Back Pain: A Spectral Clustering Approach

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Abstract We used a spectral clustering algorithm to find clusters among medical patients with lower back pain symptoms, and then we assessed the health outcomes within each cluster. First, we mapped all of the variables onto [0, 1] intervals. This allowed us to compute a similarity score between every pair of patients, using an adaptation of Pearson correlation. We then calculated the spectral (eigen) decomposition of this similarity matrix, and we used the first few eigenvectors to create a low-dimensional subspace. Finally, we performed k-means clustering in this new subspace to find four clusters. We compared the cluster means and variances for each recovery assessment variable to differentiate the health outcomes for each cluster. Lastly, we highlighted the identifying symptoms of each patient cluster by inspecting any variable whose within-cluster average is extraordinarily low or high, relative to the other clusters.

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Archives of Data Science, Series B (Online First) KIT Scientific Publishing Vol. 1, No. 1, 2019

DOI 10.5445/KSP/1000085952/07 ISSN 2510-0564

1 Introduction

Outside of some well-ordered data sets that are popular for basic clustering demonstrations, many situations do not provide a clear clustering structure. The back pain data set (see van Mechelen and Vach for details) is no different; there is a diversity of data formats and scales which inhibit any straightforward clustering procedures. In contrast, the literature shows that spectral clustering methods are particularly effective in this context (von Luxburg, 2007; Kannan et al, 2004). Specifically, similarity measures and eigen-decompositions are used to extract the underlying structure from high-dimensional data (Belkin and Niyogi, 2003; Arias-Castro et al, 2011) and to identify abstract clustering patterns (Ng et al, 2001). We rely on this flexible nature in order to handle the rougher obstacles of this data challenge.

2 Data Processing

With mixed-type data, it is challenging to incorporate both numerical and categorical data equally. The following procedures were designed to evenly consider both types of variables, without letting one type of data suppress the information of the other. In the rest of the paper, we use "validation variables" when referring to the 9 variables used only for validation purposes. All other uses of the term "variable" will refer to the variables used for cluster analysis. The validation variables are only used for cluster interpretation, so we will treat them separately in section 2.3.

2.1 Variable Transformations

For any categorical variable (including binary variables, excluding ordinal variables), we used disjunctive coding to codify a single variable with c categories into c distinct columns. An observation then receives a value of 1 in the column which corresponds to its appropriate category, as shown in Table 1. Mathematically, this will inflate the similarity score between rows of data with the same category value, as they will now appear similar across three disjunctive

columns instead of the original single column. To prevent this artificial inflation of covariance, we will assign weights of $1/\sqrt{c}$ to these columns, where *c* is the respective number of distinct categories for that variable. When we later calculate similarity scores between rows in section 3.1, this will ensure that the total weight of each categorical variable remains equal to 1, avoiding the issue of similarity inflation.

| | Category | | | Category = 1 | Category = 2 | Category = 3 |
|----------|----------|------------|----------|--------------|--------------|--------------|
| Person A | 1 | | Person A | 1 | 0 | 0 |
| Person B | 2 | \implies | Person B | 0 | 1 | 0 |
| Person C | 3 | | Person C | 0 | 0 | 1 |

Table 1: A variable with 3 categorical values is transformed into 3 binary columns. .

To preserve magnitudes between numeric and categorical variables, we linearly scaled every continuous and ordinal column to the interval [0,1]. We mapped each variable's minimum value to 0, while mapping the maximum value for each variable to 1. Each value of column \vec{y} is thereby scaled proportionally to the distance from the minimum and maximum value:

$$Mapping(\vec{y}) = \frac{\vec{y} - \min(\vec{y})}{\max(\vec{y}) - \min(\vec{y})} \in [0, 1]$$
(1)

This ensured even consideration of all variables during the clustering process; uneven magnitudes between variables would otherwise allow large variables to dominate small variables during the clustering process. Admittedly, this method is very sensitive to outliers. Within a numeric variable, if there exists a value or set of values which are much larger than the rest, then the other values will all be pushed together into a small margin as the outliers disproportionately stretch the maximum/minimum values. This may artificially reduce the variance within that specific variable, relative to other variables. Despite these concerns, this technique allowed for other useful interpretations which will be discussed in section 3.1.

2.2 Missing Value (NA) Treatment

There were two variables in the data set with an exceedingly large amount of missing values. The "musclegroup_palp" variable had 52% missing data, and the "triggerpoint" variable had 37.4% missing data.

The "Musclegroup_palp" variable mentions that roughly half of the missing values are actually not unknown quantities, but rather represent individuals who simply reported no painful muscle groups (these are not "real" missings). However, this is characteristically different from individuals who may truly experience muscle pain but simply didn't respond to this question (the "real" missings). Grouping these two responses together seems unreasonable, and we have no reliable way of distinguishing between them, so we chose to exclude this variable.

The "Triggerpoint" variable offers far less confusion. The variable summary mentions that many of the NA values here were simply recorded under the Musclepalp variable instead (not to be confused with the Musclegroup_palp variable we discussed earlier). We therefore choose to keep the Triggerpoint variable, in the expectation that many missing values here will be reconciled by the Musclepalp variable and vice-versa.

After removing the Musclegroup_palp variable, we replaced all missing values with mean imputation by column. We chose mean imputation because our algorithm relies on centering the data for correlation calculations, and mean imputation will preserve the squared error of each row (having zero effect on the correlation similarity between rows). Effectively, if either row is missing the data for that column, then that column will provide "zero information" of the similarity between those two rows, neither adding nor subtracting from the similarity measure. This is discussed in depth in section 3.1.

2.3 Validation Data

The first issue with the validation data was the different scales for each measurement. The "Gen" score is measured on a discrete scale from 1-7; the "Vasl" score is measured on a discrete scale from 0-10; and the "RMProp" score is a continuous variable ranging from 0-100. To normalize the scale between variables, we employed the standard scaling procedure of centering each column and dividing by its standard deviation.

After scaling, the main issue with the validation variables is the huge proportion of missing data. In order to ensure reliability of validation testing, our testing data only includes observations which have *at least one* value recorded for each outcome time period (2 weeks, 3 months, and 12 months). We partitioned the 9 validation variables into those three distinct time periods, and then – for each observation – we imputed any missing values with the 3-nearest-neighbour average, under Euclidean distance. The variables within each time partition are significantly correlated (see Figure 1), so the missing variables should be well-predicted by the other variables within the same time period. This justifies the usage of the k-nearest neighbour (kNN) algorithm as a strong choice for imputation. Also note that the variables were standardized to obtain equivalent scales, further assisting the reliability of kNN. For implementation of kNN, we used the R package VIM (Kowarik and Templ, 2016).



Figure 1: Correlations appear strong within a distinct time period and relatively weaker between different time periods. We use observations within a single time period to predict any other missing values within that time period. Generated with R package "corrgram" (Wright, 2017).

3 Spectral Clustering Algorithm

With a mixed-type data set and many different scales of measurement, it does not seem appropriate to run a standard clustering procedure directly within that data space. Instead, we aimed for a more well-ordered data space through construction of a similarity matrix. Groups of mutually similar observations should clump together, avoiding some common pitfalls of working with non-spherical or abstract clustering structure (von Luxburg, 2007).

3.1 Similarity Matrix

We transformed the original $n \times p$ data matrix into an $n \times n$ similarity matrix *S*. We utilized centered cosine similarity, an adaptation of Pearson correlation, to calculate pairwise similarity between rows of the data:

$$\operatorname{Corr}(\vec{x}, \vec{y}) = \frac{\sum_{k} w_{k}(x_{k} - \mu_{k})(y_{k} - \mu_{k})}{\sqrt{\sum_{k} w_{k}(x_{k} - \mu_{k})^{2} \sum_{k} w_{k}(y_{k} - \mu_{k})^{2}}} = \frac{(\vec{x} - \vec{\mu})^{T} W(\vec{y} - \vec{\mu})}{||\vec{x} - \vec{\mu}|| \cdot ||\vec{y} - \vec{\mu}||}$$
(2)

where k iterates over the data columns, w_k indicates the weight for that column, W is a diagonal matrix of column weights, and T signifies the transpose for the matrix multiplication. This calculation essentially compares rows \vec{x} and \vec{y} according to their deviation from the mean in each column. If these rows deviate from the mean in opposite directions, that variable will contribute negatively to their similarity score. If these rows deviate from the mean in the same direction, then that variable will contribute positively to their similarity score. If one row or both rows hover around the mean value, that variable will contribute zero similarity between the rows. The stronger the mean deviations, the stronger the similarity contribution.

By analysing each variable in context of its mean, correlation similarity provides a highly adaptive similarity measure for mixed type data. For binary and disjunctive categorical data, the mean reflects the proportion of 1's for each category. If we see an even split between 0's and 1's – signifying a mean value around 0.5 for that variable – then that variable will strongly distinguish those two groups (positive similarity within a group, and negative similarity between the groups). On the other hand, if a variable has a majority of observations equal to zero, then the sample mean will have a value close to zero. This will provide *weak* positive similarity to the observations in the large group, but *strong* positive similarity to the observations in the minority group (see Figure2). Intuitively, that variable acts as a unique identifier of that minority group: If most of the data acts one way, then there is likely some unifying factor within the minority group that causes it to act differently. It is harder to claim any strong identifiability within the majority group, as *most* of the data acts that way – it's not a good indicator of some identifying property, only a lack thereof.



Even Split between values of 0, 1.

Correlation similarity of (.5)(.5) = (-.5)(-.5) = .25 is given to each pair of observations with the same value. Correlation similarity of (-.5)(.5) = -.25 is given to each pair with differing values.

Uneven Split between values of 0, 1.

Correlation similarity of (-.3)(-.3) = .09 is given to observation pairs within the majority group, while (.7)(.7) = .49 similarity is assigned to members of the minority group. (.7)(-.3) = -.21 similarity is given to observations with differing values.

Recall that, to prevent inflation of similarity within categorical variables, the weights w_k have been set to 1/c for all dummy columns k (where c indicates the number of categories) and equal to 1 everywhere else.

A similar interpretation can be made with numeric data with regard to the mean, albeit perhaps less clear-cut than with binary variables. Also, as mentioned in section 2.1, outliers may skew the [0,1] interval to force a large clump of values near 0 or 1. Correlation similarity will assign strong similarity within the outlier group (if there is more than one outlier) while attributing negligible similarity within the clump of "regular" values.

This similarity measure is computed similarly to the Pearson correlation matrix. The Pearson correlation centers the data, scales each column to length one, and applies column weights before calculating $X^T X$. The correlation similarity, centers the data, scales each row to length one, and applies column weights before calculating XX^T . Both measures are reflexive (self-similarity = 1),

Figure 2: Demonstration of how the distribution of variables – specifically, the location of the mean – influences the pairwise correlation similarity. Generated with R (R Core Team, 2016).

symmetric ($\operatorname{Corr}(\vec{x}, \vec{y}) = \operatorname{Corr}(\vec{y}, \vec{x})$), and invariant to linear transformations of the variables (assuming that the correlation similarity first maps to each variable to [0,1] as discussed in section 2.1).



Figure 3: A heatmap of the correlation similarity matrix, with the values rescaled to [0,1] and the index reordered according to the final 4-cluster solution for visual clarity. White areas represent low similarity and dark regions represent high similarity. A strong clustering structure should have strong similarity to members within a cluster and low similarity between members of separate clusters. Notice that there is a strong case for two, three, or four clusters, based on this heatmap. Generated with R package "heatmap3" (Zhao et al, 2015).

One drawback of correlation similarity, with regard to numeric data, is that it relies on extreme values to identify similarity. This process can identify only 2 clusters within a single variable (assigning positive similarity to observations near the extrema), even though it is reasonable to believe that there could exist a third group of observations which contains *neutral* values clustered around the mean. This method assumes that each cluster will display extreme values (very large or very small) in at least one variable. If there are any observations that naturally cluster together with extreme values across multiple data values,

correlation similarity should identify that trend and assign those observations a large overall similarity score (close to 1).

3.2 Diffusion Map Spectral Clustering

After constructing the similarity matrix, we needed to extract a clustering structure. We adapted the popular Diffusion Map algorithm, which treats the similarity values as a probability distribution in a Markov process.

First, we mapped the entire similarity matrix (excluding diagonal elements) to a value between [0,1], using the same method described in Figure 4 (except now using the entire matrix to determine the minimum and maximum values). We then set the diagonal elements all equal to zero (detailed below). From there, we divided each row by its respective row sum, converting each row into a probability distribution with non-negative entries that sum to 1.

Given that each column of the similarity matrix represents a corresponding row, this matrix can be interpreted as a probability transition matrix between observations in the data. Given a matrix of probability distributions between data points, a Markov process lets you take any number of "steps" forward and calculate the probability of travelling from observation A to observation B. For our purposes, we postulate that this probability is large if A and B are similar to the same set of observations, while this Markov probability is conversely low if A and B do not share mutual similarities. We previously set the diagonal elements equal to zero because the diagonal probabilities correspond to self-loops, which are not interesting or useful for this algorithm.

A large number of transition steps (e.g. $t \ge 3$) tends to erase the finer details and focus on large-scale structure. A smaller number of steps (e.g. $0 \le t \le 2$) will often let the smaller clusters show themselves, allowing for more clusters. Given that *t* can also be fractional, *t* is best thought of as a "noise control" parameter. Because there is no clear resolution in the similarity structure, we are very cautious toward erasing any finer detail. We prudently chose t = 0.5, which should ideally eliminate some noise between weakly-connected observations without overriding the finer connections within smaller cluster structures.

We used the eigen-decomposition of the previous transition probability matrix to reduce the dimensions while retaining the overall similarity structure (see Nadler et al, 2006). The number of dimensions is chosen to equal the desired number of clusters, allowing enough space to separate the clusters but keeping the dimensionality low for strong clustering. For k clusters and t steps, we constructed the Diffusion Map space Ψ according to:

$$\Psi_t(x) = \left[\lambda_2^t \,\psi_2(x), \,\, \lambda_3^t \,\psi_3(x), \,\, \dots, \,\, \lambda_{k+1}^t \,\psi_{k+1}(x)\right] \tag{3}$$

where λ_p is the *p*-largest eigenvalue, ψ_p is the corresponding eigenvector, and *x* represents rows of the Diffusion Map space. Notice that we specifically chose to exclude the first eigenpair. Due to the strictly positive nature of our transition probability matrix, the first eigenvector yielded a simple weighted sum of the similarity values. This effectively clumped together all points with strong connectivity, instead of looking at *which* points were interconnected. This dimension did not prove useful for identifying separation between clusters. Moreover, the first eigenvalue was substantially larger than the following eigenvalues, and hence the first dimension would dominate the clustering structure. On the other hand, eigenpairs 2 through *k* should theoretically correspond to the dimensions *separating* clusters, which is where we wanted to focus.

Lastly, we normalized each row within this Diffusion Map Space to a unit vector, such that each vector is mapped to the unit sphere. This guarantees that we are only considering the "direction" of a vector and ignoring the magnitudes (equalizing strongly connected and weakly connected rows). For efficient eigen-decomposition, we use the R package "RSpectra" (Qiu et al, 2016).

4 Results & Insights

We varied the number of clusters between 2 to 10, comparing the results using similarity heat maps, subspace plots, and the validation variables. We chose k = 4 clusters, particularly because it led to the clearest interpretation within the validation variables. In the following section, we first interpret the clusters according to the validation variables, and then dissect each cluster in terms of its most important clustering variables.

For a baseline interpretation of the clusters, we constructed a parallel coordinates plot for each set of validation variables (see Figure 4). Recall that we centered each variable and scaled by the standard deviations; hence, in Figure 4, the vertical axis represents a cluster's standardized performance relative to each column's mean and standard deviation.



Figure 4: Each plot reads temporally from left to right. A low y-value indicates good health (according to the respective test measure) while a high y-value indicates poor health. Generated with R (R Core Team, 2016).

Figure 4 suggests certain insights to the behaviour of the clustering structure. The red cluster appears to score consistently healthily, while the green cluster scores consistently poorly over time. According to the Vasl and RMprop variables, the purple cluster starts in bad shape but heals over time, while the blue cluster conversely starts out relatively well but gets worse over time.

Interestingly, the Gen variable agrees that the red and purple clusters do better compared to the green and blue clusters, yet it seems to switch the behaviours of red/purple and green/blue. We hypothesize that the Gen variable gives less reliable interpretations because of the narrow scoring scale: Values placed in one of 7 categories, while Vasl allows for 11 categories and RMprop is measured on a continuous scale from 0–100. Further investigation is certainly warranted.

For completeness' sake, we also inspected each cluster on the original unnormalized validation variables. We still imputed the missing values using kNN on the scaled data, to equalize the distance magnitudes (otherwise the kNN algorithm would be dominated by the variable which operates on the largest scale, i.e. RMprop). We subsequently un-scaled the data by multiplying by the original standard deviations and adding the original column means, producing the exact same data space that we had initially. The results are presented in Figure 5.



Figure 5: Each plot reads temporally from left to right. A low y-value indicates good health (according to the respective test measure) while a high y-value indicates poor health. A solid line represents the cluster mean, and the dotted lines represent ± 1 standard error of the mean. Notice that Vasl and RMprop show a general recovery from the 2 week measurement to the 12 month measurement, while the Gen variable is hard to interpret in terms of recovery. Generated with R (R Core Team, 2016).

To determine the effectiveness of the clustering, we must also consider the within-cluster variance of each validation variable, instead of only measuring the cluster means. In an ideal case, we would hope to see the mean values separated by a significant magnitude of standard deviations. The within–cluster standard deviations are shown in Figure 6.



Figure 6: Each plot reads temporally from left to right. A low y-value indicates good health (according to the respective test measure) while a high y-value indicates poor health. The solid lines represent the cluster means, and the dotted lines represent ± 1 standard deviation (measured separately within each cluster). Generated with R (R Core Team, 2016).

Unfortunately, this condition is poorly reflected in all measurements except the RMprop score, which shows good separation between the green and red clusters (the "consistently healthy" and the "consistently unhealthy" clusters) but still shows strong overlap between the two middling clusters. Overall, Figure 5 suggests that we did find some real information, as the means show a significant and interpretable pattern. Unfortunately, Figure 6 shows that the clusters' separation in the validation data may not be distinct enough to classify the patients in a reliable way.

To highlight the identifying factors of each cluster, we analyse the mean of each cluster within those centered columns. We searched for any component of a cluster centroid which is near the extremes, given that all variables have been mapped to the [0,1] interval. This standardization also validates the comparison of means across different variables. Extreme averages will point to any value in which the cluster scores consistently high or consistently low. As with correlation similarity, we note that this method cannot identify variables in which a cluster scores consistently in the middle; an analysis of column variances would be required for such identification. See Tables 2 to 5 for the results of the cluster analysis.

Table 2: Cluster 1 demonstrates the best recovery outcomes, according to the validation variables. In the clustering data, Cluster 1 is characterized by low scores in the "physical pain & trouble" variables, indicating good overall health (a high score would indicate high physical pain/trouble).

| Score | Variable | Description |
|-------|----------|--|
| Low | Rm180 | "Because of my back problem, I go upstairs more slowly than usual." |
| Low | Rm140 | "I only walk short distances because of my back problem or leg pain (sciatica)." |
| Low | Rm50 | "Because of my back problem, I use a handrail to get upstairs." |
| High | Bsex0 | Sex = male. |
| Low | Rm220 | "Because of my back problem, I am doing less of the daily work around the house than I would usually do." |

| Table 3: Cluster 2 demonstrates the worst recovery outcomes, according to the validation variables. In |
|---|
| the clustering data, Cluster 2 is characterized by high scores in the "psychological distress" variables. |
| This agrees with known literature that commonly shows how psychological health is highly correlated |
| with physical well-being. |

| Score | Variable | Description |
|-------|----------|--|
| High | Start80 | "In general I have not enjoyed all the things I used to enjoy." |
| High | Start60 | "Worrying thoughts have been going through my mind a lot of the time." |
| High | Rm170 | "Because of my back problem, I am more irritable and bad tempered with people than usual." |
| High | Start10 | "My back pain has spread down my leg(s) at some time in the last 2 weeks." |
| High | Rm220 | "Because of my back problem, I am doing less of the daily work around the house than I would usually do." |

Table 4: Cluster 3 starts out with mediocre recovery symptoms but converges toward Cluster 2 over time. Interestingly, we found that Cluster 3 assigns importance to many of the same variables as cluster 1, but *in the opposite extremity*. Cluster 1 demonstrated very healthy scores in the "physical trouble" categories, while Cluster 3 clearly captures all the individuals who have poor initial physical symptoms.

| Score | Variable | Description |
|-------|----------|---|
| High | Rm140 | "I only walk short distances because of my back problem or leg pain (sciatica)." |
| High | Rm60 | "Because of my back problem, I have to hold on to something to get out of an easy chair." |
| High | Rm100 | "I find it difficult to get out of a chair because of my back problem or leg pain (sciatica)." |
| High | Rm180 | "Because of my back problem, I go upstairs more slowly than usual." |
| High | Rm50 | "Because of my back problem, I use a handrail to get upstairs." |

Table 5: Cluster 4 is characterized by healthy physical symptoms, as with Cluster 1. In the validation variables, Cluster 4 converges toward Cluster 1, and the difference between them mostly disappears by the 12-month follow-up. It seems that one of the major distinctions (most notably, male vs. female) may catalyse different recovery patterns in the short term, but converge to similar prospects for long term health and recovery.

| Score | Variable | Description |
|-------|----------|---|
| Low | Rm130 | "I have trouble putting on my socks (or stockings) because of the pain in my back or leg." |
| Low | Rm70 | "I get dressed more slowly than usual because of my back problem or leg pain (sciatica)." |
| High | Bsex1 | Sex = female. |
| Low | Rm100 | "I find it difficult to get out of a chair because of my back problem or leg pain (sciatica)." |
| Low | Rm60 | "Because of my back problem, I have to hold on to something to get out of an easy chair." |

5 Conclusions

We used a Spectral Clustering algorithm to find clusters among lower back pain symptoms in medical patients. We processed the different types of data separately such that all types of data are mapped to comparable dimensions. We computed a similarity score between every pair of patients using an adaptation of Pearson correlation and then we calculated the spectral (eigen) decomposition of this similarity matrix, reducing the dimensionality; we finally performed k-means clustering in this new subspace.

We believe that there is truly a 4-cluster structure within this data, but the partition is hard to produce reliably. At the very least, we can yield a significant 2-cluster structure (combining Cluster 1 with Cluster 4, and Cluster 2 with Cluster 3) that produces meaningful separation between positive vs. negative long-term outcomes. In the absence of finer resolution, this 2-cluster structure would be useful for identifying patients in danger of long term health risks.

Acknowledgements This work was supported by the Henry Woodward Fund. The authors would like to thank the IFCS committee, specifically Christian Hennig and Iven Van Michelen, for the opportunity to participate in the challenge.

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