About Recent Work on Sparse PCA with Applications

A short introduction

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The Standard PCA

Principal components analysis (PCA) (Jolliffe 1986) is a classical method for the dimension reduction of data in the form of n observations of a vector with p variables.
Consider feature matrix $X \in \mathbb{R}^{n \times p}$, let $X \leftarrow X - \mu$, do SVD on X that

$$X = UDV^T \tag{1}$$

Therefore, $Z = UD$ are principle components (PCs) and the columns of V are corresponding loadings of the principal components.

Problems in standard PCA:

- When p is comparable or dominates n (say, $p > n$), standard PCA is not consistent
- Each principal component is a linear combination of all the original variables and the loadings are typically nonzero, thus it is often difficult to interpret the results (derived PCs)[2]

Sparse Approximations

Zou, Hastie and Tibshirani (2006)[4],base on work of d'Aspremont (2005)[1] showed how PCA can be converted to a (naïve) elastic-net regression problem. They gave the following theorem:

Theorem 1

For each i, denote by $Z_i = U_i D_{ii}$ the ith principal component. Then $\hat{\beta}_{en}$ given by

$$\hat{\beta}_{\text{en}} = \arg\min_{\beta} \|Z_i - X\beta\|^2 + \lambda_2\|\beta\|^2 + \lambda_1\|\beta\|_1 \tag{2}$$

$\hat{V}_i = \hat{\beta}_{\text{en}}/\|\hat{\beta}_{\text{en}}\|, X\hat{V}_i$ are approximations to V_i and principal component.

Remark

Lasso: Need $n \geq k$ where k is a given amount of PCs, produces sparsity.
Elastic-Net: When $p > n$, choose some $\lambda_2 > 0$, then we can include all variables in the fitted model[3].

Sparse Approximations

Theorem 2

For any $\lambda > 0$, suppose we are considering the first k PCs, Let x_i be the ith row vector, $A_{p\times k} = [\alpha_1, \dots, \alpha_k]$ orthonormal, and $B_{p\times k} = [\beta_1, \dots, \beta_k]$, then

$$(\hat{A}, \hat{B}) = \arg\min_{A,B} \sum_{i=1}^{n} \|x_i - AB^T x_i\|^2 + \lambda \sum_{j=1}^{k} \|\beta_j\|^2 + \sum_{j=1}^{k} \lambda_{1,j} \|\beta_j\|_1, s.t. A^T A = I_{k\times k}.$$

Then $\hat{\beta}_j = cV_j, j = 1, 2, \dots, k$ where c is a constant.

It effectively transform the PCA into a regression-type problem. However, this theorem uses lasso to fit A, B, which constrains k.

An Algorithm to Minimize SPCA Criterion

1. B given A: For each j, let $Y_j^* = X\alpha_j$, then each elastic-net estimator

$$\begin{aligned}\hat{\beta}_j &= \arg\min_{\beta} \sum_{i=1}^{n} \|Y_j^* - X\beta_j\|^2 + \lambda\|\beta_j\|^2 + \lambda_{1,j}\|\beta_j\|_1 \\ &= \arg\min_{\beta} (\alpha_j - \beta)^T X^T X(\alpha_j - \beta) + \lambda\|\beta\|^2 + \lambda_{1,j}\|\beta\|_1\end{aligned} \tag{3}$$

2. A given B: Do SVD

$$X^T XB = UDV^T \tag{4}$$

set estimator $\hat{A} = UV^T$.

Algorithm 1 General SPCA Algorithm

1: Let A start at V[,1:k] which are loadings of the first k ordinary PCs.

2: Given a fixed $A = [\alpha_1, \dots, \alpha_k]$, solve the following elastic-net for $j = 1, 2, \dots, k$

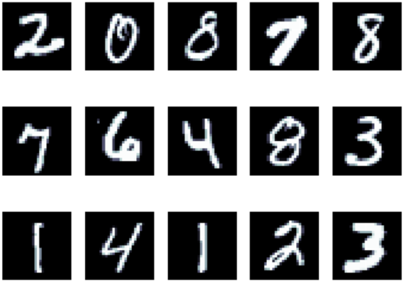
$$\beta_j = \arg\min_{\beta} (\alpha_j - \beta)^T X^T X(\alpha_j - \beta) + \lambda\|\beta\|^2 + \lambda_{1,j}\|\beta\|_1$$

3: For a fixed $B = [\beta_1, \dots, \beta_k]$, compute the SVD of $X^T XB$, then update $A = UV^T$.

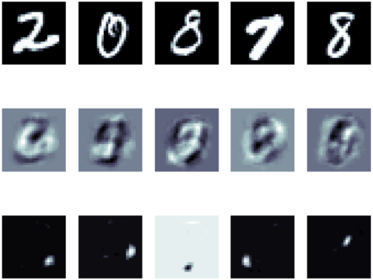
4: Repeat Steps 2-3, until convergence or the maximum number of iterations.

5: Normalization: $\hat{V}_j = \beta_j/\|\beta_j\|, j = 1, \dots, k$.

Handwritten digit recognition. Use the MNIST dataset, $28 \times 28 = 784$ pixels (features) for each picture. Set $n = 100, k = 50$. Perform both PCA and SPCA on the selected data.



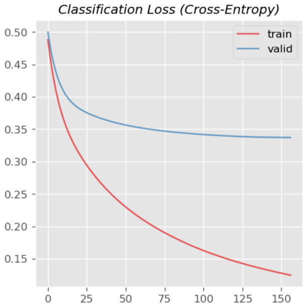
(a) Handwritten digit



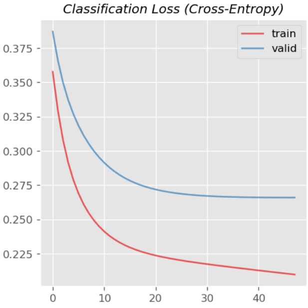
(b) PCA loadings, SPCA loadings

Figure: Comparison between loadings in PCA and SPCA

Numerical Experiment



(a) PCA



(b) SPCA

Figure: Comparison between classification error in PCA and SPCA

Preprocessing Method	Validation Error
PCA	0.337
SPCA	0.266

Reference

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