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Fast and Robust Archetypal Analysis for Representation Learning

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Abstract

We revisit a pioneer unsupervised learning technique called archetypal analysis \cite{archetypal}, which is related to successful data analysis methods such as sparse coding \cite{sparse} and non-negative matrix factorization \cite{nmf}. Since it was proposed, archetypal analysis did not gain a lot of popularity even though it produces more interpretable models than other alternatives. Because no efficient implementation has ever been made publicly available, its application to important scientific problems may have been severely limited.

Our goal is to bring back into favour archetypal analysis. We propose a fast optimization scheme using an active-set strategy, and provide an efficient open-source implementation interfaced with Matlab, R, and Python. Then, we demonstrate the usefulness of archetypal analysis for computer vision tasks, such as codebook learning, signal classification, and large image collection visualization.

1. Introduction

Unsupervised learning techniques have been widely used to automatically discover the underlying structure of data. This may serve several purposes, depending on the task considered. In experimental sciences, one may be looking for data representations that automatically exhibit interpretable patterns, for example groups of neurons with similar activation in a population, clusters of genes manifesting similar expression traits among individuals of the same cluster \cite{bioinformatics}.

A natural question is why archetypal analysis did not gain a lot of success, unlike NMF or sparse coding. We believe that the lack of efficient available software has limited the deployment of archetypal analysis to promising applications; our goal is to address this issue. First, we develop an efficient optimization technique based on an active-set strategy \cite{active_set}. Then, we demonstrate that our approach is scalable and orders of magnitude faster than existing publicly available implementations. Finally, we show that archetypal analysis can be useful for computer vision, and we believe that it could have many applications in other fields, such as neurosciences, bioinformatics, or natural language processing. We first show that it performs as well as sparse coding for learning codebooks of features in visual recognition tasks \cite{visual_recognition} and for signal classification \cite{signal_classification, signal_classification2, signal_classification3}. Second, we show that archetypal analysis provides a simple and effective way for visualizing large databases of images.

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This paper is organized as follows: in Section 2, we present the archetypal analysis formulation; Section 3 is devoted to optimization techniques; Section 4 presents successful applications of archetypal analysis to computer vision tasks, and Section 5 concludes the paper.

2. Formulation

Let us consider a matrix \( X = [x_1, \ldots, x_n] \in \mathbb{R}^{m \times n} \), where each column \( x_i \) is a vector in \( \mathbb{R}^m \) representing some data point. Archetypal analysis learns a factorial representation of \( X \); it looks for a set of \( p \) archetypes \( Z = [z_1, \ldots, z_p] \) in \( \mathbb{R}^{m \times p} \) under two geometrical constraints: each data vector \( x_i \) should be well approximated by a convex combination of a few data points only, which is useful for interpreting \( z_j \). Then, each archetype \( z_j \) becomes a linear combination of a few data points only, which is useful for interpreting \( z_j \). Moreover, the non-zero entries in \( \beta_j \) indicate in which proportions the input data points \( x_i \) are related to each archetype \( z_j \).

Another variant of sparse coding called “local coordinate coding” [26] is also related to archetypal analysis. In this variant, dictionary elements are encouraged to be close to the data points that uses them in their decompositions. Then, dictionary elements can be interpreted as anchor points on a manifold representing the data distribution.

2.1. Robust Archetypal Analysis

In some applications, it is desirable to automatically handle outliers—that is, data points \( x_i \) that significantly differ from the rest of the data. In order to make archetypal analysis robust, we propose the following variant:

\[
\min_{\alpha_i \in \Delta_p \text{ for } 1 \leq i \leq n} \min_{\beta_j \in \Delta_n \text{ for } 1 \leq j \leq p} \sum_{i=1}^n h \left( \| x_i - XB\alpha_i \|_2 \right),
\]

where \( h : \mathbb{R} \mapsto \mathbb{R} \) is the Huber loss function, which is often used as a robust replacement of the squared loss in robust statistics [11]. It is defined here for any scalar \( u \) in \( \mathbb{R} \) as

\[
h(u) = \begin{cases} 
\frac{u^2}{2} + \frac{\varepsilon}{2} u & \text{if } |u| \leq \varepsilon \\
\frac{u^2}{2} & \text{otherwise}
\end{cases}
\]

and \( \varepsilon \) is a positive constant. Whereas the cost associated to outliers in the original formulation (2) can be large since it grows quadratically, the Huber cost only grows linearly.

In Section 3, we present an effective iterative reweighted least-square strategy to deal with the Huber loss.

3. Optimization

The formulation (2) is non-convex, but it is convex with respect to one of the variables \( A \) or \( B \) when the other one is fixed. It is thus natural to use a block-coordinate descent scheme, which is guaranteed to asymptotically provide a stationary point of the problem [2]. We present such a strategy in Algorithm 1. As noticed in [5], when fixing all variables but a column \( \alpha_i \) of \( A \) and minimizing with respect
Algorithm 1 Archetypal Analysis

1: Input: Data X in $\mathbb{R}^{m \times n}$; p (number of archetypes); T (number of iterations);
2: Initialize $Z$ in $\mathbb{R}^{m \times p}$ with random columns from X;
3: Initialize B such that $Z = XB$;
4: for $t = 1 \ldots T$ do
5: for $i = 1 \ldots n$ do
6: $\alpha_i \in \arg \min_{\alpha \in \Delta_p} \|x_i - Z\alpha\|^2_2$;
7: end for
8: $R \leftarrow X - Z\alpha$;
9: for $j = 1 \ldots p$ do
10: $\beta_j \in \arg \min_{\beta \in \Delta_n} \| \frac{1}{\|\alpha\|^2_2} R\alpha^{T} + z_j - X\beta\|^2_2$;
11: $R \leftarrow R + (z_j - X\beta_j)\alpha_j$;
12: $z_j \leftarrow X\beta_j$;
13: end for
14: end for
15: Return $A$, $B$ (decomposition matrices).

Algorithm 2 Active-Set Method

1: Input: matrix $Z \in \mathbb{R}^{m \times p}$, vector $x \in \mathbb{R}^m$;
2: Initialize $\alpha_0 \in \Delta_p$ with a feasible starting point;
3: Define $A_0 = \{j \text{ s.t. } \alpha_0[j] > 0\}$;
4: for $k = 0, 1, 2 \ldots$ do
5: Solve (11) with $A_k$ to find a step $q_k$;
6: if $q_k$ is 0 then
7: Compute $\nabla f(\alpha_k) = -2Z^{T}(x - Z\alpha_k)$;
8: if $\nabla f(\alpha_k)[j] > 0$ for all $j \notin A_k$ then
9: Return $\alpha^* = \alpha_k$ (solution is optimal).
else
10: $j^* \leftarrow \min_{j \notin A_k} \nabla f(\alpha_k)[j]$;
11: $A_{k+1} \leftarrow A_k \cup \{j^*\}$;
12: end if
else
13: $\gamma_k \leftarrow \max_{\gamma \in [0, 1]} \{\text{ s.t. } \alpha_k + \gamma q_k \in \Delta_p\}$;
14: if $\gamma_k < 1$ then
15: Find $j^*$ such that $\alpha_k[j] + \gamma_k q_k[j] = 0$;
16: $A_{k+1} \leftarrow A_k \setminus \{j^*\}$;
17: end if
else
18: $A_{k+1} \leftarrow A_k$;
19: end if
20: $\alpha_{k+1} \leftarrow \alpha_k + \gamma_k q_k$;
21: end if
22: end for

3.1. Efficient Solver for QP with Simplex Constraint

Both problems (7) and (9) have the same form, and thus we will focus on finding an algorithm for solving:

$$\min_{\alpha \in \Delta_p} \left[ f(\alpha) \triangleq \|x - Z\alpha\|^2_2 \right],$$

which is a smooth (least-squares) optimization problem with a simplicial constraint. Even though generic QP solvers could be used, significantly faster convergence can be obtained by designing a dedicated algorithm that can leverage the underlying “sparsity” of the solution [1].

We propose to use an active-set algorithm [17] that can benefit from the solution sparsity, when carefully implemented. Indeed, at the optimum, most often only a small subset $A$ of the variables will be non-zero. Active-set algorithms [17] can be seen as an aggressive strategy that can leverage this property. Given a current estimate $\alpha$ in $\Delta_p$, at some iteration, they define a subset $A = \{j \text{ s.t. } \alpha[j] > 0\}$, and find a direction $q$ in $\mathbb{R}^p$ by solving the reduced problem

$$\min_{q \in \mathbb{R}^p} \|x - Z(\alpha + q)\|^2_2 \text{ s.t. } \sum_{j=1}^{p} q[j] = 0 \text{ and } q_{A^C} = 0,$$

where $A^C$ denotes the complement of $A$ in the index set $\{1, \ldots, p\}$. Then, a new estimate $\alpha' = \alpha + \gamma q$ is obtained by moving $\alpha$ onto the direction $q$—that is, choosing $\gamma$ in $[0, 1]$, such that $\alpha'$ remains in $\Delta_p$. The algorithm modifies the set $A$ until the algorithm finds an optimal solution in $\Delta_p$. This strategy is detailed in Algorithm 2. Open-source active-set solvers for generic QP exist, e.g., quadprog in Matlab, but we have found them too slow for our purpose. Instead, a dedicated implementation has proven to
be much more efficient. More precisely, we use some tricks inspired from the Lasso solver of the SPAMS toolbox [15]: (i) initialize \( A \) with a single variable; (ii) update at each iteration the quantity \( (Z_A^T Z_A)^{-1} \) by using Woodbury formula; (iii) implicitly working with the matrix \( Q = Z^T Z \) without computing it when updating \( \beta \).

As a result, each iteration of the active-set algorithm has a computational complexity of \( O(n m p + a^2) \) operations where \( a \) is the size of the set \( A \) at that iteration. Like the simplex algorithm for solving linear programs [17], the maximum number of iterations of the active-set algorithm can be exponential in theory, even though it is much smaller than \( \min(m, p) \) in practice. Other approaches than the active-set algorithm could be considered, such as the fast iterative shrinkage-thresholding algorithm (FISTA) and the penalty approach of [5]. However, in our experiments, we have observed significantly better performance of the active-set algorithm, both in terms of speed and accuracy.

### 3.2. Optimization for Robust Archetypal Analysis

To deal with the Huber loss, we use the following variational representation of the Huber loss (see, [11]):

\[
 h(u) = \frac{1}{2} \min_{w \geq \varepsilon} \left[ \frac{u^2}{w} + w \right].
\]  

(12)

which is equivalent to (6). Then, robust archetypal analysis from Eq. (5) can be reformulated as

\[
 \min_{\alpha_i \in \Delta, \beta_j \in \Delta} \left\{ \frac{1}{2} \sum_{i=1}^{n} \frac{1}{w_i} \| x_i - XB \alpha_i \|_2^2 + w_i \right\},
\]  

(13)

where the diagonal matrix \( \Gamma \) in \( R^{n \times n} \) carries the inverse of the weights \( w \) on its diagonal, thus rescaling the residual of each data point \( x_i \) by \( 1/w_i \) as in (13). Then, it is possible to show that (14) is equivalent to

\[
 \min_{\beta_j \in \Delta} \left\{ \frac{1}{\alpha^T \Gamma \alpha} \| (X - XB_{old} A) \alpha^T + z_j - X \beta_j \|^2_2 \right\},
\]  

(14)

which is carried out on Line 13 of Algorithm 3.

### 4. Experiments

We now study the efficiency of archetypal analysis in various applications. Our implementation is coded in C++ and interfaced with R, Python, and Matlab. It has been included in the toolbox SPAMS v2.5 [15]. The number of iterations for archetypal analysis was set to \( T = 100 \), which leads to a good performance in all experiments.

### 4.1. Comparison with Other Implementations

To the best of our knowledge, two software packages implementing archetypal analysis are publicly available:

- The Python Matrix Factorization toolbox (PyMF)\(^1\) is an open-source library that tackles several matrix factorization problems including archetypal analysis. It performs an alternate minimization scheme between the \( \alpha_i \)'s and \( \beta_j \)'s, but relies on a generic QP solver from CVX.\(^2\)

- The R package archetypes\(^3\) is the reference implementa-

\(^1\)http://code.google.com/p/pymf/.
\(^2\)http://cvxr.com/cvx/.
\(^3\)http://archetypes.r-forge.r-project.org/.
tation of archetypal analysis for R, which is one of the most widely used high-level programming language in statistics. Note that the algorithm implemented in this package deviates from the original archetypal analysis described in [5].

We originally intended to try all methods on matrices $X$ in $\mathbb{R}^{m \times n}$ with different sizes $m$ and $n$ and different numbers $p$ of archetypes. Unfortunately, the above software packages suffer from severe limitations and we were only able to try them on small datasets. We report such a comparison in Figure 1, where the computational times are measured on a single core of an Intel Xeon CPU E5-1620. We only report results for the R package on the smallest dataset since it diverged on larger ones, while PyMF was several orders of magnitudes slower than our implementation. We also conducted an experiment following the optimization scheme of PyMF but replacing the QP solver by other alternatives such as Mosek or quadprog, and obtained similar conclusions.

Then, we study the scalability of our implementation in regimes where the R package and PyMF are unusable. We report in Figure 2 the computational cost per iteration of our method when varying $n$ or $p$ on the MNIST dataset [13], where $m = 784$. We observe that the empirical complexity is approximately linear in $n$, allowing us to potentially learn large datasets with more than 100,000 samples, and above linear in $p$, which is thus the main limitation of our approach. However, such a limitation is also shared by classical sparse coding techniques, where the empirical complexity regarding $p$ is also greater than $O(p)$ [1].

Figure 1: Experimental comparison with other implementations. Left: value of the objective function vs computational time for a dataset with $m = 10$, $n = 507$ and $p = 5$ archetypes. Our method is denoted by arch. PyMF was too slow to appear in the graph and the R-package exhibits a non-converging behavior. Right: same experiment with $n = 600$ images from MNIST [13], of size $m = 784$, with $p = 10$ archetypes. The R package diverged while PyMF was between 100 and 1000 times slower than our approach.

Figure 2: Scalability Study. Left: the computational time per iteration when varying the sample size $n$ for different numbers of archetypes $p$. The complexity of our implementation is empirically linear in $n$. Right: the same experiment when varying $p$ and with fixed sample sizes $n$. The complexity is more than linear in $p$.

4.2. Codebook Learning with Archetypal Analysis

Many computer vision approaches have represented so far images under the form of a “bag of visual words”, or by using some variants of it. In a nutshell, each local patch (small regions of typically $16 \times 16$ pixels) of an image is encoded by a descriptor which is invariant to small deformations, such as SIFT [12]. Then, an unsupervised learning technique is used for defining a codebook of visual patterns called “visual words”. The image is finally described by computing a histogram of word occurrences, yielding a powerful representation for discriminative tasks [4, 12].

More precisely, typical methods for learning the codebook are $K$-means and sparse coding [12, 24]. SIFT descriptors are sparsely encoded in [24] by using the formulation (4), and the image representation is obtained by “max-pooling” the sparse codes, as explained in [24]. Spatial pyramid matching (SPM) [12] is also used, which includes some spatial information, yielding better accuracy than simple bags of words on many benchmark datasets. Ultimately, the classification task is performed with a support vector machine (SVM) with a linear kernel.

It is thus natural to wonder whether a similar performance could be achieved by using archetypal analysis instead of sparse coding. We thus conducted an image classification experiment by using the software package of [24], and simply replacing the sparse coding component with our implementation of archetypal analysis. We use as many archetypes as dictionary elements in [24]—that is, $p = 1,024$, and $n = 200,000$ training samples, and we call the resulting method “archetypal-SPM”. We use the same datasets as [24]—that is, Caltech-101 [9] and 15 Scenes Categorization [10, 12]. The purpose of this experiment is to demonstrate that archetypal analysis is able to learn a codebook that is as good as sparse coding and better than $K$-means. Thus, only results of similar methods are represented here such as [12, 24]. The state of the art on these data sets may be slightly better nowadays, but involves a different recognition pipeline. We report the results in Tables 1 and 2, where archetypal analysis seems to perform as well as sparse coding. Note that KMeans-SPM-$\chi^2$ uses a $\chi^2$-kernel for the SVM [12].
exploit the fact that the finding the class $k$ where tasks 

4.3. Digit Classification with Archetypal Analysis

Even though sparse coding is an unsupervised learning technique, it has been used directly for classification tasks [14, 21, 23]. For digit recognition, it has been observed in [21] that simple classification rules based on sparse coding yield impressive results on classical datasets such as MNIST [13] and USPS. Suppose that one has learned on training data a dictionary $Z_k$ in $\mathbb{R}^{m \times p}$ for every digit class $k = 0, \ldots, 9$ by using (4), and that a new test digit $x$ in $\mathbb{R}^m$ is observed. Then, $x$ can be classified by finding the class $k^*$ that best represents it with $Z_k$:

$$k^* = \arg \min_{k \in \{0, \ldots, 9\}} \left\{ \min_{\alpha \in \mathbb{R}^p} \frac{1}{2} \|x - Z_k \alpha\|_2^2 + \lambda \|\alpha\|_1 \right\}, \quad (15)$$

where $\lambda$ is set to 0.1 in [21] and the vectors $x$ are normalized. Since we want to compare archetypal analysis with sparse coding, it is thus natural to also consider the corresponding “archetype” classification rule:

$$k^* = \arg \min_{k \in \{0, \ldots, 9\}} \left\{ \min_{\alpha \in \Delta_p} \|x - Z_k \alpha\|_2^2 \right\}, \quad (16)$$

where the $Z_k$ are archetypes learned for every digit class. Note that when archetypes are made of all available training data, the convex dual of (16) is equivalent to the nearest convex hull classifier of [16]. We report the results when all the training data is used as archetypes in Table 3, and when varying the number of archetypes per class in Figure 3. We include in this comparison the performance of SVM with a Gaussian kernel, and the $K$-nearest neighbor classifier (K-NN). Even though the state of the art on MNIST achieves less than 1% test error [14, 22], the results reported in Table 3 are remarkable for several reasons: (i) the method AA-All has no hyper-parameter and performs almost as well as sparse coding, which require choosing $\lambda$; (ii) AA-All and SC-All significantly outperform K-NN and perform similarly as a non-linear SVM, even though they use a simple Euclidean norm for comparing two digits; (iii) none of the methods in Table 3 exploit the fact that the $x_i$‘s are in fact images, unlike more sophisticated techniques such as convolutional neural networks [22]. In Figure 3, neither SC nor AA are helpful for prediction, but archetypal analysis can be useful for reducing the computational cost at test time. The choice of dictionary size $K$ should be driven by this trade-off. For example, on USPS, using 200 archetypes per class yields similar results as AA-All.

Table 1: Classification accuracy (%) on Caltech-101 dataset. Following the same experiment in [24], 15 or 30 images per class are randomly chosen for training and the rest for testing. The standard deviation is obtained with 10 randomized experiments.

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>Classification Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>KMeans-SPM-χ² [12]</td>
<td>56.44 ± 0.78</td>
</tr>
<tr>
<td>KMeans-SPM [24]</td>
<td>53.23 ± 0.65</td>
</tr>
<tr>
<td>SC-SPM [24]</td>
<td>67.00 ± 0.45</td>
</tr>
<tr>
<td>archetypal-SPM</td>
<td>64.96 ± 1.04</td>
</tr>
</tbody>
</table>

Table 2: Classification accuracy (%) on Scene-15 dataset. Following the same experiment in [24], 100 images are randomly chosen for training and the rest for testing. The standard deviation is obtained with 10 randomized experiments.

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>Classification Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>KMeans-SPM-χ² [12]</td>
<td>81.40 ± 0.50</td>
</tr>
<tr>
<td>KMeans-SPM [24]</td>
<td>65.32 ± 1.02</td>
</tr>
<tr>
<td>SC-SPM [24]</td>
<td>80.28 ± 0.93</td>
</tr>
<tr>
<td>archetypal-SPM</td>
<td>81.57 ± 0.81</td>
</tr>
</tbody>
</table>

Table 3: Classification error rates (%) on the test set for the MNIST and USPS datasets. AA-All and SC-All respectively mean that all data points are used as archetypes and dictionary elements. SVM uses a Gaussian kernel.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>AA-All</th>
<th>SC-All</th>
<th>SVM</th>
<th>K-NN</th>
</tr>
</thead>
<tbody>
<tr>
<td>MNIST</td>
<td>1.51</td>
<td>1.35</td>
<td>1.4</td>
<td>3.9</td>
</tr>
<tr>
<td>USPS</td>
<td>4.33</td>
<td>4.14</td>
<td>4.2</td>
<td>4.93</td>
</tr>
</tbody>
</table>

Figure 3: Train and Test error on MNIST (left) and USPS (right) when varying the number $p$ of archetypes. All-AA means that all data points are used as archetypes.

4.4. Archetyping Flickr Requests

Data visualization has now become an important topic, especially regarding image databases from the Internet [5], or videos [8]. We focus in this section on public images downloaded from the Flickr website, and present a methodology for visualizing the content of different requests using robust archetypal analysis presented in Section 2.1.

For example, we present in this section a way to visualize the request “Paris” when downloading images uploaded in 2012 and 2013, and sorted by “relevance” according to Flickr. We first compute dense SIFT descriptors [12] for all images, and represent each image by using
a Fisher vector [20], which have shown good discriminative power in classification tasks. Then, we learn $p = 256$ archetypes. Interestingly, we observe that the Flickr request has a large number of outliers, meaning that some images tagged as “Paris” are actually unrelated to the city. Thus, we choose to use the robust version of archetypal analysis in order to reduce the influence of such outliers. We use similar heuristics for choosing $\varepsilon$ as in the robust statistics literature, resulting in $\varepsilon = 0.01$ for data points that are $l_2$-normalized.

Even though archetypes are learned in the space of Fisher vectors, which are not displayable, each archetype can be interpreted as a sparse convex combination of data points. In Figure 4 we represent some of the archetypes learned by our approach; each one is represented by a few training images with some proportions indicated in red (the value of the $\beta_j$’s). Classical landmarks appear in Figure 4a, which is not surprising since Flickr contains a large number of vacation pictures. In Figure 4b, we display several archetypes that we did not expect, including ones about soccer, graffiti, food, flowers, and social gatherings. In Figure 4c, some archetypes do not seem to have some semantic meaning, but they capture some scene composition or texture that are common in the dataset. We present the rest of the archetypes in the supplementary material, and results obtained for other requests, such as London or Berlin.

In Figure 5, we exploit the symmetrical relation between data and archetypes. We show for four images how they decompose onto archetypes, indicating the values of the $\alpha_i$’s. Some decompositions are trivial (Figure 5a); some others with high mean squared error are badly represented by the archetypes (Figure 5c); some others exhibit interesting relations between some “texture” and “architecture” archetypes (Figure 5b).

5. Discussions

In this paper, we present an efficient active-set strategy for archetypal analysis. By providing the first scalable open-source implementation of this powerful unsupervised learning technique, we hope that our work will be useful for applying archetypal analysis to various scientific problems. In particular, we have shown that it has promising applications in computer vision, where it performs as well as sparse coding for prediction tasks, and provides an intuitive visualization technique for large databases of natural images. We also propose a robust version, which is useful for processing datasets containing noise, or outliers, or both.

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References

(a) Archetypes representing (expected) landmarks.  
(b) Less expected archetypes.  
(c) Archetypes representing scene composition.

Figure 4: Some archetypes learned from 36 600 pictures corresponding to the request “Paris” downloaded from Flickr.

(a) Image with trivial interpretation.  
(b) Image with interesting interpretation.  
(c) Image with bad (non-sparse) reconstruction.

Figure 5: Decomposition of some images onto the learned archetypal set.