Introduction to Principal Components Analysis[1]

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Abstract.
Understanding the inverse equivalent width – luminosity relationship (Baldwin Effect), the topic of this meeting, requires extracting information on continuum and emission line parameters from samples of AGN. We wish to discover whether, and how, different subsets of measured parameters may correlate with each other. This general problem is the domain of Principal Components Analysis (PCA). We discuss the purpose, principles, and the interpretation of PCA, using some examples from QSO spectroscopy. The hope is that identification of relationships among subsets of correlated variables may lead to new physical insight.

1. Introduction

The point of all statistics is simplification. The amount of data the world can throw at us would swamp Einstein: we have to simplify to survive. Statistics is the art of extracting simple comprehensible facts that tell us what we want to know for practical reasons, from the floods of data washing over us.

Consider the fuel consumption of cars, for example. Every car will be different, depending on its model, year, maintenance state, and the aggression level of its driver. To fully characterize the fuel economy of cars in the USA would require a different number for every car/driver combination: that is, more than 10^8 numbers. For most purposes, however, such as working out the nation's likely oil usage, these 10^8 numbers can be replaced with one: the average fuel consumption. An enormous simplification!

Principal Components Analysis (PCA) is a tool for simplifying one particular class of data. Imagine that you have n objects (where n is large), and you can measure p parameters for each of them (where p is also large). For example, the objects could be the n QSO researchers attending a meeting in La Serena, and the parameters could be the p things you know about each of them: e.g.,

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[1]This paper is for our friends Leah Cutter and Mike Brotherton, who announced their engagement during the La Serena meeting.

their heights, weights, number of publications, frequent flier miles and the fuel consumption of their cars. Let us imagine that you want to investigate how these p parameters are related to each other. For example, do astronomers who spend most of their lives in airports publish more? Does this depend on how fat they are? Do people with inefficient cars fly more, or is it only the smart ones (with lots of publications) that do so? Do these correlations represent real causal connections, or it it just that once you get tenure you buy a new car, become fat, stop publishing and give lots of invited talks in exotic foreign locations?

The traditional way of dealing with this type of problem is to plot everything against everything else and look for correlations. Unfortunately, as the number of parameters increases, this rapidly becomes impossibly complicated. It is easy to get lost in the web of parameters, each of which correlates more or less well with some combination of the other parameters. The human brain can cope with two or three parameters easily. By plotting all the different variables against each other separately, we can just about learn something about $5 - 7$ variables. But once we are beyond this, the human brain needs help.

PCA is specifically designed to help in situations like this: when you know lots of things about lots of objects, and want to see how all these properties are inter-related. Basically, PCA looks for sets of parameters that always correlate together. By grouping these into one new parameter, an enormous saving in complexity can be achieved with minimal loss of information.

PCA is one of a family of algorithms (known as multivariate statistics) designed to handle complex problems of this sort. It was first widely applied in the social sciences. The most infamous early application of PCA was to intelligence testing. You can test the intellectual ability of people in many ways. For example, you could give a sample of n people a set of p exams, with questions testing their creativity, memory, math skills, verbal skills etc. Do people who score well on one test score well on all? Or do the scores break up into sub-groups, such as verbal or logical scores, which correlate well with the scores on other similar tests? PCA was applied to these exercises, and it was found that nearly all the scores correlate well with each other. Thus, it was claimed, a single underlying variable (known as IQ) can be used to replace all the individual scores, and once you know someone's IQ, you can accurately predict their performance on all the tests. (See Steven Jay Gould's 'The Mismeasure of Man' for a hilarious account of the misuse of this application of PCA.)

2.   Overview

The task of PCA is then, given a sample of n objects with p measured quantities for each, i.e. p variables, x_j $(j = 1, \ldots, p)$, find a set of p new, orthogonal (i.e. independent) variables, $\xi_1, \ldots, \xi_i, \ldots, \xi_p$, each one a linear combination of the original variables, x_j:

$$\xi_i = a_{i1}x_1 + \cdots + a_{ij}x_j + \cdots + a_{ip}x_p$$

Determine the constants a_{ij} such that the smallest number of new variables account for as much of the variance of the sample as possible. The ξ_i are called principal components.

If most of the variance in the original data can be accounted for by just a few of the p new variables, we will have found a simpler description of the original dataset. A smaller number of variables may point to a way of classifying the data. More interesting, beyond the realm of statistical description, the PCA, by showing which original variables correlate together, may lead to new physical insight. Of course it will sometimes happen that the observed variables are uncorrelated, or at least, lead to no dominant principal components. That may be useful to know, but not very interesting.

The concept of PCA is usually introduced either algebraically, through co-variance matrices, or geometrically. We will first give a geometrical overview, then illustrate with examples and interpretation. Many textbooks on multivariate statistics give rigorous mathematical treatments (e.g., Kendall 1980).

3.   A Geometrical Approach to Principal Components Analysis

Consider the case of p variables. The data of n QSOs are represented by a large cloud in p-dimensional space. If two or more parameters are correlated, the cloud will be elongated along some direction in hyper-space defined by their axes. Large extensions can arise when a few parameters are correlated, or when smaller correlated variations occur for a substantial number of variables.

PCA identifies these extended directions and uses them as a set of axes for the parameterization of the multidimemsional space. Following the analysis, each QSO can be represented by its coordinates in the new space. The new axes are identified sequentially: PCA first finds the most extended direction in the original p-dimensional space by minimizing the sums of squares of the deviations from that direction. This direction forms the first principal component (often called eigenvector 1), and accounts for the largest single linear variation among measured QSO properties. Next we consider the $(p-1)$-dimensional hyper-plane orthogonal to the first principal component. We then search for the direction that represents the greatest variance in $(p-1)$-space, thus defining the second principal component. This process is continued, defining a total of p orthogonal directions.

4.   Examples using Real Data

4.1.   PCA with Two Variables

Consider the case of 22 QSOs each with measured values of X-ray spectral index α_x (defined by $F_\nu \propto \nu^{-\alpha_x}$ between 0.15 keV and 2keV), and FWHM Hβ (full width at half maximum for the broad Hβ emission line). The data points are distributed in an elongated cloud in 2 dimensions, as shown in Fig. 1. It is standard practice to subtract the mean value from each variable, and normalize by dividing by the standard deviation. One can find the direction of the first principal component axis by rotating an axis to align with the direction of maximum elongation, actually maximum variance, of the data. The result of this is shown by the dashed line labeled PC1 in Fig. 2. Because the points remain the same distance from the origin, by Pythagoras' theorem, maximizing the variance along PC1 is equivalent to minimizing the sums of squares of the
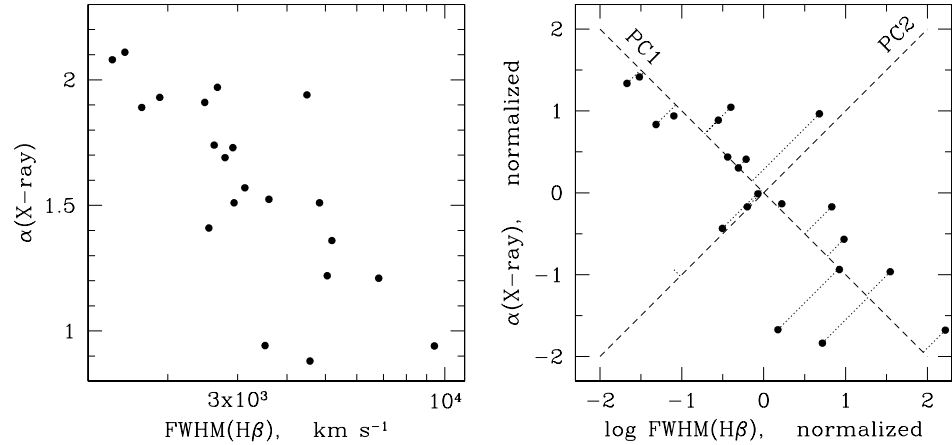
Figure 1.   An important optical correlation, soft X-ray spectral index vs. width of the broad Hβ emission line. Left: In natural units. Right: In normalized units, with mean subtracted, then divided by the standard deviation. The dashed line shows the direction of the first principal component (PC1), representing the maximum deviation of the cloud of data points. Dotted lines project the data points onto this direction. PC1 represents the direction that minimizes the sums of the squares of the lengths of the dotted lines. The value (score) of PC1 for a given point is the distance of the point from the origin, projected onto PC1. Similarly the lengths of the dotted lines represent the values of PC2 for each data point.

distances of the points from this line through the origin; these distances are shown as dotted lines. The distance of a point from the origin, projected onto the direction PC1 represents the value (score) of the first principal component for that data point. Clearly, PC1 is a linear combination of the original input variables. The variance of PC1 is 1.764 – rather more than the unit variance of the original variables. The total variance of the sample is the sum of the variances for each variable, in this case, 2. Because the new coordinates are found simply by rotation, the distance of the points from the origin remains unchanged, so the total variance remains the same. Thus the first principal component accounts for $1.764/2 = 88.2\%$ of the total sample variance. The remaining variance of the sample can be accounted for by the projection of the data points onto the axis PC2, perpendicular to PC1 – or $0.236/2 = 11.8\%$. These projections (lengths of the dotted lines) are the values or scores of the second principal component.

We have succeeded in defining a new variable, a linear combination of α_x and log FWHM Hβ, that accounts for most of the variation within the sample (PC1). The interpretation of this parameter is a hotly contended topic (e.g., Pounds, Done & Osborne 1995, Laor et al. 1997, Brandt & Boller 1998). Is PC2 of any significance? The astronomer, with knowledge of the measurement uncertainties, may have more hope of addressing this. If the original variables

had been uncorrelated, we could still define PC1 and PC2 mathematically, but we would be no better off as a result of the analysis.

4.2.   PCA with More Variables

Table 1.   Input Data

PG Name	log L_{1216}[a]	α_x	log FWHM Hβ	FeII/ Hβ	log EW [OIII]	log FWHM CIII]
0947+396	45.66	1.51	3.684	0.23	1.18	3.520
0953+414	45.83	1.57	3.496	0.25	1.26	3.432
1001+054	44.93	. . .	3.241	0.82	0.85	3.424
1114+445	44.99	0.88	3.660	0.20	1.23	3.654
1115+407	45.41	1.89	3.236	0.54	0.78	3.403
1116+215	46.00	1.73	3.465	0.47	1.00	3.446
1202+281	44.77	1.22	3.703	0.29	1.56	3.434
1216+069	46.03	1.36	3.715	0.20	1.00	3.514
1226+023	46.74	0.94	3.547	0.57	0.70	3.477
1309+355	45.55	1.51	3.468	0.28	1.28	3.406
1322+659	45.42	1.69	3.446	0.59	0.90	3.351
1352+183	45.34	1.52	3.556	0.46	1.00	3.548
1402+261	45.74	1.93	3.281	1.23	0.30	3.229
1411+442	44.93	1.97	3.427	0.49	1.18	3.275
1415+451	45.08	1.74	3.418	1.25	0.30	3.434
1425+267	45.72	0.94	3.974	0.11	1.56	3.666
1427+480	45.54	1.41	3.405	0.36	1.76	3.300
1440+356	45.23	2.08	3.161	1.19	1.00	3.192
1444+407	45.92	1.91	3.394	1.45	0.30	3.479
1512+370	46.04	1.21	3.833	0.16	1.76	3.546
1543+489	46.02	2.11	3.193	0.85	0.00	. . .
1626+554	45.48	1.94	3.652	0.32	0.95	3.631
Number	22	21	22	22	22	21
Mean	45.56	1.57	3.498	0.56	0.99	3.446
Std dev'n	0.47	0.38	0.212	0.40	0.47	0.129

[a]Log of continuum luminosity at 1216Å in units of erg s^{-1} (H$_o$ = 50 km s^{-1} Mpc^{-1}, q$_o$ = 0.5.) FWHM are in km s^{-1}; rest-frame equivalent widths (EW) are in Å.

PCA achieves its real usefulness in multivariate problems. We perform a PCA[1] on the small sample of 22 QSOs discussed by Wills et al. (1998a,b), using a subset of the available measured properties shown in Tables 1 and 2. Unavoidably, there are missing data, so the number of objects available depends

[1]Several widely available statistical packages include a task for Principal Components Analyses (Statistical Package for the Social Sciences – SSPS, Statistical Analysis System – SAS, Minitab – Minitab Reference Manual 1992).

on the variables chosen for the PCA. Many correlations are plotted, and the Pearson correlation coefficients tabulated, by Wills et al. (this volume).

Table 2.   Input Data, continued

PG Name	log EW Lyα	log EW CIV	CIV/ Lyα	log EW CIII]	SiIII/ CIII]	NV/ Lyα	λ1400/ Lyα
0947+396	2.08	1.78	0.45	1.24	0.306	0.179	0.143
0953+414	2.19	1.78	0.40	1.24	0.164	0.189	0.093
1001+054	2.25	1.76	0.40	1.43	0.443	0.462	0.174
1114+445	2.27	1.85	0.42	1.48	0.222	0.175	0.092
1115+407	1.90	1.51	0.33	1.14	0.385	0.228	0.134
1116+215	2.14	1.71	0.34	1.20	0.440	0.254	0.126
1202+281	2.72	2.41	0.69	1.87	0.164	0.154	0.098
1216+069	2.12	1.95	0.54	1.20	0.037	0.121	0.056
1226+023	1.64	1.44	0.45	1.00	0.280	0.174	0.018
1309+355	2.01	1.68	0.41	1.15	0.303	0.131	0.064
1322+659	2.19	1.85	0.41	1.30	0.291	0.135	0.097
1352+183	2.14	1.80	0.41	1.29	0.357	0.203	0.116
1402+261	1.91	1.59	0.39	1.09	0.568	0.227	0.161
1411+442	. . .	1.88	. . .	1,42	0.314	. . .	0.093
1415+451	2.32	1.78	0.29	1.40	0.688	0.210	0.142
1425+267	. . .	2.17	. . .	1.43	0.398	. . .	0.055
1427+480	2.03	1.82	0.49	1.21	0.265	0.126	0.117
1440+356	2.14	1.54	0.21	1.05	0.747	0.141	0.092
1444+407	1.99	1.34	0.21	1.06	0.809	0.335	0.164
1512+370	2.02	2.05	0.75	1.28	0.228	0.182	0.050
1543+489	1.93	1.60	0.44	. . .	. . .	0.398	0.174
1626+554	2.14	1.80	0.39	1.36	0.197	0.217	0.118
Number	20	22	20	21	21	20	22
Mean	2.11	1.78	0.421	1.279	0.362	0.212	0.108
Std dev'n	0.21	0.24	0.131	0.194	0.199	0.091	0.043

Tables 1 and 2 also present, for each variable, the number of data points, the mean and the standard deviation. Notice the completely different units for different measured parameters. Clearly, from our two dimensional example, one can see in Fig. 1 or 2 that the deviations from PC1, hence PC1 itself, will depend on the units chosen (the weighting of the variables). In order to weight the variables more or less equally, after subtracting the mean values, we normalize by the variance. The choice of weights is a difficult issue, and depends on the user's knowledge of the data, and preferences, as well as the use to which the results will be put. The results of performing a PCA on these normalized variables are shown in Table 3. Columns (2)–(6) show the first 5 out of a total of 13 principal components. The first row gives the variances (eigenvalues) of the data along the direction of the corresponding principal component. The sums of all the variances add up to the sums of the variances of the input variables,

in this case, 13. By convention, the principal components are given in order of their contribution to the total variance. This is given as 'Proportion' in the second line, and the 'Cumulative' proportion on the third line. Thus, among the parameters we have chosen to use, the first principal component contributes 50% of the spectrum-to-spectrum variance, the second 22%, the third, 12%. The first two principal components together contribute 71% of the variance, the first 3, 84%, and the first 4, nearly 90%.

Table 3.   Results of Eigenanalysis – The Principal Components[a]

	PC1	PC2	PC3	PC4	PC5
Eigenvalue	6.4505	2.8157	1.5879	0.6257	0.5698
Proportion	0.496	0.217	0.122	0.048	0.044
Cumulative	0.496	0.713	0.835	0.883	0.927
Variable	PC1	PC2	PC3	PC4	PC5
$\log L_{1216}$	0.053	0.535	−0.123	−0.029	−0.405
α_x	0.295	−0.198	0.079	0.485	−0.155
FWHM Hβ	−0.330	0.077	−0.357	−0.082	−0.141
Fe II/Hβ	0.341	−0.140	0.003	−0.487	−0.212
log EW [O III]	−0.310	0.016	0.255	0.394	−0.095
log FWHM C III]	−0.198	0.077	−0.623	0.054	0.402
log EW Lyα	−0.177	−0.502	−0.006	−0.143	0.033
log EW C IV	−0.336	−0.262	0.048	−0.050	−0.303
C IV/Lyα	−0.342	0.062	0.025	−0.074	−0.584
log EW C III]	−0.262	−0.413	−0.124	−0.176	−0.008
Si III]/C III]	0.342	−0.149	−0.018	−0.311	−0.116
N V/Lyα	0.231	−0.050	−0.573	0.107	−0.288
$\lambda 1400$/Lyα	0.223	−0.351	−0.225	0.441	−0.216

[a] 18 of 22 QSO spectra used; 4 cases contain missing values.

The columns of numbers for each principal component represent the weights assigned to each input variable. Thus PC1 = $0.053 \times x_1 + 0.295 \times x_2 - 0.330 \times x_3 + \ldots$, where x_1, x_2, and x_3 are the values of the normalized variables corresponding to log L$_{1216}$, α_x, FWMH Hβ, etc. By convention these weights are chosen so that the sum of their squares = 1. This arbitrarily fixes the scale of the new variable. The sign of the new variable is therefore arbitrary.

4.3.   Interpretation

The first principal component is elongated with variance 6.5 times that of any individual measurements, and accounts for about half the total variance. This is therefore likely to be highly significant. If all measured, normalized quantities contributed equally to PC1, they would all have weight 0.277 ($1/\sqrt{13}$ for 13 variables), but each variable contributes more or less than this. One way to test the significance of the contribution of any one measured variable, is to perform

the PCA without that variable, then check the significance of the correlation between that variable and the scores of the new principal component. This procedure shows that all measured variables except L_{1216}, log FWHM CIII], and log EW Lyα, correlate with PC1, but correlations involving NV/Lyα and $\lambda1400$/Lyα are not very strong. PC2, accounting for 22% of the variance in this dataset, appears to link the EW Lyα, EW CIV, and EW CIII] with L_{1216}, so EW CIV and EW CIII] appear to contribute to both PC1 and PC2, but EW Lyα contributes predominantly to PC2. Is PC2 a significant component? A similar correlation test shows that individually the EWs do anti-correlate with L_{1216}, but this result depends on the lowest EWs for the highest luminosity QSO PG1226+023 and the highest EWs for the low luminosity QSO PG1202+281. However L_{1216} correlates significantly (Pearson's ordinary correlation coefficient $= -0.77$) with PC2 formed when L_{1216} is excluded. Thus there is a significant overall correlation between EW and L_{1216}, although a larger sample is clearly needed to investigate the individual EW correlations. Another test may be to check correlations between observed measurements for those measurements that contribute to only one significant principal component – for example, C IV/Lyα vs. Fe II/Hβ (see Fig. and Table of Wills et al. in this volume).

As a rule-of-thumb, any principal component with variance greater than 1, should be considered seriously. It is also worth investigating any principal component with variance rather greater than that of the remaining principal components. In our example, this could mean the first three principal components.

PCA is a linear analysis. Tests should be performed to check on the linearity of the principal components. If a linear analysis is valid, plotting the scores of PC1 vs. PC2 should show a normal distribution consistent with no correlation between the two. Mathematically, there cannot be a correlation, but a non-random distribution of points, or individual outlying points, may indicate non-linearity of the relationships – or some other problem with the uniformity of the data-set. Outliers could be rejected and the analysis repeated, or a transform of co-ordinates, for example to logarithmic co-ordinates, may reduce the problem to a linear analysis. A PCA performed using the ranks rather than the actual (normalized) measurements may be more robust to both non-random distributions and outliers. (Compare the present results with those from the analysis of the ranks, in Table 2 of the other PCA paper in this volume.) These tests are an important tool for examining non-linearities in the data, and for discovering individual unusual objects.

5.   Some Examples from the Literature

Increasing awareness of statistical methods has led to the establishment of the Statistical Consulting Center For Astronomy at Penn State University (Akritas et al. 1997, Feigelson et al. 1995, see also http://www.stat.psu.edu/scca/ and www.astro.psu.edu/statcodes), and a series of conference and other volumes devoted to statistics in astronomy (Murtagh & Heck 1987; Feigelson, Babu, & Jogesh 1992), including PCA.

PCA is being increasingly applied in astrophysics. Investigations of low and high redshift galaxies depend on their classification (by morphology, photome-

try, kinematics, etc.), in terms of the purely observational "fundamental plane", a subspace of the p-dimensional parameter space (Djorgovski & Davis 1987, see also an interesting PCA paper by M. Han 1995). The same area of astronomy has also extensively applied 'neural network' techniques for the automated classification of galaxy images, and more (Odewahn 1998; Rawson, Bailey & Francis 1996.)

An example similar to that presented here, using a subset of the parameters we consider, but for a much larger sample, is provided in the paper by Boroson & Green (1992). Other examples of PCA analyses are given and discussed by Whitney (1983a, b), and Murtagh and Heck (1987). Some PCAs have a larger number of variables than input observables, $p > n$. This results in a singular matrix and therefore requires modifications to the techniques to solve the eigenvector equations. These techniques are discussed, for example, by Wilkinson (1978), and mentioned by Mittaz, Penston, & Snijders (1990). This situation occurs in 'Spectral PCA'. The principles are identical, but the number of variables is larger than the number of QSO spectra. Here the QSO spectra are divided into many discrete bins, by wavelength or log (wavelength) (or velocity), and the p variables are the fluxes in these p bins. An excellent example and discussion of interpretation is given by Francis et al. (1992)[2]. For another example, see Wills, Brotherton, Wills & Thompson (1997). Spectral PCA also finds application to spectral time variability. For example, Mittaz et al. (1990) analyze the spectra of NGC 4151 at 59 epochs, binning each spectrum in wavelength space (1375 bins). A more recent example is given by Türler & Courvoisier (1998).

Recommended for further reading, is chapter 6 from Manly's 'Multivariate Statistical Methods' (1994), which gives a good brief discussion of the method, with useful insights into interpretation. A more rigorous mathematical treatment, together with discussion, is given by *the* great researcher and expositor of statistics M. Kendall (Chapters 1 and 2 of 'Multivariate Analysis'.)

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[2]The spectral PCA code is available from the web: http://msowww.anu.edu.au/~ pfrancis/

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