The Stochastic Complexity of Principal Component Analysis

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Abstract—PCA (principal component analysis) and its variants are ubiquitous techniques for matrix dimension reduction and reduced-dimension latent-factor extraction. For an arbitrary matrix, they cannot, on their own, determine the size of the reduced dimension, but rather must be given this as an input. NML (normalized maximum likelihood) is a universal implementation of the Minimal Description Length principle, which gives an objective compression-based criterion for model selection.

This work applies NML to PCA. A direct attempt to do so would involve the distributions of singular values of random matrices, which is difficult. A reduction to linear regression with a noisy unitary covariate matrix, however, allows finding closed-form bounds on the NML of PCA.

Index Terms—minimum description length, normalized maximum likelihood, principal component analysis, unsupervised learning, model selection

I. INTRODUCTION

Let $X$ be an $n \times m$ matrix (we will focus on long and narrow matrices, for which $n \gg m$). In machine learning, it is very common to approximate it by a “simpler” product of matrices $W$ and $Z^T$ of lower dimensions $n \times k$ and $k \times m$, respectively (for $k \leq m$). Among others, these include probabilistic principal component analysis, independent-factor analysis, and non-negative matrix factorization (see [11], [18], [2]). We will focus specifically on the simple PCA (principal component analysis),

$$\arg \min_{W,V : \text{rank}(W) = \text{rank}(V) = k} \|X - WZ^T\|_F^2. \quad (1)$$

The lower-dimension product is not guaranteed to losslessly approximate the original matrix. In fact, the famous Eckart-Young-Mirsky Theorem - whose properties we will use throughout - essentially guarantees some loss:

**Theorem 1. (Eckart-Young-Mirsky)** Let $X = U\Lambda V^T$ be the SVD (singular value decomposition) of $X$, with $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)$, and $U$ and $V$ unitary. Let $U_k$ and $V_k$ be the matrices of the first $k$ columns of $U$ and $V$, respectively. Then

$$\|X - WZ^T\|_F^2 \geq \|X - U_k \text{diag}(\lambda_1, \ldots, \lambda_k) V_k\|_F^2 = \sum_{i=k+1}^m \lambda_i^2, \quad (2)$$

and so $W = U_k \text{diag}(\lambda_1, \ldots, \lambda_k), Z = V_k, is optimal$.

The motivation for the reduced dimension is uncovering a structure that is, in some sense, “truer”, or “more useful”. As the theorem shows, though, loss minimization, in itself, will not lead us to the reduced dimension.

One approach for this type of problem - the MDL (minimum description length) approach - uses compression as a way to select from among such models (see the Related Works part later). In particular, the following NML (normalized maximum likelihood) minimizes the worst-case expected description regret relative to a fixed class of codes (see [17], [1]):

**Definition 1. Normalized Maximum Likelihood** Let $X$ be distributed by a model specified by some parameter(s) $\Phi$. The NML is defined as

$$f_{\text{NML}}(X) = \frac{f(X; \hat{\Phi}(X))}{\int f(Y; \hat{\Phi}(Y))dY}, \quad (3)$$

where

- $\hat{\Phi}(X)$ is the maximal likelihood (ML) estimator of $\Phi$ given $X$.
- $f(X; \hat{\Phi}(X))$ is the ML of $X$ assuming that the true parameters are $\hat{\Phi}(X)$.

The logarithm of the right-hand side of equation (3) is the stochastic complexity, and the logarithm of its numerator is the parametric complexity.

In the rest of the paper, we prove the following theorem:

**Theorem 2.** Let $s(X : k)$ be the stochastic complexity of a $k$-dimensional PCA reduction of $X$. Then

$$2s(X : k) \leq (nm - kn) \ln \left( \sum_{i=k+1}^m \frac{\lambda_i^2}{nm} \right) + nk \ln \left( \|X^TX\|_F^2 \right)$$

$$+ (mn - kn - 1) \ln \left( \frac{mn}{mn - kn} \right) - (nk + 1) \ln(nk) + \Delta s,$$

where

$$-nk\epsilon^2 \|X^TX\|_F^2 \leq \Delta s \leq nk\epsilon^2 \|X^TX\|_F^2 + nk \ln \left( \frac{2\epsilon}{\sqrt{\epsilon}} \right). \quad (5)$$
Outline We continue this section with definitions and notations, and related work. Section [II] shows the main idea of reducing the problem to the NML of linear regression via elimination of some of the optimization parameters. Section [III] details the specific reductions. Section [IV] shows numerical experiments. Section [V] concludes and discusses further work.

Definitions and Notations We will use lowercase letters (s) for scalars, underlined lowercase letters (±) for column vectors, uppercase letters (X) for matrices, and calligraphic (B) for sets. A single subscript for a matrix denotes a matrix row (Xi). f(x), f(x; y), f(x | y) denote the density of some x, the density of some x assuming some other parameter is y, and the density of some x conditional on some other random variable being y, respectively. ||X||F = (Σi,jX2i,j)1/2 is the Forbenius norm, and D(x | y) is the Kullback-Leibler distance.

Related Work [2], [18] contain excellent overviews of matrix factorization. In particular, PCA appears in the classic [6], [14], [10], [17], [8], [9], [1] describe MDL and NML, in particular, for model selection. [16] uses cross validation approximations for PCA dimension estimation, and [3] does so using an analysis of the conditional distribution of the singular values of a Wishart matrix. To the best of my knowledge, there are no works on NML forms for PCA.

II. MAIN IDEA

To formulate expression (1) for NML, we can use the generative model shown in the factor diagram (see [3]) in Figure 1. In this model, k ∼ U(1, m) determines the dimension of Wk and Vk, X = WkVkT + Υ, where Υ ∼ N(0, τIκ). Note that they do not appear in the original problem (at least in this form). The distribution of k hardly affects the stochastic complexity, and any distribution assigning a positive probability to any value of 1, . . . , m could be used. Regarding the Gaussian additive noise Υ,

\[ \text{arg max}_{W_k, V_k} f(X; k) = \text{arg max}_{W_k, V_k} \frac{1}{(2\pi)^{n/2}} e^{-\frac{||X-W_kV_k^T||^2}{2\tau^2}} \]

(6)

where (a) follows from Theorem 1. It is thus just a convenient construct, therefore.

While it is conceptually possible to calculate the NML of PCA by inserting equation (6) into equation (3), but the denominator requires integrating over the eigenvalues of arbitrary matrices, which is difficult. Instead, consider the problem in Figure 3 (discussed in greater detail in Section III), where both the number of parameters and the loadings matrix are known. This simpler problem is more similar to linear regression, whose NML has a closed form (see [16]). Of course, in the original problem, the loadings matrix is not known, but rather requires optimization as well. The following lemma, however, relates the NML of a problem depending on a number of parameters, to the same problem where one of them is fixed.

Fig. 1. Equivalent factor graph of PCA. The dimension k is a-priori uniform, and the observed matrix X is the product of the score and loadings matrices, with additive noise Υ distributed i.i.d. N(0, τIk).

Fig. 2. Parametric complexity using only a subset of the features. For each X, there are an optimal A(X) and b(x), but we wish to bound this by expressions in which for each X, b is constant.

Lemma 1. Let \( \mathcal{B} = \{b_1, \ldots, b_\ell\} \) be a finite set (for some \( \ell \)). Then

\[ \int \hat{f}(X | A(X), b(X)) dX \leq \sum_{b \in \mathcal{B}} \int \hat{f}(X | A(X), b) dX. \]

(7)

Furthermore, if

\[ \hat{b}(x) = \arg \min_b \hat{f}(X | A(X), b), \]

then

\[ \int \hat{f}(X | A(X), \hat{b}(X)) dX \geq \max_{b \in \mathcal{B}} \int \hat{f}(X | A(X), b) dX. \]

(9)
Proof. For inequality (7)

\[ \int f(X | \hat{A}(X), \hat{b}(X)) dX = \sum_b \int_{X: \hat{b}(X) = b} f(X | \hat{A}(X), \hat{b}) dX \]

where (a) follows from condition (8). Since this is true for horizontal level. Corresponds to moving the disks until they are at the same
Figure 2, this corresponds to bounding by considering the sum of all planes, then slicing them by vertical levels.

For inequality (9), consider an arbitrary \( b' \in B \). Then

\[ \int f(X | \hat{A}(X), \hat{b}(X)) dX = \sum_{b: \hat{b}(X) = b} \int f(X | \hat{A}(X), \hat{b}) dX \]

where (a) follows from the non-negativity of densities. In Figure 3, this corresponds to bounding by considering the sum of all planes, then slicing them by vertical levels.

\[ \max_{i \in \{1,...,|V_k|\}} \frac{K_i(X; k)}{s(X; k)} \leq \frac{\sum_{i=1}^{\frac{|V_k|}{2}} [s_i(X; k)]}{\frac{|V_k|}{2}} \]

Furthermore, we will see in Appendix A the following lemma:

**Lemma 2.**

\[ \ln \left( |V_k| \right) \leq mk \ln \left( \frac{2}{\epsilon + 1} e^{-\left( \frac{1 + \epsilon + \frac{\epsilon^2}{2}}{\epsilon} \right)} \right) + (k - 1) \ln \left( \frac{\epsilon + \frac{m^2}{\pi}}{\pi} \right) \]

Let \( V_k^\epsilon \), a known quantized loadings matrix, be the \( i \)th item in \( V_k^\epsilon \). To calculate its NML, note that Figure 3 is very similar to linear regression (whose NML is known), except that \( W_k \) and \( X \) are matrices instead of vectors. This can be easily remedied, though, by considering the problem

\[ \hat{x} = V_k^\epsilon \hat{w} + \hat{v} \]

where \( \hat{v} \) and \( \hat{w} \) each have length \( nm \), \( \hat{V}_k^\epsilon \) is \( mn \times kn \), and \( \hat{w} \) has length \( km \). This is the dashed part of Figure 3 and has known NML (see equation (19) in [16])

\[ s_i^\epsilon(X; k) = \left( nm - kn \right) \ln (\hat{\tau}) + nk \ln \left( \| \hat{V}_k^\epsilon \hat{w} \|_F^2 \right) + (nm - kn - 1) \ln \left( \frac{\text{mm}}{mn - kn} \right) - (nk + 1) \ln (nk) \]

**III. THE REDUCTIONS**

Let \( v_{i,j} \) be the elements of the unitary matrix \( V \) from Theorem 1. By the Cauchy-Schwartz Inequality, \(|v_{i,j}| \leq 1\). Let \( \epsilon \leq \frac{1}{m} \) be a number such that \( \frac{1}{\epsilon} \) is an integer. We can quantize \( v_{i,j} \), into one of \( \frac{1}{\epsilon} + 1 \) entries, each distance \( \epsilon \) from each other, resulting in the matrix \( V' \). It is simple to see from Theorem 1 that this quantization alters the objective in expression (11) by at most \( \epsilon^2 \).

Tolerating this relaxation, therefore, and using Lemma 1, we can reduce the original problem to that in Figure 3 where

\[ \frac{\epsilon}{W} \]

\[ \frac{\epsilon}{V} \]

\[ \frac{\epsilon}{U} \]

\[ \frac{\epsilon}{W} \]

\[ \frac{\epsilon}{V} \]

\[ \frac{\epsilon}{U} \]

\[ \frac{\epsilon}{W} \]

\[ \frac{\epsilon}{V} \]

\[ \frac{\epsilon}{U} \]
However, we need the NML to be expressed in terms from the original problem.

It is well known (see [11]) that

$$\hat{w} = \begin{bmatrix} (V_k^T V_k)^{-1} V_k^T X_1^T \\ \vdots \\ (V_k^T V_k)^{-1} V_k^T X_n^T \end{bmatrix}.$$ 

Furthermore, for the $j$th range,

$$\hat{W}_j = (V_k^T V_k)^{-1} V_k^T X_j^T 
\simeq (I_k + \epsilon (V_k^T E + E^T V_k))^{-1} V_k^T X_j^T 
\simeq (I_k - \epsilon (V_k^T E + E^T V_k)) V_k^T X_j^T,$$

where (a) follows from [15] equation (191). Therefore,

$$(V_k + \epsilon E) \hat{W}_j \simeq (I_k - \epsilon (V_k^T E + E^T V_k)) X_j^T,$$

and, finally,

$$\left| \ln \left( \frac{\|V_k^T \hat{w}_j\|^2}{F} \right) - \ln \left( X_j^T X_j \right) \right| \lessapprox \epsilon^2.$$ (13)

We now prove Theorem 2.

Proof. In equation (12), we replace $\hat{\tau}$ using Theorem 2 and $\hat{V}_k \hat{w}$ using equation (13). We use the resulting expression - which is independent from $i$ (the element of $V_k^i$) - in Lemma 1.

IV. Numerical Experiments

For numerical experiments we use the Dow-Jones Industrial Index (DJIA), with up to one year of 30 closing prices. We transform the $i,j$th entry, $c_{i,j}$ denoting the closing price of stock $j$ at day $i$, to $100 \frac{c_{i,j} - c_{i,j-1}}{c_{i,j-1}}$, i.e., the relative closing price in percentage [19]). In the following, Orig is this matrix; Lin5 is a matrix whose first 5 columns are the original ones, and the last 25 are a random linear combination of the first 10; with $N(0, 0.1)$ noise added; Lin10 is the same, but with the last 20 generated from the first 10.

Figure [5] shows the Scree plots for the three datasets. The optimal dimensions are not apparent from them. Nevertheless, Figure [6] shows that the relative difference between the bounds from Theorem 2 are small, and Figure [7] shows the optimal $k$ lower and upper bounds as a function of $n$.

V. Conclusions and Future Work

In this work we used an NML-calculation technique based on reducing a problem, through eliminating some of its
original dimensions. We used this to bound the NML of PCA. The simple technique is general, and might be applicable to problems in other domains. In some cases (e.g., probabilistic principal component analysis, independent latent factor analysis, decompositions to low-dimension plus sparse, etc.), closed solutions are not known even for the simpler, reduced, problem. The numerical properties of the algorithms, in conjunction with an MCMC approximation for the parametric complexity, could be used to efficiently calculate the NML numerically; this remains a topic for further work.

APPENDIX

A. Number of Quantized Unary Matrices

We prove here Lemma 2. Let \( v_i, v_j \) be two columns of a unitary matrix (perhaps the one), and \( v_i', v_j' \) be their quantized counterparts. Simple arithmetic shows that

\[
|v_i' \cdot v_j' - v_i \cdot v_j| \leq \epsilon + \frac{m\epsilon^2}{4}.
\]

We will see that

\[
P \left( |v_i' \cdot v_j' - v_i \cdot v_j| \leq \epsilon + \frac{c^2}{4} \right) 
\]

\[
\leq \epsilon - m \left( \frac{1+\epsilon+c^2}{\pi} \right)^{k-1},
\]

where \( (a) \) follows from the Taylor series of \( \sin \) (see [4], Chapter 5). Using the well-known bound (see [3], Chapter 5),

\[
D \left( x \mid y \right) \geq \frac{(x-y)^2}{2y}, \quad (x \leq y)
\]

and \( (a) \) follow from the Chernoff bound (see [13], Chapter 5).

For the second part of inequality (15), applying inequality (14) twice on the left side, and once on the right side, we have

\[
\frac{|v_i' - v_i|}{\sqrt{m}} \leq \sqrt{\frac{1+\epsilon+c^2}{\sqrt{m}}}
\]

where \( (a) \) and \( (b) \) follow from the Taylor expansion of \( (1+x)^n \).

The events in these probabilities are necessary (although not sufficient) conditions.

\[
P \left( \sum_{k=1}^{m} \left| (v_i'k)^2 \right| \leq 1 + \epsilon + \frac{m\epsilon^2}{4} \right) 
\]

\[
\leq \epsilon - m \left( \frac{1+\epsilon+c^2}{\sqrt{m}} \right)^{k-1},
\]

\[
(1+\epsilon+c^2) \left( \frac{1}{\sqrt{m}} - 1 \right)^2 \geq \left( \frac{1+\epsilon+c^2}{\sqrt{m}} \right)^2 - \frac{1}{\sqrt{m}}\leq \frac{1+\epsilon+c^2}{\sqrt{m}}
\]

where \( (a) \) and \( (b) \) follow from the Taylor expansion of \( (1+x)^n \).

For the second part of inequality (15), applying inequality (14) twice on the left side, and once on the right side, we have

\[
\frac{|v_i' - v_i|}{\sqrt{m}} \leq \sqrt{\frac{1+\epsilon+c^2}{\sqrt{m}}}
\]

The proofs for the second part of inequality (15).

\[
\left( \frac{1+\epsilon+c^2}{\sqrt{m}} \right)^2 \geq \left( \frac{1+\epsilon+c^2}{\sqrt{m}} \right)^2 - \frac{1}{\sqrt{m}}\leq \frac{1+\epsilon+c^2}{\sqrt{m}}
\]

where \( (a) \) and \( (b) \) follow from the Taylor expansion of \( (1+x)^n \).

\[
\frac{|v_i' - v_i|}{\sqrt{m}} \leq \sqrt{\frac{1+\epsilon+c^2}{\sqrt{m}}}
\]

The references for the second part of inequality (15).