Principal Component Analysis: Data Reduction and Simplification

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The primary purpose of principal component analysis (PCA) is to reduce the dimension of a large data set containing interrelated variables into a more concise data set that retains most of the existing variations. The objective of this paper is to intuitively and mathematically explain why this analysis works and how it can be applied to experimental data. A 6061 aluminum rod with attached strain gages was subjected to a torsion test using a Tinius Olsen Bench Type Torsion Testing Machine and torque, shear strain (γ), and angle of twist (φ) were measured and recorded from the test. Although the relationships among the three measured variables are well known, PCA was performed on the test data to rediscover these correlations. The results of the analysis did indeed identify the most significant relationships within the test data, and revealed the material linearity of the test specimen.

I. Introduction

The primary purpose of principal component analysis (PCA) is to reduce the dimension of a large data set which contains interrelated variables into a smaller, simpler set that retains most of the variations among the data [1]. PCA has the ability of extracting the most significant variations between variables to reveal the sometimes simple relationship among large sets of data. It does this by transforming the original basis in which the data is expressed into a more “meaningful” basis [2]. These new bases are called the principal components of the data and are derived in such a way that the first few retain most of the variations exhibited in the original data.

Oftentimes in experimentation, the experimenter does not known the dynamics of the system that he or she is observing and, as the goal of all experiments, seeks to understand the relationships among the measured data. Depending on the complexity of the system, there can be a large number of variables, m, recorded over several trails, n, during the experiment. It would then be necessary to decipher the important relationships within an $m \times n$ set of

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entries which, in most cases, is not a trivial task. In addition to the sheer volume of the data, noise and redundancy further compounds the difficulty of the task.

II. Derivation

To fully understand the intuitive derivation of PCA, some basic linear algebra and mathematical statistics knowledge must be known. As an aid, Appendix A briefly defines the statistical expressions used heavily in the following section. The mathematical derivation uses the method of Lagrange multipliers which is explained in Appendix B for the benefit of the reader.

A. Intuitive Derivation

PCA makes an initial assumption that ensures the implementation and results of the analysis are both simple and clear to interpret. This assumption is linearity which greatly simplifies the problem in two ways by (1) restricting the potential set of bases and (2) further assuming that the data set is continuous [2].

Returning to the goal of PCA, we seek a linear transformation matrix $P$, to re-express the original $m \times n$ data set matrix $X$, into the data in the new bases $Y$.

$$P_{m \times m}X_{m \times n} = Y_{m \times n}$$

It can be immediately noticed that $P$ is a square matrix whose rows are the new basis for the columns of $X$. Under additional assumptions, the row vectors of $P$ will become the coefficients or loadings of the principal components of the data set $X$. If the signal-to-noise ratio in the collected data is reasonably higher than unity, then PCA assumes that the dynamics of interest in the observed system lie within the directions of largest variance. The new criterion for $P$ becomes to maximize the variance in $X$.

The original data may also include redundancy which simply adds dimensionality to the data set, but no new additional information. The goal is to express the original data in the smallest form possible; therefore, it is necessary to eliminate redundant data from the set. Fortunately, mathematical statistics provides a way to compare the relationship between different variables. The covariance is an extension of the variance in a two dimensional case. Covariance is a measure of how much two dimensions or variables vary from the mean with respect to each other [3]. The covariance of the data $X$ can be expressed as
\[ C_X = E\left( XX^T \right) \]

or the expectation of \( X \) by \( X \) transpose. The columns of \( X \), \( \{ x_1, x_2 \ldots x_n \} \), contain an \( m \) number of variables and thus the matrix multiplication will yield a square \( m \times m \) covariance matrix with elements \( i, j = 1, 2 \ldots m \). The diagonal elements where \( i = j \) represent the variance while the non-diagonal terms represent the covariance between the \( i^{th} \) and \( j^{th} \) terms.

In terms of redundancy, a high covariance corresponds to high redundancy between the two variables, and conversely a low covariance corresponds to low redundancy. If two variables are independent of one another, then the covariance is zero. Now with this new knowledge, we wish the covariance matrix of the new data set, \( C_Y \), to be a diagonal matrix which in turn identifies variance and minimizes redundancy. The bases or row vectors \( \{ p_1, p_2 \ldots p_m \} \) are orthogonal to one another due to the linearity assumption. For simplicity, these rows are taken in the unit directions and therefore \( P \) becomes an orthogonal matrix.

Summarizing the requirements of PCA leads to the intuitive proof:

\[ C_Y = E\left( YY^T \right) \]

Substituting \( Y = PX \),

\[ = E\left[ PX(PX)^T \right] \]
\[ = PE\left( XX^T \right)P^T \]

From linear algebra, \( XX^T \) is a symmetric matrix which can be expressed in terms of its normalized eigenvectors \( Q \) and its diagonal eigenvalues \( \Lambda \) as

\[ XX^T = QAQ^T. \]

Suppose that \( P \) is selected in such a way that it is equal to the normalized eigenvectors of \( XX^T \) or in other words \( Q = P^T \).

\[ = Q^T E\left( QAQ^T \right)Q \]
\[ = \left( QQ^T \right) E\left( \Lambda \right)\left( QQ^T \right) \]

The property \( Q^T = Q^T \) is derived from linear algebra and can thus be used to simplify the expression.
\[
\begin{align*}
\mathbf{C}_Y &= \mathbf{E}(\Lambda) \\
\Rightarrow \mathbf{YY}^T &= \Lambda
\end{align*}
\]

It can be seen that the sought after \( \mathbf{P} \) is actually the orthogonal matrix containing the eigenvectors of \( \mathbf{X} \), and the variances of interest are the diagonals of \( \Lambda \), or the eigenvalues of \( \mathbf{X} \). If the eigenvalues are ordered along the main diagonal from largest to smallest, the first principal component of \( \mathbf{X} \) is \( \mathbf{p}_1\mathbf{x}_1 \), the second would be \( \mathbf{p}_2\mathbf{x}_2 \), and so on. The larger eigenvalues correspond to the most important or “principal” components. It is hopeful to uncover the relationships among the measured \( m \) variables by \( p \) principal components where \( p \ll m \).

**B. Mathematical Derivation**

Suppose there is a vector \( \mathbf{x} \) that contains an \( m \) number of random variables and \( \mathbf{a}_1 \) is a vector or \( m \) constants. We would like to define a linear function of \( \mathbf{a}_1^T \mathbf{x} \) with maximum variance. So taking the transpose of \( \mathbf{a}_1 \) and multiplying it by the elements of \( \mathbf{x} \) yields

\[
\mathbf{a}_1^T \mathbf{x} = \alpha_{11}x_1 + \alpha_{12}x_2 + \cdots + \alpha_{1m}x_m = \sum_{j=1}^{m} \alpha_{1j}x_j.
\]

Hopefully the variations in the random variables can be identified by a few principal components say \( p \) where \( p \) is much smaller than \( m \) \( (p \ll m) \). The goal is to maximize the variance of the principal component \( \mathbf{a}_k^T \mathbf{x} \) that corresponds to the \( k^{th} \) largest value. Given the covariance matrix of \( \mathbf{x} \), which will be designated by \( \Sigma \), the variance of \( \mathbf{a}_k^T \mathbf{x} \) or \( \text{var}(\mathbf{a}_k^T \mathbf{x}) = \mathbf{a}_k^T \Sigma \mathbf{a}_k \). There must be a constraint on \( \mathbf{a}_k \) to make it finite; therefore, it is required to be of unit length or \( \mathbf{a}_k^T \mathbf{a}_k = 1 \).

The constrained problem becomes

\[
\begin{align*}
\text{Maximize} & \quad \mathbf{a}_k^T \Sigma \mathbf{a}_k \\
\text{Subject to} & \quad \mathbf{a}_k^T \mathbf{a}_k - 1 = 0
\end{align*}
\]

This problem can be solved using the method of Lagrange multipliers where \( \lambda \) is the Lagrange multiplier and the Lagrangian function becomes

\[
\text{Maximize} \quad \mathbf{a}_k^T \Sigma \mathbf{a}_k + \lambda (\mathbf{a}_k^T \mathbf{a}_k - 1).
\]
Differentiate with respect to $a_k$, 

$$\Sigma a_k + \lambda a_k = 0$$

$$(\Sigma + \lambda I) a_k = 0.$$ 

This result is the familiar eigenvector problem where $\lambda$ is the eigenvalue and $a_k$ is the eigenvector of $\Sigma$, respectively. To maximize the variance, the largest $\lambda$ must be chosen. Therefore the $k^{th}$ principal component becomes the largest $\lambda_k$ along with its eigenvector $a_k$ or $\lambda_k a_k$. To find the $k+1$ principal component, $a_k^T x$ and $a_{k+1}^T x$ must be independent of one another. In mathematical terms, the covariance of $a_k^T x$ and $a_{k+1}^T x$ is zero. This is expressed as follows

$$\text{cov} \left(a_k^T x, a_{k+1}^T x\right) = a_k^T \Sigma a_k = \lambda_k a_k^T a_k = 0.$$ 

Similar to the constraint placed on $a_k$, $a_{k+1}$ will be restricted to a unit vector. Once again the constrained problem becomes

Maximize $a_k^T \Sigma a_{k+1}$

Subject to $a_k^T a_{k+1} - 1 = 0$, $a_{k+1} a_k = 0$

The Lagrangian function becomes

Maximize $a_k^T \Sigma a_{k+1} + \lambda \left(a_{k+1}^T a_{k+1} - 1\right) + \phi \left(a_{k+1}^T a_k\right)$. 

Differentiate with respect to $a_{k+1}$, 

$$\Sigma a_{k+1} + \lambda a_{k+1} + \phi a_k = 0.$$ 

Multiply by $a_k^T$, 

$$a_k^T \Sigma a_{k+1} + \lambda a_k^T a_{k+1} + \phi a_k^T a_k = 0.$$ 

Noticing that the first two terms are equal to zero and $a_k^T a_k = 1$, $\phi = 0$ the expression becomes

$$\Sigma a_{k+1} + \lambda a_{k+1} = 0$$

$$(\Sigma + \lambda I) a_{k+1} = 0.$$
Once again, the maximum variance occurs at the largest $\lambda$ designated as $\lambda_{k+1}$ and the $k+1$ principal component is $\lambda_{k+1} \mathbf{a}_{k+1}$. Furthermore, it can be proven that the principal components of $\mathbf{x}$ are the eigenvalues $\lambda_k$, where $k = 1, 2 \ldots m$ coupled with its corresponding eigenvector $\mathbf{a}_k$ ordered from largest to smallest.

### III. Experimental Application

Principal component analysis was performed on some experimental data to interpret the relationships among the measured variables. A 6061 aluminum rod with attached strain gages was subjected to a torsion test using a Tinius Olsen Bench Type Torsion Testing Machine and torque, shear strain ($\gamma$), and angle of twist ($\phi$) were measured and recorded from the test. Although the relationships among the three measured variables are well known, PCA was performed on the test data to rediscover these correlations.

#### A. Theory

The externally applied torque induces a shear stress within the rod symbolized by $\tau$. Shear stress acts in a direction perpendicular to the normal direction of the surface upon which it acts. In the simple case of an applied torque, the shear stress produced is

$$\tau = \frac{Tr}{J}$$  \hspace{1cm} (3.1)

where,

$T$ = Torque

$r$ = radius

$J$ = polar moment of inertia

The material properties also influence the amount of shear stress produced in the body and how much strain is present. This material property is called the shear modulus of elasticity, $G$. Simply, the stress-strain relationship is given by

$$\tau = G\gamma$$  \hspace{1cm} (3.2)

where $\gamma$ is called the shear strain. This linear relationship between stress and strain within the elastic range of a material is known as material linearity. Along with shear strain, the angle of twist can be computed as well by the equation
\[ \phi = \frac{TL}{JG} \]  

(3.3)

where \( L \) is the length of the rod.

**B. Methodology**

A solid aluminum rod with a diameter of 0.76 inches and a length of 15.25 inches was clamped at both ends in the torsion testing machine and the two attached strain gages, one oriented in the ± 45° direction, were connected to a VISHAY Instruments Division P-3500 Digital Strain Indicator in a half-bridge configuration. Once both machines were calibrated, a torque was applied to one end of the rod while the other end remained fixed. The torque was increased from 0 to 800 in-lb by increments of 200 in-lb and the corresponding strain was measured from the strain indicator, and the angle of twist was recorded from the torsion machine. The setup of the experiment can be seen in Fig. 1.

![Experiment Setup](image.png)

Figure 1: Experiment Setup

**C. Results**

The results of the experiment are presented in Table 1 and are subsequently plotted in Figs. 2 and 3.
Table 1: Experimental Results

<table>
<thead>
<tr>
<th>Torque (in-lb)</th>
<th>Strain</th>
<th>Angle of Twist (Rads)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>200</td>
<td>0.000593</td>
<td>0.02618</td>
</tr>
<tr>
<td>400</td>
<td>0.001188</td>
<td>0.06108</td>
</tr>
<tr>
<td>600</td>
<td>0.001781</td>
<td>0.08726</td>
</tr>
<tr>
<td>800</td>
<td>0.002372</td>
<td>0.11690</td>
</tr>
</tbody>
</table>

Figure 2: Torque vs. Strain

Figure 3: Torque vs. Angle of Twist (φ)
There is no surprise that there is a linear relationship between torque vs. strain, and torque vs. angle of twist. Setting Eq. 3.1 and 3.2 equal to one another and solving for torque $T$,

$$T = \frac{JG}{r} \gamma. \quad (3.4)$$

Since $J$, $G$, and $r$ are all constants, the coefficient can be replaced by a single constant. This constant can be further interpreted as the slope of Fig. 1. Solving for $T$ from Eq. 3.3,

$$T = \frac{JG}{L} \phi. \quad (3.5)$$

Similarly, the slope of Fig. 2 is equal to the coefficient.

Suppose that these relations are not known and the goal is to determine them by analyzing the collected data. It would be beneficial to know how much influence each measured parameter has on one another. This is the function of principal component analysis (PCA). The MATLAB code found in Appendix C performs PCA on the data collected in Table 1. The output is shown below in Figs. 4-8.

<table>
<thead>
<tr>
<th>Torque (in-lb)</th>
<th>Strain (Rads)</th>
<th>Angle of Twist (Rads)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>200.000000</td>
<td>0.000593</td>
<td>0.026180</td>
</tr>
<tr>
<td>400.000000</td>
<td>0.001188</td>
<td>0.061087</td>
</tr>
<tr>
<td>600.000000</td>
<td>0.001781</td>
<td>0.087266</td>
</tr>
<tr>
<td>800.000000</td>
<td>0.002372</td>
<td>0.116937</td>
</tr>
</tbody>
</table>

Coefficients

$$1.0e+010 *$$

5.3325
0.0000
0.0000

Principal Components (Columns)

<table>
<thead>
<tr>
<th>1.0000</th>
<th>0.0000</th>
<th>-0.0001</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000</td>
<td>1.0000</td>
<td>0.0001</td>
</tr>
<tr>
<td>0.0001</td>
<td>-0.0001</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Explained

100.000
0.0000
0.0000
Data after PCA

<table>
<thead>
<tr>
<th>Torque (in-lb)</th>
<th>Strain (με)</th>
<th>Angle of Twist (Rads)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-400.00</td>
<td>-0.444</td>
<td>0.000698</td>
</tr>
<tr>
<td>-200.00</td>
<td>-0.435</td>
<td>-0.002618</td>
</tr>
<tr>
<td>0.00</td>
<td>1.024</td>
<td>0.002793</td>
</tr>
<tr>
<td>200.00</td>
<td>1.033</td>
<td>-0.000524</td>
</tr>
<tr>
<td>400.00</td>
<td>-1.178</td>
<td>-0.000349</td>
</tr>
</tbody>
</table>

Figure 4: MATLAB Output

Figure 5: Torque vs. Strain – MATLAB Figure
Figure 6: Torque vs. Angle – MATLAB Figure

Figure 7: Torque vs. Strain along 1st and 2nd PCs
D. Discussion

The standard x-y axes, represented by the black dashed lines in Figs. 5 and 6, do not align with the directions of largest variance within the data. A more “meaningful” basis, generated by the principal components shown by the red dashed lines in the same figures, would help identify the most significant relationships among the collected variables. These new axes are simply a rotation of the standard x-y axes in the directions of largest variance. Figures 5 and 6 show the data in its re-expressed form along the first and second principal components.

The column labeled “Explained” in the MATLAB output shown in Fig. 4 is the total variance explained by each of the principal components. Since the first principal component explains 100% of the variance, it is only necessary to retain the first principal component to preserve all the variations in the data. It is no coincidence that the first principal component is the zero mean representation of the collected torque data. The foresight afforded by Eq. 3.4 and 3.5 confirms the analysis because both strain and angle of twist are only dependent on torque in this experiment. Although PCA does not explicitly give these expressions, it leads the experimenter to this overall conclusion.
IV. Conclusion

Principal component analysis is an effective data reduction tool derived from the operations of linear algebra. The objective to find the relationships among measured variables is greatly simplified by this analysis, and the results are clear. Although the dimension of the analyzed experimental data was relatively small, the linear stress-strain relationship (i.e., material linearity) was rediscovered by the first principal component involving the measured variable torque. Using the assumptions of linearity and largest variance, the task of the experimenter to decipher the unknown variations within a system can become more focused by eliminating redundancy and targeting the most relevant variables of interest.
Appendix A: Mathematical Expectation, Variance, and Covariance

Mathematical Expectation

The mathematical expectation is a statistical expression which provides the average per trial of a finite set of values as they occur over a large number of trials. An “average” is the result of experiment, whereas a “mathematical expectation” is an advance judgment as to what that average is likely to be [4]. The average or mean of a set of values is a single number that can replace every value in that set and not change the sum. Given a set of values with \( m \) members, where \( n_1 \) of them possess the value \( x_1 \), and \( n_2 \) members have the value \( x_2 \), etc., the mathematical expression for the average is

\[
m\bar{x} = \sum x_j n_j
\]

Dividing both sides of the equation by \( m \) yields

\[
\mu_1(x) = \bar{x} = \frac{1}{m} \sum x_j n_j
\]

If the summation of the total number of trials were expanded, the result is given by

\[
\bar{x} = \frac{n_1}{m} x_1 + \frac{n_2}{m} x_2 + \ldots + \frac{n_a}{m} x_a
\]

Since the average is derived from actually performing an experiment, it is impossible to know the average in advance, but there is a way to predict the average with acceptable accuracy. Bernoulli’s Theorem states that the difference between \( n_1/m \) and the probability \( p_1 \) becomes smaller as the total number of independent trials \( m \) increases. Mathematically speaking,

\[
\bar{x} \approx x_1 p_1 + x_2 p_2 + \ldots + x_a p_a
\]

Therefore the definition of the mathematical expectation is as follows:

If \( x \) can take only the values \( x_1, x_2, \ldots, x_a \) and zero, the probability of each being \( p(x_1), p(x_2), \ldots, p(x_a) \) and \( p(0) \), the mathematical expectation of \( x \) is [4]
The moment of expectation or “i’th expectation” can also be expressed as

$$\varepsilon_i (x) = \sum_{j=0}^{n} x_j p(x_j)$$

It is interesting to note that the $p(x_j)$ remains the same because the probability of $x_j$ occurring is the same as $x_j$.

One must be careful when performing the mathematical expectation. As initially mentioned in this section, two criteria must be satisfied for the expectation to work as designed: the set of values must be finite, and a large number of independent trials must be performed to minimize the difference between the true average and the expected value of x.

**Variance**

Variance is a measure of dispersion within a one dimensional set of data and provides insight as to how the set of numbers relate to one another. Before variance can be defined, it is necessary to know another concept called deviation which is the basis for the calculation of variance. If a set of data contains numbers $x_1, x_2, \ldots, x_a$ which occur $n_1, n_2, \ldots, n_a$ times, respectively, and the mean of this set of values is $\bar{x}$, the corresponding deviations from the mean are as follows:

$$d_1 = x_1 - \bar{x}$$
$$d_2 = x_2 - \bar{x}$$
$$\ldots$$
$$d_a = x_a - \bar{x}$$

Similarly, given that the set of values have an expectation $\varepsilon$, the deviation from the expectation is

$$\delta_1 = x_1 - \varepsilon$$
$$\delta_2 = x_2 - \varepsilon$$
$$\ldots$$
$$\delta_a = x_a - \varepsilon$$
The second expectation of $\delta$ can be expressed as

$$
\varepsilon_2(\delta) = \sum p(x_j)(x_j - \varepsilon)^2
$$

Expanding the right hand side yields,

$$
\varepsilon_2(\delta) = \sum x_j^2 p(x_j) - 2 \varepsilon \sum x_j p(x_j) + \varepsilon^2 \sum p(x_j)
$$

Noticing that the first term by definition is the second expectation of $x$, $\sum x_j p(x_j)$ is the expectation, and $\sum p(x_j) = 1$, the final result can be expressed as,

$$
\varepsilon_2(\delta) = \varepsilon_2(x) - [\varepsilon_1(x)]^2
$$

This expression is also known as the variance of $x$ or $\text{var}(x)$. It is defined as the second expectation of $x$ minus the first expectation of $x$ squared.

$$
\text{var}(x) = \varepsilon_2(x) - [\varepsilon_1(x)]^2
$$

**Covariance**

The covariance is an extension of the variance in a two dimensional case. Covariance is a measure of how much two dimensions vary from the mean with respect to one another [3]. The expression for covariance presents itself by taking the variance of the function, $f = x + y$.

$$
\text{var}(x + y) = \text{var}(x) + \text{var}(y) + 2[\varepsilon_1(xy) - \varepsilon_1(x) \varepsilon_1(y)]
$$

Where,

$$
\text{covar}(xy) = \varepsilon_1(xy) - \varepsilon_1(x) \varepsilon_1(y).
$$

Covariance is a weak indication of dependence between variables in the sense that if the covariance is not zero, then the variables are not independent, but the converse cannot be said. The sign of the covariance is more important.
than its magnitude. If the covariance is positive, the two variables are directly proportional to one another meaning as one increases, the other also increases and vice versa. When the covariance is a negative value, an inverse proportionality exists between the variables where as one variable increases or decreases the second variable will behave oppositely. Lastly, if two variables are independent, their covariance is zero [3].

**Covariance Matrix**

The covariance matrix, as the name suggests, is a square, symmetric matrix which contains the covariance measurements between variables. Although the covariance can only be taken between two dimensions at one time, the covariance matrix expresses the covariance of multiple variables as they relate to each other. The covariance matrix can be expressed as

\[
C_{ij} = E(x_i x_j^T)
\]

Where each element equals

\[
C_{ij} = E(x_i, x_j)
\]

For example if a data set has the three dimensions \(x, y\), and \(z\), its covariance matrix is

\[
C = E(x, y, z)
\]

\[
C = E(x, x) E(x, y) E(x, z) \\
E(y, x) E(y, y) E(y, z) \\
E(z, x) E(z, y) E(z, z)
\]

Since the covariance is the multiple of the variance of two variables with respect to their means, it is commutative and therefore the order of multiplication does not change the product. Thus \(E(x, y) = E(y, x)\) and the matrix is symmetric. Also noticing that the main diagonal is the covariance of a variable with respect to itself, it can simply be identified as variance.
Appendix B: Method of Lagrange Multipliers

Lagrange Multipliers

There are several methods to develop optimality criteria for unconstrained optimization problems, but in reality, most engineering problems are subject to constraints on the design variables. Particularly, the optimization problem may involve equality constraints. Therefore, a method to convert the equality constrained problem into an unconstrained problem, while satisfying all equality constraints is required to optimize engineering problems. The method of Lagrange multipliers is such a method which performs the necessary conversion and identifies optimal points with the aid of unspecified parameters known as Lagrange multipliers [5].

Suppose it is required to minimize a function with \( n \) variables subject to one equality constraint:

\[
\begin{align*}
\text{Minimize} & \quad f(x_1, x_2, \ldots, x_n) \\
\text{Subject to} & \quad h_i(x_1, x_2, \ldots, x_n) = 0
\end{align*}
\]

The method of Lagrange multipliers converts this problem to the following unconstrained optimization problem:

\[
\begin{align*}
\text{Minimize} & \quad L(x, \nu) = f(x) - \nu h_i(x)
\end{align*}
\]

The unconstrained function \( L(x, \nu) \) is called the Lagrangian function and \( \nu \) is the unspecified constant called the Lagrange multiplier which can either be positive or negative. It can be seen that if a given \( \nu \) minimizes \( L(x, \nu) \) with respect to \( x \) occurs at a given \( x \), and that \( x \) satisfies the equality constraint \( h_i(x) \), then that \( x \) minimizes the equality constrained problem.

Consider the following example,

\[
\begin{align*}
\text{Minimize} & \quad f(x) = x_1^2 + x_2^2 \\
\text{Subject to} & \quad h_i(x) = 2x_1 + x_2 - 2 = 0
\end{align*}
\]

The Lagrangian problem becomes

\[
\begin{align*}
\text{Minimize} & \quad L(x, \nu) = x_1^2 + x_2^2 - \nu(2x_1 + x_2 - 2)
\end{align*}
\]
Setting the gradient of $L$ with respect to $x$ equal to zero,

$$\frac{\partial L}{\partial x_1} = 2x_1 - 2v = 0$$

$$\Rightarrow x_1^* = v$$

$$\frac{\partial L}{\partial x_2} = 2x_2 - v = 0$$

$$\Rightarrow x_2^* = \frac{v}{2}$$

The Hessian matrix of $L(x, v)$ with respect to $x$ can test whether the point $x^*$ is a minimum.

$$H_L(x, v) = \begin{bmatrix}
\frac{\partial^2 L}{\partial x_1^2} & \frac{\partial^2 L}{\partial x_1 \partial x_2}
\frac{\partial^2 L}{\partial x_2 \partial x_1} & \frac{\partial^2 L}{\partial x_2^2}
\end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

The Hessian matrix is positive definite which implies that the function is concave down. So $x_1^*$ and $x_2^*$ is the global minimum. Substituting these points into $h_i(x)$ yields $v^* = 4/5$. Therefore, the constrained minimum is located at $x_1^*$ = 4/5, $x_2^*$ = 2/5, and $\min f(x) = 4/5$. Similarly, the maximum of a function can be identified using Lagrange multipliers. Also the Lagrange multiplier method can be applied to several equality constraints. The general problem is as follows

Minimize $f(x)$

Subject to $h_k(x) = 0 \quad k = 1, 2, ..., K$

The Lagrange function becomes

$$\text{Minimize} \quad L(x, v) = f(x) - \sum_{k=1}^{K} v_k h_k$$
% This example implements principal component analysis on data collected 
% from a torsion test on 6061 aluminum. 
% The three variables measured were Torque (in-lb), Strain (micro), and 
% Angle of twist (deg). The data was measured in 5 increments.

clear
clc

format('short')
% populate measured torques
torque = [0 200 400 600 800];

% populate measured strains
strain = [0 593 1188 1781 2372];
strain = strain.*10^-6;%convert to microstrain

% populate measured angle of twist
angle = [18.5 20 22 23.5 25.2];
angle = angle - 18.5*ones(1,5);%subtract the offset angle
angle = angle.*pi/180;%convert to radians

% populate data set
data = [torque; strain; angle];
table = data;
mn = mean(data,2);
data = data - repmat(mn,1,5);%subtract the mean from the collected data

% display table of values
fprintf('	%s		%s		%s
','Torque','Strain','Angle of Twist');
fprintf('	%s						%s

','(in-lb)','(Rads)');
for i = 1:5
   fprintf('%f		%f		%f
',torque(1,i),strain(1,i),angle(1,i));
end

% calculate the covariance of the data
sigma = cov(data*data');

% calculate the eigenvalues and eigenvectors of the covariance matrix
[PC,coeffs] = eig(sigma);%PC are the eigenvectors and coeffs are the 
eigenvalues
coeffs = diag(coeffs);%capture values on the main diagonal

% sort the coefficients in descending order
[des_coeffs,index] = sort(coeffs,1,'descend');
PC = PC(:,index);%order the principal components with their corresponding 
coeffs

% display Coefficients, PCs, and Interpretation
fprintf('
Coefficients
')
disp(des_coeffs);
fprintf('Principal Components (Columns)
')
disp(PC);
fprintf('Explained
')
total_var = sum(des_coeffs);% sum the variances
% percentage of how much data is explained by each PC
first = des_coeffs(1,1)/total_var;
second = des_coeffs(2,1)/total_var;
third = des_coeffs(3,1)/total_var;
expl = [first,second,third];
disp(expl')

% apply principal components to the data
new_data = PC'*data;

pc_torque = new_data(1,1:5);
pc_strain = new_data(2,1:5);
pc_angle = new_data(3,1:5);

% display new data
fprintf('
Data after PCA
');
fprintf('%s	%s	%s
','Torque','Strain','Angle of Twist');
fprintf('%s	%s	%s
','(in-lb)','(Rads)');
for i = 1:5
    fprintf('%2f	%2f	%6f
',pc_torque(1,i),pc_strain(1,i),pc_angle(1,i));
end

% display figures of original data and standard axis
figure(1)
plot(data(2,:),data(1,:),'ob')
xlabel('Strain')
ylabel('Torque')
hold on;
x = min(data(2,:)):max(data(2,:))
y1 = PC(1,1)/PC(2,1)*x;
y2 = PC(2,2)/PC(1,2)*x;
plot(x,y1,'--r',x,y2,'--r')
axis square
title('Torque vs. Strain')
xlabel('Strain')
ylabel('Torque (in-lb)')
hold on;
x1 = min(data(2,:)):max(data(2,:))
y1 = 0*x1;
x2 = 0*x1;
y2 = min(data(1,:)):max(data(1,:));
plot(x1,x2,'--k',x2,y2,'--k')
figure(2)
plot(data(3,:),data(1,:),'ob')
xlabel('Angle')
ylabel('Torque')
hold on;
x = min(data(3,:)):max(data(3,:))
y1 = PC(1,1)/PC(3,1)*x;
y2 = PC(3,3)/PC(1,3)*x;
plot(x,y1,'--r',x,y2,'--r')
axis square
title('Torque vs. Angle of Twist')
xlabel('Angle (rad)')
ylabel('Torque (in-lb)')
hold on;
\begin{verbatim}
x1 = min(data(3,:)):(max(data(3,:))-min(data(3,:)))/10:max(data(3,:));
y1 = 0*x1;
x2 = 0*x1;
y2 = min(data(1,:)):(max(data(1,:))-min(data(1,:)))/10:max(data(1,:));
plot(x1,x2,'--k',x2,y2,'--k')

% display figures of original data along PCs
figure(3)
plot(new_data(1,:),new_data(2,:),'ob')
title('Torque vs. Strain along 1st and 2nd PCs')
xlabel('1st Principal Component')
ylabel('2nd Principal Component')
hold on;
x1 = min(new_data(1,:)):(max(new_data(1,:))-min(new_data(1,:)))/10:max(new_data(1,:));
y1 = 0*x1;
x2 = 0*x1;
y2 = min(new_data(2,:)):(max(new_data(2,:))-min(new_data(2,:)))/10:max(new_data(2,:));
plot(x1,x2,'--r',x2,y2,'--r')

figure(4)
plot(new_data(1,:),new_data(3,:),'ob')
title('Torque vs. Angle of Twist along 1st and 2nd PCs')
xlabel('1st Principal Component')
ylabel('2nd Principal Component')
hold on;
x1 = min(new_data(1,:)):(max(new_data(1,:))-min(new_data(1,:)))/10:max(new_data(1,:));
y1 = 0*x1;
x2 = 0*x1;
y2 = min(new_data(3,:)):(max(new_data(3,:))-min(new_data(3,:)))/10:max(new_data(3,:));
plot(x1,x2,'--r',x2,y2,'--r')
\end{verbatim}
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References


