Robust Principal Component Analysis on Graphs

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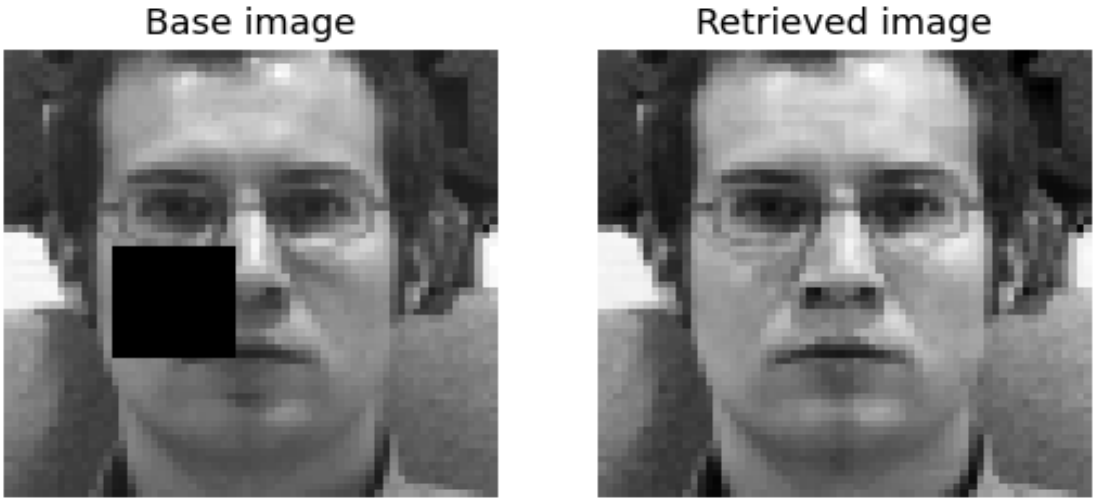

Figure 1: Low-rank reconstruction of corrupted images using the proposed method of [1].

1 ABSTRACT

Principal Component Analysis (PCA) is a very popular method for dimensionality reduction, and is used by thousands accross the world to provide 2D or 3D visualisations and insights about high-dimension data. It is used in a variety of different fields, such as image processing, finance, biology, and computer vision, to name only a few of them. In this work, we present a benchmark of different variants of PCA, which aim to tackle some of the issues of the original PCA algorithm that prevent it from being used in many real-life situations.

2 INTRODUCTION

As mentionned in the abstract, PCA is a useful tool for dimensionnality reduction. More specifically, given a matrix $X \in \mathbb{R}^{n \times p}$, it solves the following optimization problem:

$$\begin{aligned} \min_{Q,U} \quad & ||X - UQ^T||_F^2 \\ \text{subject to} \quad & Q^T Q = I \end{aligned}$$

where $||.||_F$ designates the Frobenius norm. It can be shown that this problem actually has a closed-form solution given by the principal components of X.

However, the main drawback of PCA is that it is very sensitive to noise, corrupted data and outliers and thus cannot be used in many real-world applications. The sensitivity to noise has been partially solved by the introduction of a robust variant of PCA, RPCA [3]. However, this algorithm is very slow on large datasets, which makes it impractical for many applications. This motivated the introduction of another PCA variant called GLPCA [2] which uses graph Laplacian regularization to improve the robustness of the algorithm while keeping the computational cost low. Finally, a third variant of PCA similar to the previous ones has been proposed by the authors of [1] to improve the robustness of the algorithm while keeping the computational cost low.

This project aims to provide a simple and efficient implementation of those main variants of the PCA algorithm, as well as a benchmark of those methods on different tasks (clustering and low-rank recovery for corrupted data on real-life and artificial datsets).

3 ALGORITHMS

In this section, we are going to present the algorithms we implemented and compared for the benchmark. We can divide them into two categories: factorized and non-factorized models. The first category regroups the original PCA algorithm and its variants which aim to learn two matrix factors U and Q such that $X \approx UQ$. Those models often have the constraint $Q^T Q = I$, which, in the case of the original PCA, can be understood as the orthonormality condition of the eigenvectors basis of $X^T X$. On the other hand, the second category regroups PCA variants which try to learn a low-rank matrix L such that $X = L + S$, where S is sparse. For example, the original PCA algorithm, as well as GLPCA and RGLPCA are factorized models, while RPCA and the new variant introduced in [1] are non-factorized models.

3.1 Classical PCA

We used Scikit-Learn implementation of PCA, which simply computes the SVD of X and creates a low-rank approximation by using the first k singular vectors of X.

3.2 Robust PCA

We implemented (see algorithm 1) the algorithm described in [3] using the ADMM [4] (Alternating Direction Method of Multipliers) and following as closely as possible the pseudo-code provided in the paper. This algorithm solves the following convex optimization problem:

$$\begin{aligned} \min_{L,S} \quad & ||L||_* + \lambda||S||_1 \\ \text{subject to} \quad & L + S = X \end{aligned}$$

where $||.||_*$ is the nuclear norm and $||.||_1$ is the ℓ_1 norm. This problem is solved iteratively by alterning between phases of optimization over L and over S.

3.3 Graph-Laplacian PCA (GLPCA)

We also implement the Graph-Laplacian PCA (GLPCA) method proposed by Jiang et. al. in [2]. In this method, the authors propose to use additional information about the data in the form of a graph $\mathcal{G}$ to perform the data dimensionality reduction.

The idea is to incorporate the graph Laplacian of $\mathcal{G}$ in the objective function of the PCA algorithm in the form of a regularization term. Here, the Laplacian embedding [**?**] is used as the regularization term.

The model obtained is,

$$\begin{aligned} &\min_{Q,U} ||X - UQ^T||_F^2 + \alpha Tr(Q^T(D-W)Q) \\ &\text{subject to } Q^TQ = I \end{aligned}$$

where D is the degree matrix of $\mathcal{G}$ and W is the adjacency matrix of $\mathcal{G}$.

A closed form solution is obtained by differentiating the objective function with respect to U and Q and setting the result to zero. The authors easily show that this leads to setting Q equal to the k smallest eigenvectors of the matrix,

$$G_\alpha = -X^TX + \alpha L,$$

where $L = D - W$ and setting $U = XQ$. To make the terms in G_α comparable, the authors propose a simple reformulation of the problem by introducing a new parameter β such that $\alpha = \frac{\beta}{1-\beta}\frac{\lambda_n}{\xi_n}$, where λ_n and ξ_n are the smallest eigenvalues of X^TX and $L = D-W$ respectively. The new problem can be written as,

$$\begin{aligned} &\min_{Q,U} TrQ^T\left[(1-\beta)(I - \frac{X^TX}{\lambda_n}) + \beta\frac{L}{\xi_n}\right]Q \\ &\text{subject to } Q^TQ = I \end{aligned}$$

A closed form solution for Q is obtained by solving for the k smallest eigenvectors of the matrix

$$G_\beta = (1-\beta)(I - \frac{X^TX}{\lambda_n}) + \beta\frac{L}{\xi_n}$$

and setting $U = XQ$.

3.4 Robust GLPCA (RGLPCA)

A robust version of the GLPCA (RGLPCA) is proposed in [**?**]. The authors propose to use almost the same objective function as GLPCA, but with a different norm for the PCA term. This new norm is the $L_{2,1}$ norm first introduced by Ding et. al. in [**?**] and defined by

$$||A||_{2,1} = \sum_{j=1}^{n}\sqrt{\sum_{i=1}^{p}A_{ij}^2}.$$

Ding et. al. show that this norm is more robust to outliers than the Frobenius norm since it is less sensitive to data points (rows of X) with unrealistic values (use of the L^1 norm between data points). They also show that this norm has better theoretical properties than the L^1 norm. For instance, it converses the rotational invariance property of the Frobenius norm (that is lost with the L^1 norm) and it directly relates to the covariance matrix of the data.

The RGLPCA model is obtained by solving the following optimization problem,

$$\begin{aligned} \min_{Q,U} \quad & ||X - UQ^T||_{2,1} + \alpha Tr(Q^T(D-W)Q) \\ \text{subject to} \quad & Q^TQ = I \end{aligned}$$

The Augmented Lagrangian Multiplier (ALM) method is used to solve this problem. The ALM is an iterative method that solves a sequence of minimization problems that depend on a Lagrange multiplier C and a penalty parameter μ, which are updated at each iteration. In the case of RGLPCA, the authors introduce $E = X - UQ^T$ and show that a sub-problem of the ALM method can be written as,

$$\begin{aligned} \min_{Q,U,E} \quad & ||E||_{2,1} + \alpha Tr(Q^TLQ) + \frac{\mu}{2}||E - X + UQ^T + \frac{C}{\mu}||_F^2 \\ \text{subject to} \quad & Q^TQ = I \end{aligned}$$

To solve a sub-problem, the authors propose to solve iteratively, for a fixed E,

$$\begin{aligned} \min_{Q,U} \quad & \frac{\mu}{2}||E - X + UQ^T + \frac{C}{\mu}||_F^2 + \alpha Tr(Q^TLQ) \\ \text{subject to} \quad & Q^TQ = I \end{aligned}$$

using the GLPCA method with $\tilde{X} = E - X + \frac{C}{\mu}$ and $\tilde{\alpha} = \frac{2\alpha}{\mu}$ (from which $\tilde{\beta}$ is then computed). Then, fixing Q and U, we solve for E,

$$\min_E \quad ||E||_{2,1} + \frac{\mu}{2}||E - X + UQ^T + \frac{C}{\mu}||_F^2$$

which solution is known to be,

$$e_i = \max(1 - \frac{1}{\mu||a_i||}, 0)a_i$$

where a_i is the i-th row of $X - UQ^T - \frac{C}{\mu}$. No justification of the validity of this decomposition method to solve the sub-problem is given in the paper. Finally, at the end of each iteration, the Lagrange multiplier C and the penalty parameter μ are updated as follows,

$$C = C + \mu(E - X + UQ^T)$$

$$\mu = \rho\mu.$$

3.5 RPCA on graphs

Finally, we implemented (see algorithm 4) the RPCA on graphs algorithm described in [1] which claims to be more robust than the previous ones while keeping the computational cost low. This algorithm solves the following convex optimization problem:

$$\begin{aligned} \min_{L,S} \quad & ||L||_* + \lambda||S||_1 + \gamma Tr(L\phi L^T) \\ \text{subject to} \quad & L + S = X \end{aligned}$$

Where ϕ is the graph Laplacian of $\mathcal{G}$ and γ is a hyperparameter of the algorithm. As the previous methods, it uses the ADMM [4] algorithm to solve this problem by alterning phases of optimization over L and over S.

4 EXPERIMENTAL SETUP

For the benchmark, we compared these algorithms on two different tasks: low-rank recovery for corrupted data and clustering. For the low-rank recovery task, we used the CMU PIE dataset which is a dataset of images of faces with different angles and lighting. For the clustering task, we used the AT&T dataset which is another dataset of images of faces.

4.1 Low-rank recovery for corrupted data

For this task, we used the PIE dataset, and more specifically 20 64×64 images of the same 40 people under different lighting with a constant camera angle, and corrupted them by adding a single random black block of 25% of the image dimensions to each sample. We then used the different algorithms to recover the concatenation of the original images from the concatenation of the corrupted ones. The main hypothesis here is that this long concatenation matrix will be well approximated by a low-rank matrix, since the difference in lighting and corruption is supposed to be sparse. We evaluated the different methods mostly by visual inspection of the results, but also by computing the mean squared error between the original and recovered images.

4.2 Clustering

For this task, we used the AT&T dataset, and more specifically 400 112×92 images aggregated in 40 equally sampled classes (each class corresponding to one individual). We then compute the low-rank approximation of the concatenation of the images, and used the resulting matrix as a feature matrix for clustering. We then evaluated the different methods by computing the labels produced by the KMeans algorithm trained on this feature matrix, and comparing them with the original labels of the dataset. We compared the different methods by computing the error between, as well as the Adjusted Rand Index (ARI) as well as the Normalized Mutual Information (NMI). These metrics can be easily computed given the confusion matrix and the raw labels:

$$ARI = 2\frac{TP \times TN - FN \times FP}{(TP + FN) \times (FN + TN) + (TP + FP) \times (FP + FN)}$$

$$NMI = \frac{I(y_{\text{true}}, y_{\text{pred}})}{\sqrt{H(y_{\text{true}}) \times H(y_{\text{pred}})}}$$

where TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives, FN is the number of false negatives, $I(y_{\text{true}}, y_{\text{pred}})$ is the mutual information between y_{true} and y_{pred}, and $H(y)$ is the entropy of y.

5 RESULTS

6 LIMITATIONS

7 CONCLUSION

8 APPENDIX

8.1 Pseudo-code

In order to make notations more concise, we will define the following shrinkage and singular value tresholding operators (defined on the space of square matrices):

$$\begin{cases} \mathcal{S}_\tau(\mathbf{Z}) = \text{sign}(\mathbf{Z}) \times \max(\mathbf{0}, |\mathbf{Z}| - \tau\mathbf{I}) \\ \mathcal{D}_\tau(\mathbf{Z}) = \mathbf{U}\mathcal{S}_\tau(\Sigma)\mathbf{V}^T \text{ with } \mathbf{Z} = \mathbf{U}\Sigma\mathbf{V}^T \end{cases}$$

Algorithm 1 RPCA algorithm

Require: $\mathbf{X} \in \mathbb{R}^{p \times n}$, ε, n_{iter}
  $\lambda \leftarrow \frac{1}{\sqrt{\max(m,n)}}$
  $\mu \leftarrow \frac{\max(m,n)}{4 \times ||\mathbf{X}||_1}$
  $\mathbf{S} \leftarrow \mathbf{0}$
  $\mathbf{Y} \leftarrow \mathbf{0}$
  for $i = 1$ **to** n_{iter} **do**
    $\mathbf{L} \leftarrow \mathcal{D}_\mu(\mathbf{X} - \mathbf{S} + \frac{1}{\mu}\mathbf{Y})$
    $\mathbf{S} \leftarrow \mathcal{S}_{\frac{\lambda}{\mu}}(\mathbf{X} - \mathbf{L} + \frac{1}{\mu}\mathbf{Y})$
    $\mathbf{Y} \leftarrow \mathbf{Y} + \mu(\mathbf{X} - \mathbf{L} - \mathbf{S})$
    if $||\mathbf{X} - \mathbf{L} - \mathbf{S}||_F \leqslant \varepsilon$ **then**
      break
    end if
  end for
  return L, S

Algorithm 2 GLPCA algorithm

Require: $\mathbf{X} \in \mathbb{R}^{p \times n}$, $\mathcal{G}$, β
  $\mathbf{W} \leftarrow adj(\mathcal{G})$
  $\mathbf{D} \leftarrow diag(\{d_1, d_2, ..., d_{n_{\text{nodes}}}\})$
  $\mathbf{L} \leftarrow \mathbf{D} - \mathbf{W}$
  $\lambda_n \leftarrow \Re(\max(eigenval(\mathbf{X}^T\mathbf{X})))$
  $\xi_n \leftarrow \Re(\max(eigenval(\mathbf{L})))$
  $\mathbf{G}_\beta \leftarrow (1 - \beta)(\mathbf{I} - \frac{1}{\lambda_n}\mathbf{X}^T\mathbf{X}) + \frac{\beta}{\xi_n}\mathbf{L}$
  $\mathbf{Q} \leftarrow \Re(eigenvect(\mathbf{G}_\beta))$
  $\mathbf{U} \leftarrow \mathbf{X}\mathbf{Q}$
  return Q, U

Algorithm 3 RGLPCA algorithm

Require: $\mathbf{X} \in \mathbb{R}^{p \times n}$, $\mathcal{G}$, β, k, ρ, n_{iter}
  $\mathbf{X}_0 \leftarrow \mathbf{X}$
  $\beta_0 \leftarrow \beta$
  $\mathbf{E} \leftarrow \mathbf{1}$
  $\mathbf{C} \leftarrow \mathbf{1}$
  $\mu \leftarrow 1$
  $\mathbf{W} \leftarrow adj(\mathcal{G})$
  $\mathbf{D} \leftarrow diag(\{d_1, d_2, ..., d_{n_{\text{nodes}}}\})$
  $\mathbf{L} \leftarrow \mathbf{D} - \mathbf{W}$
  $\xi \leftarrow \Re(max(eigenval(\mathbf{X}_0^T \mathbf{X}_0)))$
  for $i = 1$ **to** n_{iter} **do**
    $\mathbf{X}_i \leftarrow \mathbf{X} - \mathbf{E} - \frac{1}{\mu}\mathbf{C}$
    $\lambda \leftarrow \Re(\max(eigenval(\mathbf{X}_i^T \mathbf{X}_i)))$
    $\alpha \leftarrow \frac{2\beta_0 \lambda}{\mu(1-\beta_0)\xi}$
    $\beta \leftarrow \frac{\alpha\xi}{\lambda + \alpha\xi}$
    $\mathbf{Q}, \mathbf{U} \leftarrow GLPCA(\mathbf{X}, \mathcal{G}, \beta, k)$
    $\mathbf{A} \leftarrow \mathbf{X}_k - \mathbf{U}\mathbf{Q}^T - \frac{1}{\mu}\mathbf{C}$
    $\mathbf{a} \leftarrow (||\mathbf{A}_1||_2, ||\mathbf{A}_2||_2, ..., ||\mathbf{A}_m||_2)$
    $\mathbf{E} \leftarrow \mathcal{S}_{\frac{1}{\mu}}(\mathbf{a})$
    $\mathbf{C} \leftarrow \mathbf{C} + \mu(\mathbf{E} - \mathbf{X} - \mathbf{U}\mathbf{Q}^T)$
    $\mu \leftarrow \rho\mu$
  end for
  return $\mathbf{Q}$, $\mathbf{U}$, $\mathbf{E}$

Algorithm 4 RPCA on graphs algorithm

Require: $\mathbf{X} \in \mathbb{R}^{p \times n}$, $\mathcal{G}$, n_{iter}, γ, ε
  $\mathbf{A} \leftarrow adj(\mathcal{G})$
  $\mathbf{D} \leftarrow diag(\{d_1, d_2, ..., d_{n_{\text{nodes}}}\})$
  $\boldsymbol{\phi} \leftarrow D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$
  $\lambda \leftarrow \frac{1}{\sqrt{\max(p,n)}}$
  $\mathbf{L} \leftarrow random(p, n)$
  $\mathbf{W} \leftarrow random(p, n)$
  $\mathbf{S} \leftarrow random(p, n)$
  $r_1 \leftarrow 1$
  $r_2 \leftarrow 1$
  $\mathbf{Z}_1 \leftarrow \mathbf{X} - \mathbf{L} - \mathbf{S}$
  $\mathbf{Z}_2 \leftarrow \mathbf{W} - \mathbf{L}$
  for $i = 1$ **to** n_{iter} **do**
    $\mathbf{H}_1 \leftarrow \mathbf{X} - \mathbf{S} + \frac{1}{r_1}\mathbf{Z}_1$
    $\mathbf{H}_2 \leftarrow \mathbf{W} + \frac{1}{r_2}\mathbf{Z}_2$
    $\mathbf{H} \leftarrow \frac{1}{r_1 + r_2}(r_1\mathbf{H}_1 + r_2\mathbf{H}_2)$
    $\mathbf{L} \leftarrow \mathcal{D}_{\frac{2}{r_1+r_2}}(\mathbf{H})$
    $\mathbf{S} \leftarrow \mathcal{S}_{\frac{\lambda}{r_1}}(\mathbf{X} - \mathbf{L} + \frac{1}{r_1}\mathbf{Z}_1)$
    $\mathbf{W} \leftarrow r_2(\gamma\boldsymbol{\phi} + r_2\mathbf{I})^{-1}(L - \frac{1}{r_2}Z_2)$
    $\mathbf{Z}_1 \leftarrow \mathbf{Z}_1 + r_1(\mathbf{X} - \mathbf{L} - \mathbf{S})$
    $\mathbf{Z}_2 \leftarrow \mathbf{Z}_2 + r_2(\mathbf{W} - \mathbf{L})$
    if $||\mathbf{X} - \mathbf{L} - \mathbf{S}||_F \leqslant \varepsilon$ **then**
      break
    end if
  end for
  return $\mathbf{L}$, $\mathbf{S}$

8.2 Figures

REFERENCES

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