placed in the ii^{th} position.

We will now show that $\mathbf{AE} = \mathbf{ED}$. We can examine the columns of the right-hand and left-hand sides of the equation.

$$\begin{array}{rrcl} \text{Left hand side :} & \mathbf{AE} & = & [\mathbf{Ae_1}\ \mathbf{Ae_2}\ \ldots\ \mathbf{Ae_n}] \\ \text{Right hand side :} & \mathbf{ED} & = & [\lambda_1\mathbf{e_1}\ \lambda_2\mathbf{e_2}\ \ldots\ \lambda_n\mathbf{e_n}] \end{array}$$

Evidently, if $\mathbf{AE} = \mathbf{ED}$ then $\mathbf{Ae_i} = \lambda_i\mathbf{e_i}$ for all i. This equation is the definition of the eigenvalue equation. Therefore, it must be that $\mathbf{AE} = \mathbf{ED}$. A little rearrangement provides $\mathbf{A} = \mathbf{EDE}^{-1}$, completing the first part the proof.

For the second part of the proof, we show that a symmetric matrix always has orthogonal eigenvectors. For some symmetric matrix, let λ_1 and λ_2 be distinct eigenvalues for eigenvectors $\mathbf{e_1}$ and $\mathbf{e_2}$.

$$\begin{aligned} \lambda_1\mathbf{e_1}\cdot\mathbf{e_2} &= (\lambda_1\mathbf{e_1})^T\mathbf{e_2} \\ &= (\mathbf{Ae_1})^T\mathbf{e_2} \\ &= \mathbf{e_1}^T\mathbf{A}^T\mathbf{e_2} \\ &= \mathbf{e_1}^T\mathbf{Ae_2} \\ &= \mathbf{e_1}^T(\lambda_2\mathbf{e_2}) \\ \lambda_1\mathbf{e_1}\cdot\mathbf{e_2} &= \lambda_2\mathbf{e_1}\cdot\mathbf{e_2} \end{aligned}$$

By the last relation we can equate that $(\lambda_1 - \lambda_2)\mathbf{e_1}\cdot\mathbf{e_2} = 0$. Since we have conjectured that the eigenvalues are in fact unique, it must be the case that $\mathbf{e_1}\cdot\mathbf{e_2} = 0$. Therefore, the eigenvectors of a symmetric matrix are orthogonal.

Let us back up now to our original postulate that $\mathbf{A}$ is a symmetric matrix. By the second part of the proof, we know that the eigenvectors of $\mathbf{A}$ are all orthonormal (we choose the eigenvectors to be normalized). This means that $\mathbf{E}$ is an orthogonal matrix so by theorem 1, $\mathbf{E}^T = \mathbf{E}^{-1}$ and we can rewrite the final result.

$$\mathbf{A} = \mathbf{EDE}^T$$

. Thus, a symmetric matrix is diagonalized by a matrix of its eigenvectors.

5. For any arbitrary $m \times n$ matrix $\mathbf{X}$, the symmetric matrix $\mathbf{X}^T\mathbf{X}$ has a set of orthonormal eigenvectors of $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \ldots, \hat{\mathbf{v}}_n\}$ and a set of associated eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. The set of vectors $\{\mathbf{X}\hat{\mathbf{v}}_1, \mathbf{X}\hat{\mathbf{v}}_2, \ldots, \mathbf{X}\hat{\mathbf{v}}_n\}$ then form an orthogonal basis, where each vector $\mathbf{X}\hat{\mathbf{v}}_i$ is of length $\sqrt{\lambda_i}$.

All of these properties arise from the dot product of any two vectors from this set.

$$\begin{aligned} (\mathbf{X}\hat{\mathbf{v}}_i)\cdot(\mathbf{X}\hat{\mathbf{v}}_j) &= (\mathbf{X}\hat{\mathbf{v}}_i)^T(\mathbf{X}\hat{\mathbf{v}}_j) \\ &= \hat{\mathbf{v}}_i^T\mathbf{X}^T\mathbf{X}\hat{\mathbf{v}}_j \\ &= \hat{\mathbf{v}}_i^T(\lambda_j\hat{\mathbf{v}}_j) \\ &= \lambda_j\hat{\mathbf{v}}_i\cdot\hat{\mathbf{v}}_j \\ (\mathbf{X}\hat{\mathbf{v}}_i)\cdot(\mathbf{X}\hat{\mathbf{v}}_j) &= \lambda_j\delta_{ij} \end{aligned}$$

The last relation arises because the set of eigenvectors of $\mathbf{X}$ is orthogonal resulting in the Kronecker delta. In more simpler terms the last relation states:

$$(\mathbf{X}\hat{\mathbf{v}}_i)\cdot(\mathbf{X}\hat{\mathbf{v}}_j) = \begin{cases} \lambda_j & i = j \\ 0 & i \neq j \end{cases}$$

This equation states that any two vectors in the set are orthogonal.

The second property arises from the above equation by realizing that the length squared of each vector is defined as:

$$\|\mathbf{X}\hat{\mathbf{v}}_i\|^2 = (\mathbf{X}\hat{\mathbf{v}}_i)\cdot(\mathbf{X}\hat{\mathbf{v}}_i) = \lambda_i$$

APPENDIX B: Code

This code is written for Matlab 6.5 (Release 13) from Mathworks[13]. The code is not computationally efficient but explanatory (terse comments begin with a %).

This first version follows Section 5 by examining the covariance of the data set.

```
function [signals,PC,V] = pca1(data)
% PCA1: Perform PCA using covariance.
%     data - MxN matrix of input data
%            (M dimensions, N trials)
%  signals - MxN matrix of projected data
%       PC - each column is a PC
%        V - Mx1 matrix of variances

[M,N] = size(data);

% subtract off the mean for each dimension
mn =  mean(data,2);
data = data - repmat(mn,1,N);

% calculate the covariance matrix
covariance = 1 / (N-1) * data * data';

% find the eigenvectors and eigenvalues
[PC, V] = eig(covariance);
```

[13] http://www.mathworks.com

```
% extract diagonal of matrix as vector
V = diag(V);

% sort the variances in decreasing order
[junk, rindices] = sort(-1*V);
V  = V(rindices);
PC = PC(:,rindices);

% project the original data set
signals = PC' * data;
```

This second version follows section 6 computing *PCA* through *SVD*.

```
function [signals,PC,V] = pca2(data)
% PCA2: Perform PCA using SVD.
%     data - MxN matrix of input data
%            (M dimensions, N trials)
%  signals - MxN matrix of projected data
%       PC - each column is a PC
%        V - Mx1 matrix of variances

[M,N] = size(data);

% subtract off the mean for each dimension
mn =  mean(data,2);
data = data - repmat(mn,1,N);

% construct the matrix Y
Y = data' / sqrt(N-1);

% SVD does it all
[u,S,PC] = svd(Y);

% calculate the variances
S = diag(S);
V = S .* S;

% project the original data
signals = PC' * data;
```

APPENDIX C: References

Bell, Anthony and Sejnowski, Terry. (1997) “The Independent Components of Natural Scenes are Edge Filters.” *Vision Research* 37(23), 3327-3338.
[A paper from my field of research that surveys and explores different forms of decorrelating data sets. The authors examine the features of PCA and compare it with new ideas in redundancy reduction, namely Independent Component Analysis.]

Bishop, Christopher. (1996) *Neural Networks for Pattern Recognition.* Clarendon, Oxford, UK.
[A challenging but brilliant text on statistical pattern recognition. Although the derivation of PCA is tough in section 8.6 (p.310-319), it does have a great discussion on potential extensions to the method and it puts PCA in context of other methods of dimensional reduction. Also, I want to acknowledge this book for several ideas about the limitations of PCA.]

Lay, David. (2000). *Linear Algebra and It's Applications.* Addison-Wesley, New York.
[This is a beautiful text. Chapter 7 in the second edition (p. 441-486) has an exquisite, intuitive derivation and discussion of SVD and PCA. Extremely easy to follow and a must read.]

Mitra, Partha and Pesaran, Bijan. (1999) "Analysis of Dynamic Brain Imaging Data.” *Biophysical Journal.* 76, 691-708.
[A comprehensive and spectacular paper from my field of research interest. It is dense but in two sections "Eigenmode Analysis: SVD" and "Space-frequency SVD" the authors discuss the benefits of performing a Fourier transform on the data before an SVD.]

Will, Todd (1999) "Introduction to the Singular Value Decomposition" Davidson College. *www.davidson.edu/academic/math/will/svd/index.html*
[A math professor wrote up a great web tutorial on SVD with tremendous intuitive explanations, graphics and animations. Although it avoids PCA directly, it gives a great intuitive feel for what SVD is doing mathematically. Also, it is the inspiration for my "spring" example.]