Maximum Likelihood Estimation in Principal Component Analysis with Noise Perturbation: a Gaussian Model.

by M.S Keane* and J.L Philoche**

Abstract

In Principal Component Analysis, an estimation of a parametrized gaussian model with noise is investigated. We define an estimate that relies only on the explanatory variables: the M.L. estimate.

1 Introduction and main Theorem

The estimation of mean and covariants by maximum likelihood (M.L.E.) out of an i.i.d. sample of Gaussian random vectors has been treated extensively in the literature since the pioneering work of Anderson (1963), and later Muirhead (1982), etc. It turns out that part of these results are only available through delicate combinatorial or insufficiently explicited arguments which give little insight with respect to the mathematical structure of the problem.

One of the purposes of this paper is to present an alternative approach to this question. By doing so, we provide some improvements with respect to both theorem formulations and proofs.

In many situations, n independent observations are taken on p correlated variables with, of course, $n > p$. Let $Y \in \mathbb{R}^p$ be gaussian $\mathcal{N}_p(\mu, \Sigma)$; the parameters μ and Σ being unknown. We assume that the q largest eigenvalues of Σ are distinct (of course $q < p$), and that the remaining $(p-q)$ eigenvalues are equal and non null.

Interpretation: the q explanatory variables are associated to the q greatest eigenvalues, the noise corresponding to the smallest (multiple) eigenvalue.

Denoting by $(\lambda_i)_{1\leq i\leq p}$ the eigenvalues of Σ, we look for the M.L.E of μ and Σ satisfying:

$$\lambda_1 > \lambda_2 > \cdots \lambda_q > \lambda_{q+1} = \cdots = \lambda_p > 0 \ . \qquad (1)$$

So we are dealing with a situation with a noise.

Among other tools, the proof of Theorem 1 relies on methods of differential geometry. Part (II) of Theorem 1 provides a concrete way for computation of this maximum likelilood out of the data. Theorem 2 gathers the technical tools for the proof of Theorem 1.

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We prove a Theorem which gives in particular the M.L.E of μ and Σ, satisfying (1); the data are $y_1, y_2, \cdots, y_n$, i.i.d. from $\mathcal{N}_p(\mu, \Sigma)$, the density of $y = (y_1, y_2, \cdots, y_n)^\top$ is:

$$(2\pi)^{-n/2}[(\det(\Sigma))^{-n/2}] \exp[-\frac{1}{2}(y-\mu)^\top \Sigma^{-1}(y-\mu)],$$

up to multiplicative an positive constants, the loglikelihood is:

$$\mathcal{L}_n(\mu, \Sigma) = -\ln[\det(\Sigma)] - \mathrm{Tr}(S\Sigma^{-1}) - \langle \overline{y} - \mu, \Sigma^{-1}(\overline{y} - \mu) \rangle, \tag{2}$$

with $\overline{y} := \frac{1}{n}\sum_{i=1}^{n} y_i$, the empirical mean; and $S := \frac{1}{n}\sum_{i=1}^{n}(y_i - \overline{y})(y_i - \overline{y})^\top$, the empirical covariance operator. Since, $\langle \overline{y} - \mu, \Sigma^{-1}(\overline{y} - \mu) \rangle \geq 0$, with equality iff $\mu = \overline{y}$; *for any fixed* Σ, $\mathcal{L}_n(\mu, \Sigma)$ has a unique maximum: $\widehat{\mu} = \overline{x}$. Therefore one has to find the maximum of the function L, for $\Sigma \in \mathcal{U} \subset \mathcal{M}^+$, the subset $\mathcal{U}$ being defined by (1), and $L(\Sigma) := -\ln(\det(\Sigma)) - \mathrm{Tr}(S\Sigma^{-1})$. Here $\mathcal{M}^+$ denotes the set of symmetric and positive definite operators. It is clear that the eigenvalues of S are distinct (a.s), we denote them by $s_1 > s_2 > \cdots s_p > 0$.

Theorem 1 *(I) On $\mathcal{U}$, L attains a maximum for a unique $\widehat{\Sigma}$ characterized by (i) and (ii):*

(i) the q greatest eigenvalues of $\widehat{\Sigma}$ are the same as the corresponding ones in S: $\widehat{\lambda}_j = s_j$, $(1 \leq j \leq q)$, with (resp.) the same eigendirections.

(ii) the $(p-q)$ smallest eigenvalues $\widehat{\lambda}_j$ (of $\widehat{\Sigma}$), $(q+1 \leq j \leq p)$ are equal to:

$$\widehat{\lambda} = \frac{1}{p-q} \sum_{k=q+1}^{p} s_k \; ;$$

here the eigenspace is the subspace orthogonal to all eigendirections of (i),

(II) Moreover, any maximizing sequence: $[i.e\{\Sigma_n \in \mathcal{U}\}_{n\in\mathbb{N}} \; ; \lim_{n\to\infty} L(\Sigma_n) = L(\widehat{\Sigma})]$ converges to $\widehat{\Sigma}$.

Remark: Part (II) of Theorem 1 provides an algorithm which gives a concrete way for the computation of the M.L.E. out of the data.

2 Biographical comments

Theorem 1 appears already in the literature [7] with a different proof, though not entirely explicit. In [9] the author mentions that this theory does not hold, when some of the λ_i are equal, nevertheless he guesses the correct result without proof. In [1], 11.3, the situation is quite similar to what is done in [7] ; but the situation seems better settled ; in [2], Theorem 2, T.W. Anderson gives a rather technical combinatorial proof of Theorem 1, (I).

The proofs of theorem 1 part (I) given [1], [2], [7] and [9] cannot give any direct proof of our Theorem 1 part (II).

In the following, it is convenient to use a change of variables, setting $\Theta = \Sigma^{-1}$,. $\mathcal{V} := \{\Theta \in \mathcal{M}^+ \; ; \Theta^{-1} \in \mathcal{U}\}$, $F(\Theta) := L(\Theta^{-1})$, so $F(\Theta) = \ln(\det\Theta) - \mathrm{Tr}(S\Theta)$.

3 Existence of a maximum

Lemma 1 *(Existence of a maximum) Let $\overline{\mathcal{V}}$ the closure of $\mathcal{V}$ in $\mathcal{M}^+$, the function F reaches a maximum on $\overline{\mathcal{V}}$.*

Proof We establish that F tends to $-\infty$, as Θ tends to ∞ on $\mathcal{M}^+$, i.e that for every $a \in \mathbf{R}$, $\{\Theta \in \mathcal{M}^+ ; F(\Theta) \geq a\}$ is compact, so F admits a maximum on every closed set ($\neq \emptyset$) of $\mathcal{M}^+$, [particulary on the $\overline{\mathcal{W}}_{\mathbf{k}}, (\mathbf{k} \in K)$, introduced below].

(*i*) on one hand, $\mathrm{Tr}(S\Theta) \geq \dfrac{\|\Theta\|}{\|S^{-1}\|}$:

In fact, let $\Theta = \sum_{j=1}^{p} \rho_j Q_j$ a representation of Θ, where the Q_j are orthogonal projectors of rank 1, and $\rho_p \geq \rho_j > 0$, $(j \leq p)$.
As $\rho_p = \|\Theta\|$, and S is positive, $\mathrm{Tr}(SQ_j) \geq 0$, thus:

$$\begin{aligned} \mathrm{Tr}(S\Theta) &\geq \rho_p \mathrm{Tr}(SQ_p) \\ &\geq \rho_p \min\{\mathrm{Tr}(SQ);\ Q \text{ orthogonal projector, with } \mathrm{rk}(Q) = 1\}\ ; \end{aligned}$$

the minimum is reached for Q projector on the subspace of S corresponding to the smallest eigenvalue: $s_p = \|S^{-1}\|^{-1}$;
on the other hand $\ln(\det\Theta) \leq p \ln \|\Theta\|$, therefore $F(\Theta) \to -\infty$, as $\|\Theta\| \to \infty$.

(*ii*) As ρ_1 is the smallest eigenvalue of Θ, so $\rho_1 = \|\Theta^{-1}\|^{-1}$ and:

$$\begin{aligned} \ln(\det\Theta) &\leq (p-1)\ln\rho_p + \ln\rho_1 \\ &\leq (p-1)\ln\|\Theta\| - \ln\|\Theta^{-1}\|\ . \end{aligned}$$

Thus, as $\mathrm{Tr}(S\Theta) \geq 0$, $F(\Theta) \to -\infty$, when $\|\Theta^{-1}\| \to \infty$, $\|\Theta\|$ being bounded. □

Let $\overline{\mathcal{V}}$ be the closure of $\mathcal{V}$ in $\mathcal{M}^+$. $\overline{\mathcal{V}}$ is also the set of the elements of $\mathcal{M}^+$, the eigenvalues of which satisfy:

$$0 < \rho_1 \leq \rho_2 \leq \cdots \leq \rho_q \leq \rho_{q+1} = \cdots = \rho_p\ . \tag{3}$$

We shall use the fact that $\overline{\mathcal{V}}$ admits the following partition: For fixed $p > q$, we denote by K the set of families of integers $\mathbf{k} := \{k_1, \cdots k_{|\mathbf{k}|}\}$, such that $k_i - k_{i-1} \geq 1$,$(1 \leq i \leq |K|)$, [convention $k_0 = 0$]; $k_{|\mathbf{k}|-1} \leq q, k_{|\mathbf{k}|} = p$; The set K has exactly 2^q elements.
Interpretation: *the k_i, $(i \geq 1)$ gives the position of the strict inequalities in (3).*
For each $\mathbf{k} \in K$, let $\mathcal{W}_{\mathbf{k}}$ denote the subset of $\mathcal{M}^+$, the eigenvalues of which satisfy $\rho_j = \rho_{k_i}$, $(k_{i-1} < j \leq |\mathbf{k}|)$, and $\rho_{k_{i-1}} \leq \rho_{k_i}$,$(k_i \leq j \leq k_i$,$(2 \leq i \leq |\mathbf{k}|)$; then:

- $\overline{\mathcal{V}} = \sum_{\mathbf{k} \in K} \mathcal{W}_{\mathbf{k}}$ (partition of $\overline{\mathcal{V}}$), [in particular $\mathcal{V} = \mathcal{W}_{\mathbf{k}_0}$, where $\mathbf{k}_0^i = i$].
- Each $\mathcal{W}_{\mathbf{k}}$ is a smooth, finite dimensional manifold imbedded in $\mathcal{M}^+$, hence a point of $\overline{\mathcal{V}}$, at which F reaches a maximum is a critical point of the restriction of F to one of the $\mathcal{W}_{\mathbf{k}}$.

Actually Theorem 1 is a particular case of the following result:

Theorem 2 *For every $\mathbf{k} \in K$, the restriction of F to $\mathcal{W}_{\mathbf{k}}$ reaches a maximum at a unique point $\widetilde{\Theta}_k$. As in Theorem (1), the maximizing sequences converge.*

4 Proofs of the main results

Lemma 2 *$\widetilde{\Theta} \in \mathcal{W}_{\mathbf{k}}$ is a critical point of F iff:*

(i) there is a simultaneous diagonalization of $\widetilde{\Theta}$ and S,

(ii) there exist an ordered partition $\pi = \{\pi_1, \cdots, \pi_{|\mathbf{k}|}\}$ of $\{1, \cdots, p\}$, with $|\pi_i| = k_i - k_{i-1}$, such that:

$$\widetilde{\rho}_{k_i}^{-1} = \frac{1}{k_i - k_{i-1}} \sum_{j \in \pi_i} s_j, \ (1 \leq i \leq |\mathbf{k}|).$$

In particular, F has, at least, one critical point in $\mathcal{W}_{\mathbf{k}}$, namely the point, denoted $\widetilde{\Theta}_{\mathbf{k}}$, corresponding to the partition $\pi^{\mathbf{k}}$ defined by $\pi_i^{\mathbf{k}} = \{k_{i-1} + 1, \cdots, k_i\}$, $(1 \leq i \leq |\mathbf{k}|)$.

Proof It is classical that the tangent space to $\mathcal{W}_{\mathbf{k}}$ at $\Theta \in \mathcal{W}_{\mathbf{k}}$ is linearly generated by the spectral projectors $P_1, \cdots, P_{|\mathbf{k}|}$ of $\Theta = \sum_{i=1}^{|\mathbf{k}|} \rho_{k_i} P_i$, [tangent to the affine sub-manifold generated by the elements of $\mathcal{W}_{\mathbf{k}}$ of the form $\sum_{i=1}^{|\mathbf{k}|} \nu_{k_i} P_i$] and the commutators $(\Theta A - A\Theta)$, with $A \in L(\mathbf{R}^p)$ antisymmetric, [tangent to the orbit of Θ under the action of $SO(p)$].

For any $X \in L(\mathbf{R}^p)$, symmetric [tangent to $\mathcal{M}^+$], we have

$$< F'(\Theta), X >= \mathrm{Tr}\{\Theta^{-1} X\} - \mathrm{Tr}\{SX\} \ ,$$

(here $<,>$ denotes the duality bracket). Beginning with the subspace generated by the $\Theta A - A\Theta$, as $\mathrm{Tr}\{\Theta^{-1}(\Theta A - A\Theta)\} = 0$, the condition $< F'(\Theta), (\widetilde{\Theta} A - A\widetilde{\Theta}) >= 0$ is equivalent to:

$$-\mathrm{Tr}\{S(\widetilde{\Theta} A - A\widetilde{\Theta})\} = \mathrm{Tr}\{(SA - AS)\widetilde{\Theta}\} = 0 \ ;$$

then, representing the operators by their matrix in an (orthonormal) basis where S is diagonal: if, for $i \neq j$, the only non zero coefficients of $A^{(i,j)}$ are $A_{ij}^{(i,j)} = -A_{ji}^{(i,j)} = 1$, then:
$\mathrm{Tr}\{SA^{(i,j)} - A^{(i,j)}S)\widetilde{\Theta}\} = 2(s_i - s_j)\widetilde{\Theta}_{ij}$, thus the condition is equivalent to $\widetilde{\Theta}_{ij} = 0$, $(i \neq j)$.
If $\pi_i \subset \{1, \cdots p\}$ is such that the range of the spectral projector $\widetilde{P}_i$ of $\widetilde{\Theta}$ is generated by the eigenspaces of S corresponding to the eigenvalues $\{s_j\}_{j \in \pi_i}$.
The condition $< F'(\Theta), \widetilde{P}_i >= 0$ can be written:

$$(k_i - k_{i-1})\widetilde{\rho}_{k_i}^{-1} = \mathrm{Tr}\{\Theta^{-1}\widetilde{P}_i\} = \sum_{j \in \pi_i} s_j. \ \square$$

Lemma 3 *(Comparing the values of F on the different critical points in $\mathcal{W}_{\mathbf{k}}$) Let $\widetilde{\Theta} \in \mathcal{W}_{\mathbf{k}}$ a critical point of F, distinct of $\widetilde{\Theta}_{\mathbf{k}}$, then: $F(\widetilde{\Theta}) < F(\widetilde{\Theta}_{\mathbf{k}})$.*

Proof First, we remark that, for every critical point $\widetilde{\Theta} \in \overline{\mathcal{V}}$, $\mathrm{Tr}\{S\widetilde{\Theta}\} = p$; it is sufficient to establish: $\det(\widetilde{\Theta}_{\mathbf{k}}) > \det(\widetilde{\Theta})$, or $\det(\widetilde{\Sigma}_{\mathbf{k}}) > \det(\widetilde{\Sigma})$.

But, $\sum_{1\le j\le p} \frac{\widetilde{\lambda}_j^{\mathbf{k}}}{\widetilde{\lambda}_j} = \sum_{1\le j\le p} s_j\widetilde{\rho}_j$; as $s_j > s_{j-1}$ and $\widetilde{\rho}_j > \widetilde{\rho}_{j-1}$, $(2 \le j \le p)$, for any permutation $\sigma \in \mathfrak{S}_p$, we have: (see [4], Th 368, p. 261)

$$\sum_{1\le j\le p} s_j\,\widetilde{\rho}_j \le \sum_{1\le j\le p} s_j\,\widetilde{\rho}_{\sigma(j)} \ .$$

Furthermore, there exists (at least) one permutation $\underline{\sigma}$ such that

$$\sum_{1\le j\le p} \widetilde{\rho}_{\underline{\sigma}(j)} = \mathrm{Tr}\{S\widetilde{\Theta}\} = p \ ,$$

hence $\sum_{1\le j\le p} \frac{\widetilde{\lambda}_j^{\mathbf{k}_j}}{\widetilde{\lambda}_j} \le p$. Put it differently, if $m := p^{-1} \sum_{1\le j\le p} \frac{\widetilde{\lambda}_j^{\mathbf{k}}}{\widetilde{\lambda}_j}$, then $m \le 1$. Finally, using the well-known inequality, comparing the geometric and the arithmetic mean, we obtain:

$$\frac{\det(\widetilde{\Sigma}^{\mathbf{k}})}{\det(\widetilde{\Sigma})} = \prod_{1\le j\le p} \frac{\widetilde{\lambda}_j^{\mathbf{k}}}{\widetilde{\lambda}_j} < m^p \le 1 \ .$$

The inequality is strict, if $\widetilde{\Theta} \ne \widetilde{\Theta}_{\mathbf{k}}$, because the $\left\{\frac{\widetilde{\lambda}_j^{\mathbf{k}}}{\widetilde{\lambda}_j}\right\}_{1\le j\le p}$ are not all equal. □

Lemma 4 *(Comparison of the values of F at points $\widetilde{\Theta}_{\mathbf{k}}$) If $\mathbf{k}_1, \mathbf{k}_2 \in K, \mathbf{k}_1 \ne \mathbf{k}_2$, are such that $\overline{\mathcal{W}}_{\mathbf{k}_2} \subset \overline{\mathcal{W}}_{\mathbf{k}_1}$, $(\mathcal{W}_{\mathbf{k}_1} \ne \mathcal{W}_{\mathbf{k}_2})$, then $F(\widetilde{\Theta}_{\mathbf{k}_2}) < F(\widetilde{\Theta}_{\mathbf{k}_1})$; particulary, for every $\mathbf{k} \in K$, $\mathbf{k} \ne \mathbf{k}_0$, $F(\widetilde{\Theta}_{\mathbf{k}}) < F(\widetilde{\Theta}_{\mathbf{k}_0})$, [recall: $\mathcal{V} = \mathcal{W}_{\mathbf{k}_0}$].*

Proof Again it is sufficient to get: $\det(\widetilde{\Sigma}_{\mathbf{k}_1}) < \det(\widetilde{\Sigma}_{\mathbf{k}_2})$. The condition $\mathcal{W}_{\mathbf{k}_2} \subset \overline{\mathcal{W}}_{\mathbf{k}_1}$ is equivalent to $\mathbf{k}_2 \subset \mathbf{k}_1$ and $\mathbf{k}_2 \ne \mathbf{k}_1$; but, if $\pi^{\mathbf{k}_1}$ and $\pi^{\mathbf{k}_2}$ are the partitions corresponding to $\widetilde{\Theta}_{\mathbf{k}_1}$ and $\widetilde{\Theta}_{\mathbf{k}_2}$, $\mathbf{k}_2 \subset \mathbf{k}_1$ means that any elements of $\pi^{\mathbf{k}_2}$ is an union of elements of $\pi^{\mathbf{k}_1}$; thus for any $i \in \{1, \cdots, |\mathbf{k}_2|\}$ the common eigenvalue $\widetilde{\lambda}_j^{\mathbf{k}_2}$, $(j \in \pi_i^{\mathbf{k}_2})$ of $\widetilde{\Sigma}_{\mathbf{k}_2}$ is the mean of the eigenvalues $\widetilde{\lambda}_j^{\mathbf{k}_1}$, $(j \in \pi_i^{\mathbf{k}_2})$ of $\widetilde{\Sigma}_{\mathbf{k}_1}$, thus, using again the same inequality, we obtain:

$$\prod_{j\in\pi_i^{\mathbf{k}_2}} \widetilde{\lambda}_j^{\mathbf{k}_1} \le \prod_{j\in\pi_i^{\mathbf{k}_2}} \widetilde{\lambda}_j^{\mathbf{k}_2} \ ,$$

with strict inequality for at least one $i \in \{1, \cdots, |\mathbf{k}_2|\}$, if $\mathbf{k}_2 \ne \mathbf{k}_1$, so:

$$det(\widetilde{\Sigma}_{\mathbf{k}_1}) = \prod_{1\le i\le|\mathbf{k}_2|} \prod_{j\in\pi_i^{\mathbf{k}_2}} \widetilde{\lambda}_j^{\mathbf{k}_1} < \prod_{1\le i\le|\mathbf{k}_2|} \prod_{j\in\pi_i^{\mathbf{k}_2}} \widetilde{\lambda}_j^{\mathbf{k}_2} = \det(\widetilde{\Sigma}_{\mathbf{k}_2}) \ .$$

Particularly, $\mathbf{k} \subset \mathbf{k}_0$, for every $\mathbf{k} \in K$. □

Remark: The convergence of a maximizing sequence, (at every stage of the proof), is an easy consequence of: As F tends to $-\infty$, at infinite (proof of lemma 1), any maximizing sequence is bounded, thus a converging subsequence can be chosen out of this sequence: clearly, let l $(l \in \overline{\mathcal{W}}_{\mathbf{k}})$ denotes its limit, of course $F(l) = F(\widetilde{\Theta}_{\mathbf{k}})$; hence $l = \widetilde{\Theta}_{\mathbf{k}}$ (lemma 4), since $\widetilde{\Theta}_{\mathbf{k}}$ is the unique maximum of F in $\overline{\mathcal{W}}_{\mathbf{k}}$.

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