Mode Hunting using Pettiest Components Analysis

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Abstract
Principal component analysis has been used to reduce dimensionality of datasets for a long time. In this paper, we will demonstrate that in mode detection the components of smallest variance, the pettiest components, are more important. We prove that when the data follows a multivariate normal distribution, by implementing “pettiest component analysis” when the data is normally distributed, we obtain boxes of optimal size in the sense that their size is minimal over all possible boxes with the same number of dimensions and given probability. We illustrate our result with a simulation revealing that pettiest component analysis works better than its competitors.

Keywords: Bump hunting, Dimension reduction, Mode detection, Patient rule induction method, Principal components analysis, Space rotation.

1. Introduction

Principal components analysis is a widely used method in data analysis which reduces the dimension by projecting on the orthogonal rotation that maximizes the variance (Mardia et al., 1979, Ch. 8). Due to the simple mechanism and good compatibility with different regression methods, principal components analysis is used in many scenarios, especially dealing in \( p \gg n \) datasets. Even in regression and learning settings, most practitioners prefer to discard the components of the input with the smallest variance, using just the first few principal components. This is called principal components regression. But we should be careful about some potential pitfalls when applying principal components analysis on regression models. As Jolliffe demonstrated in a classic paper, we can easily find some ordinary examples in which small-variance components become equally important, if not more, than large-variance ones (Jolliffe, 1982). Hadi and Ling have also presented three cautionary notes on using principal components regression, mainly due to issues arising from multicollinearity (Hadi and Ling, 1998). In the end, maybe the strongest reason to question principal components regression is that the dependent variables are never used in principal components analysis. As Cox said, it is hard to see any reason “why the dependent variable should not be closely tied to the least important principal components” (Cox, 1968, p. 272). Here we will call those least important...
principal components pettiest components. Nevertheless, using principal components regression is not totally invalid. Actually, discarding the pettiest components does give satisfying results in many situations. In fact, Artemiou and Li gave conditions under which the first few leading principal components have a higher probability of correlating with the dependent variable than the small-variance ones (Artemiou and Li, 2009).

All these arguments are informative but none, to the best of our knowledge, have tried to make a systematic use of the pettiest components in their own right. That is, most criticisms have focused on the negative aspect of finding isolated counterexamples showing that principal components regression is not desirable, based on the underlying assumption that the leading principal components are better, but none has focused on the positive aspect of systematically selecting the pettiest components. In this article we take advantage from these pettiest components. In fact, a modification of a mode hunting algorithm will show that the smallest regions of the same probability are achieved using the pettiest components. Intuitively, the result presented here follows this very simple idea: In a space $S \subset \mathbb{R}^p$, define a $\beta$-mode of a continuous distribution as the region of the space with the smallest volume constrained to have a probability $\beta$. Assume the underlying distribution of a $p$-dimensional vector $x$ is a multivariate normal, and that we project it to a $p'$-dimensional space, with $p' < p$. Then the box that minimizes the size, among all possible boxes of probability $\beta$, is the one projected over the subspace of the orthogonal variables with the smallest variance.

This work can be seen as a continuation of Díaz-Pachón et al. (2017), where the optimality, in terms of smallest volume, of the $p$-dimensional box centered around the mean in the direction of the eigenvectors was proved for a multivariate normal distribution. The next obvious step, the reduction of dimensionality to $p'$ dimensions, is accomplished here; but contrary to common practice, we show that the optimal $p'$-box is obtained when the $p$-dimensional box in the previous step is projected to the subspace of the $p'$ pettiest components.

Several questions and comments arise from this situation. First, finding a general solution for the set of minimum volume in the class $C$ of all the Borel sets with probability $\beta$ in $\mathbb{R}^d$ seems in general intractable; therefore we consider the next big thing: the more manageable class $C' \subset C$ of all hyper-rectangles $I_1 \times \cdots \times I_p$, where $I_i$ are intervals in $\mathbb{R}$. Second, we define a $\beta$-mode and not the $\beta$-mode, because there can be more than one Borel set with identical hyper-volume and probability $\beta$ in the space; in fact, in many situations not only global but local $\beta$-modes are of interest. Third, we talk about $\beta$-modes in general, instead of simply modes, because we are interested on regions of positive probability. And fourth, out of the previous considerations, there are no spaces without $\beta$-modes; i.e., even if $S$ is of finite volume and the underlying distribution is uniform we have uncountable $\beta$-modes, though these will not be very informative; on the other hand, if $S$ has infinite Lebesgue measure, a continuous distribution in $S$ will have at least a $\beta$-mode.

Why the interest in the $\beta$-regions with the smallest volume? An answer among many approaches lies in the fact that such regions might contain a large amount of relative Shannon information. To see this, imagine $S = [0, 1]$ and suppose a non-uniform distribution $\phi$ in this space whose $\beta$-mode $I$ is unique in the sense that if there is another set $I'$ with probability $\beta$, then the volume of the symmetric difference $I \triangle I'$ is zero. For definiteness, let $I = [a, b]$. Then, calling $U$ the uniform distribution over $S$, we have that $I_+(I)$, defined as $\log(\phi(I)/U(I)) = \log(\beta/(b-a))$, is maximal over all the other intervals
in $S$. That is, for any other interval $I^*$ with $\phi(I^*) = \beta$, then $I_+(I) - I_+(I^*) > 0$. $I_+$ is called active information; it is the information added by $\phi$ with respect to a baseline distribution, in this case $U$ (Díaz-Pachón et al., 2020). Active information was introduced in the context of search problems (Dembski and Marks II, 2009a,b, Díaz-Pachón and Marks II, 2020), and has also been used to detect modes in multivariate analyses (Díaz-Pachón et al., 2019).

Besides the theoretical curiosity of finding such a region, there is a vast number of applications. Since there are uncountably infinite regions of probability $\beta$ in a $p$-dimensional support of a continuous distribution, even when $p = 1$, the smallest region of probability $\beta$ will tell us that the data is highly concentrated inside such region. This is of course of interest in many fields, for instance in tumor detection by image recognition in medicine, where a high concentration of points around a small region can help on early detection; or in more accurate predictions based on closeness to a given target, as in the Netflix recommendations algorithm. Many more come easily to mind.

Yet, mode detection continues being a difficult problem, specially in multivariate settings. One of the most famous ways to approach it, specially in computer vision, is via the mean-shift algorithm by kernel density estimation (Fukunaga and Hostetler, 1975). It works well when $p = 2$ having amenable asymptotic properties (Parzen, 1962, de Valpine, 2004). However, it becomes very slow when $p > 2$, though when the shape of the density is known, the speed improves (Cule et al., 2010). More recently, Ruzankin and Logashov introduced a fast mode estimator with time complexity $O(pn^2)$, whereas other estimators time complexity is $O(pn^4)$, where $n$ is the number of observations (Ruzankin and Logashov, 2020).

2. Basic notions

2.1. Components

Suppose there is a $p$-dimensional dataset of $n$ observations $\{x_1, \ldots, x_p\}_n^1$ with covariance matrix $\Sigma$. The problem is to solve the eigenvalue question $\Sigma a = \lambda a$. From the solution, we get the eigenvectors $a_1, \ldots, a_p$, and respective eigenvalues $\lambda_1, \ldots, \lambda_k$. The original $p$-dimensional input space will be $\mathcal{X}(p)$, and the space after the rotation in the direction of its $p$ eigenvectors, $\mathcal{X}'(p)$.

We will call these eigenvectors components, and their corresponding eigenvalue will be their variance. Then, sorting the components in order of increasing variance, the $k$ principal components will be the $k$ components with the largest variances; and the $k$ pettiest components will be the $k$ components with the smallest variance.

2.2. Patient rule induction method

The patient rule induction method (PRIM) is a greedy algorithm designed for bump hunting. A bump can be roughly defined as a region on the response variable with higher mean, compared to other places. Here we outline briefly the algorithm. More details can be found in Friedman and Fisher (1999).

Assume we have a dataset $\{y, x\}_n^1$ where $x = \{x_1, x_2, \ldots, x_p\}$ is a continuous random vector. $f(x)$ is the target function. The input domain $\mathcal{X}(p)$ is here called $S$. Defining
\[ \bar{f}_B \text{ and } \bar{f} \text{ as} \]

\[ \bar{f}_B = \frac{\int_B f(x)p(x)dx}{\int_B p(x)dx}, \]

\[ \bar{f} = \int_S f(x)p(x)dx, \]

where \( p(x) \) is the density function of \( x \), the method aims to find a box \( B \subset S \) in which \( \bar{f}_B/\bar{f} \) is maximized under the constraint that \( B \) is not too small. In fact, the probability of \( B \) is defined at the outset by a tuning meta-parameter \( \beta \) for the smallest permitted box size. In practice, \( \bar{f}_B/\bar{f} \) will be replaced by its corresponding estimator.

The algorithm is divided in three stages. First there is a peeling: Beginning with the whole input space \( S \), a whole class of eligible boxes for removal is set up. This class is made of sets of the form

\[ b_{j-} = \{ x \mid x_j < x_{j(\alpha)} \}, \]

\[ b_{j+} = \{ x \mid x_j > x_{j(1-\alpha)} \}, \]

where \( x_{j(\alpha)} \) is an \( \alpha \)-quantile. If a box \( b^* \) is in the eligible set, and without it the remaining \( S \setminus b^* \) will give the maximum average value of response variable, \( b^* \) is the specific box selected to remove in this loop. Formally we write

\[ b^* = \arg \max_b \text{ave}[y_i \mid x_i \in B - b], \]

where \( \text{ave} \) is the average. Update the new box as \( B = S \setminus b^* \) and run the same procedure on \( B \). The process is iterated until the final box \( B \) has probability \( \beta \). The peeling procedure is shown in Fig. 1.

After peeling, a second step called pasting is performed in order to correct for the greediness of peeling. We will not consider pasting in this paper. Finally, the third step is called covering, which means that after the peeling stage, the final box \( B \) is deleted from \( S \), and then the whole procedure of peeling is repeated in \( S \setminus B \).

Figure 1: The peeling procedure in PRIM.
2.3. Fast patient rule induction method

PRIM has at least three shortcomings. First, it is computationally expensive; second, it does not behave well in the presence of collinearity; and third, even in a small number of dimensions, it cannot detect multiple bumps (Polonik and Wang, 2010). For this reason, Dazard and Rao developed a modified algorithm called local sparse bump hunting in which the patient rule induction method is subsumed (Dazard and Rao, 2010). The local sparse bump hunting algorithm uses a recursive partition algorithm, say classification and regression trees, in order to divide the space $\mathcal{X}(p)$ in several regions $S_1, \ldots, S_R$; then applies sparse principal components analysis inside each particular region $S_i$ in order to reduce the dimension of each region in the partition; and finally applies the patient rule induction method to each rotated and projected subspace induced by $S_i$. The local sparse bump hunting algorithm has been successfully applied to detect heterogeneity of colon tumors, dividing colon cancer patients into two subpopulations with different genetic/molecular profiles in all stages of cancer (Dazard et al., 2012).

Elaborating on local sparse bump hunting, a new modified algorithm called fastPRIM was developed in order to find the minimal volume of boxes with probability $\beta$ when the distribution is a multivariate normal (Díaz-Pachón et al., 2017, Algorithm 4). More accurately, the modes can be defined as $\beta$-modes; i.e., contiguous regions, not necessarily unique, with the smallest volume and probability $\beta$. Since the mode and the mean of the normal distribution coincide, mode hunting in this case is equivalent to finding a box of probability $\beta$ centered around the mean. In fastPRIM the space is first rotated in the direction of its eigenvectors, and then the patient rule induction is applied in the direction of the rotation. It turns out that in this setting the whole peeling and pasting iteration is reduced to one single step. That is, fastPRIM chooses the centralized box such that each side of the box is parallel to an axis of the input space and whose vertices are located at the quantiles $2^{-1}(1 \pm \beta^{1/p})$ of the corresponding variable, where $\beta_T = \sum_{k=1}^{t} \beta(1-\beta)^{k-1} = 1 - (1-\beta)^t$ is the probability measure after $t$ steps of covering. As a result, we obtain a rectangular Lebesgue set, or say a square set in probability, centralized at the zero point.

Therefore, from a sampling viewpoint fastPRIM is consistent: calculating the average of all the points inside the final centered box and taking this average as the center of our box, we know by the law of large numbers that the final box will be centered around the origin. Since the mean and the mode coincide in the normal distribution, as $n \to \infty$, the procedure is approaching a box whose center is the true mode. This is so with or without dimension reduction.

3. Pettiest components analysis with fastPRIM

The fastPRIM algorithm satisfies the following optimality property: when the data is multivariate normal, say $\mathcal{N}(0, \Sigma)$, the box with the smallest volume subject to have probability $\beta$ is found in the direction of the rotation of the $p$ principal components; that is, the box centered around the mean of probability $\beta$ in $\mathcal{X}'(p)$ (Díaz-Pachón et al., 2017, Proposition 1). However, no result in Díaz-Pachón et al. (2017) dealt with dimension reduction. This article goes one step further: it shows that if we are going to consider reduction of dimensionality, say to $p' < p$, we should consider pettiest components instead of principal components.
Starting thus with the space $X'(p')$, let $B_i$ be the final box obtained by fastPRIM on an input space $X'(p')$, where $i$ indicates a specific way of choosing $p'$ variables from $p$ variables. The collection of all such boxes will be $B$. The Lebesgue measure of the box $B \in B$ with probability measure $\beta$ is $\Vol(B|\beta)$. In the input space $X'(p')$ spanned by the pettiest components, we write that specific box as $B$.

**Theorem 1.** Let $X$ be a $p$-random vector such that its components $X_1, \ldots, X_p$ are independent of each other and have normal distribution $N(0, \sigma_1^2), \ldots, N(0, \sigma_p^2)$, respectively. Apply fastPRIM on each possible projection space $X'(p')$ with same probability $\beta$. Then,

$$\arg \min_{B \in B} \Vol(B|\beta) = B.$$  

**Proof.** There are $\binom{p}{p'}$ ways to choose $p'$ dimensions from $p$. For $X_1, \ldots, X_p$ following independent normal distributions, we write $X_j \sim N_j(0, \sigma_i^2)$, $(j = 1, \ldots, p)$. From the fact that the final box $B$ in fastPRIM is a square in probability, the marginal probability measure of every $B \in B$ is $\beta^{1/p'}$. Because all boxes $B \in B$ are centralized at zero, the Lebesgue measure of $X_j$, subject to a probability $\beta^{1/p'}$, can be calculated by the equation $P(-k\sigma_j < X_j < k\sigma_j) = \beta^{1/p'}$. Here $k$ only depends on $\beta^{1/p'}$ and it has nothing to do with $j$. Therefore, the edge length of $B_i$ in the $X_j$ direction is $2k\sigma_j$. Then,

$$\Vol(B_i|\beta) = \prod_{j^{(i)}=1}^{p'} 2k\sigma_{j^{(i)}} = (2k)^{p'} \prod_{j^{(i)}=1}^{p'} \sigma_{j^{(i)}},$$

where $j^{(i)}$ denotes the $p'$ variables in the choice of $B_i$. Since a fix $\beta$ implies a fix $k$, the minimum of $\Vol(B_i|\beta)$ can thus be obtained by minimizing $\prod_{j^{(i)}=1}^{p'} \sigma_{j^{(i)}}$. But this only requires the $\sigma_{1^{(i)}}, \ldots, \sigma_{p^{(i)}}$ to have the smallest values, which is achieved by choosing the $X_{1^{(i)}}, \ldots, X_{p^{(i)}}$ with the smallest variances. That is, the $p'$ pettiest components. The corresponding box found by fastPRIM with pettiest components is $B$. □

Using Theorem 1, we can easily show that the same conclusion is true for any multivariate normal distribution input under fastPRIM.

**Theorem 2.** Let $X$ be a $p$-random vector distributed as $N_p(0, \Sigma)$. Apply fastPRIM on each possible projection space $X'(p')$ with same probability $\beta$. Then,

$$\arg \min_{B \in B} \Vol(B|\beta) = B$$

**Proof.** For a multivariate normal distribution input, to rotate the space in the direction of its $p$ components is equivalent to solve the eigenvalue equation of covariance matrix $\Sigma$. The rotation will produce a diagonal matrix $D$ with eigenvalues as its diagonal elements. This new matrix $D$ is the covariance matrix of the components, which implies that they are all independent of each other and follow a normal distribution. So the problem is reduced to an instantiation of Theorem 1. Thus the result holds as before. □

**4. Simulation**

We generate a dataset with 300 observations and 100 dimensions, which follow the multivariate normal distribution $N_p(0, \Sigma)$. The covariance matrix $\Sigma$ is assumed to have
its first two diagonal elements as 1, and \(\text{cov}(x_1, x_2) = 0.7\); the last two diagonal elements are 12 with \(\text{cov}(x_{99}, x_{100}) = 8\); the remaining diagonal elements are 6 and all other places are 0. A pure PRIM, no rotation nor reduction, with ten iterations of covering, is then applied for contrast purposes. The result is shown in Fig. 2 for the first two dimension. We now standardize the dataset to use the correlation matrix and apply the rotation in the direction of the eigenvectors. Once the rotation is performed, the two new variables with larger variances are the principal components, and the two variables with smaller variances are the pettiest components. The next step is to run both PRIM and fastPRIM on the two principal components and the two pettiest components, both with \(\beta = 0.1\). The results are shown in Fig. 3. Each box results from a whole peeling period and the order of the boxes after ten stages of covering is shown by grading color. The fastPRIM algorithm exhibits nested rectangular boxes instead of the PRIM’s messy ones with. There is a striking difference in both algorithms results between principal and pettiest components: the final boxes obtained by fastPRIM are almost five times smaller than those of its competitor.

Table 1 shows the quantitative results in terms of the empirical density over volume of the box. Looking at it by columns, we can compare the different methods under the same covering step. First, the classical PRIM results in too small densities, thus rendering it completely useless. This in the end comes as no surprise considering the curse of dimensionality. In this sense Table 1 also reveals the benefits of dimension reduction, since any of the other options will do much better. That is, using principal or pettiest components analysis to reduce dimensionality, from 100 dimensions to 2 in our example, we get much better densities. In fact, fastPRIM improves the densities even more. However, the optimal improvement comes when the pettiest components are used; in this case, the densities show an increase of an order of magnitude. Finally, looking at the table by rows, one can track the variations of the densities during covering procedures. There is an interesting contrast in that for PRIM the density starts from a really small value and then increases monotonically; whereas for all other cases, a final decrease is accomplished as expected, though it is not monotonic.

Table 2 shows bias and variance by different method. The bias was calculated as the distance between the mean value and the origin. The results were obtained by 100 times simulations from the same distribution used before. We can see that the variance of PRIM is too high, compared to the other mechanisms with the dimension reduction, corresponding to what we would expect. Also, PRIM with principal components and fastPRIM with principal components have variances that are close, but there is a huge shrinkage of bias between the two methods. The same is true for PRIM and fastPRIM both with pettiest components. This illustrates the superiority of fastPRIM in this scenario. Finally, notice that pettiest components is producing a tenfold decrease in variance, whether we are looking at PRIM or to fastPRIM; the bias also decreases. The final outcome is that fastPRIM with pettiest components, having least variance and bias among all the strategies, minimizes the mean squared error.

5. Summary

Even though it is well known that pettiest components can sometimes explain better a response than principal components, they have been treated more like counter-examples, anomalies to be avoided, than as a tool themselves. However, in this article we showed
that pettiest components can be systematically used in order to find the best β-modes in multivariate datasets, provided that the data is distributed normal. In this sense, the fact that it had not been noted before is surprising. This finding goes against the general notion that principal components are more informative, since, as shown in the
Table 1: Density of boxes per volume by different method

| Method       | 1    | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   |
|--------------|------|------|------|------|------|------|------|------|------|------|
| PRIM         | 1.07e-73 | 1.57e-73 | 1.76e-73 | 2.14e-73 | 2.59e-73 | 3.04e-73 | 3.45e-73 | 3.87e-73 | 4.26e-73 | 4.65e-73 |
| PRIM-Principal | 15.7 | 16.7 | 14.2 | 14.7 | 14.3 | 14.2 | 14.0 | 13.9 | 13.8 | 13.0 |
| fastPRIM-Principal | 16.3 | 15.6 | 16.2 | 16.3 | 14.5 | 13.2 | 13.1 | 13.1 | 12.7 | 11.8 |
| PRIM-Pettiest | 182 | 168 | 187 | 152 | 155 | 142 | 130 | 132 | 132 | 127 |
| fastPRIM-Pettiest | 215 | 240 | 237 | 218 | 207 | 186 | 189 | 177 | 169 | 161 |

Table 2: Empirical variance and bias by method

| Method       | Variance | Bias   |
|--------------|----------|--------|
| PRIM         | 104      | 0.310  |
| PRIM-Principal | 2.28   | 0.145  |
| PRIM-Pettiest | 0.204  | 0.1    |
| fastPRIM-Principal | 2.23 | 0.00579 |
| fastPRIM-Pettiest | 0.149 | 0.000653 |

Introduction, the box with the smallest size also maximizes the active information relative to the uniform distribution.

Given the mean’s lack of robustness even in low dimensions, and the prevalence of big data and large-dimensions analyses, the importance of mode-based statistics and learning is becoming more relevant Chacón (2020). To mention just one case, a recent analysis in affecting computing used for autism therapy is performed around modes, not the mean Rudovic et al. (2019). Consequently, new theory and methods are required in order to better detect modes, but this task is difficult and elusive. The importance of fastPRIM in mode hunting is dictated by the central limit theorem. The setback of this approach is the curse of dimensionality, as Vapnik explains in the Introduction of his book (Vapnik, 1998, pp. 4–6). Therefore, even though there is some optimality that is reached just by rotating the information in the direction of the eigenvalues, if fastPRIM is going to be useful it will need to reduce dimensionality.

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