Intrinsic Dimension Estimation by Maximum Likelihood in Probabilistic PCA

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Abstract

A central issue in dimension reduction is choosing a sensible number of dimensions to be retained. This work demonstrates the asymptotic consistency of the maximum likelihood criterion for determining the intrinsic dimension of a dataset in a isotropic version of Probabilistic Principal Component Analysis (PPCA). Numerical experiments on simulated and real datasets show that the maximum likelihood criterion can actually be used in practice and outperforms existing intrinsic dimension selection criteria in various situations. This paper exhibits as well the limits of the maximum likelihood criterion and recommends in specific situations the use of the AIC criterion.

Index Terms

Probabilistic PCA, isotropic model, dimension reduction, intrinsic dimension, maximum likelihood, asymptotic consistency.

1 INTRODUCTION

The analysis of high-dimensional data has become an important problem in statistical learning and dimension reduction has a central place in such studies. Among all existing methods, Principal Component Analysis (PCA) [13] and its probabilistic version (PPCA) [24], [25] are two popular techniques. A central issue in dimension reduction is choosing a sensible number of dimensions to be retained. We refer to [7] for a review on this topic. Two kind of approaches have been proposed in the last decades for intrinsic dimension estimation.

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Local methods

The local approach estimates the topological dimension (defined as the basis dimension of the tangent space of the data manifold) from the information contained in sample neighborhoods. Fukanaga-Olsen's algorithm [12] consists of estimating the rank of the covariance matrix computed locally on a Voronoi tessellation. In [6], the Voronoi tessellation is computed thanks to a topology representing network. The algorithms proposed by Pettis *et al.* [19] and Verver-Duin [27] are based on the analysis of the distances from one point to its nearest neighbors. The main limitation of local approaches is their sensitivity to outliers.

Global methods

The global approach consists of unfolding the whole dataset into a linear subspace. The estimated intrinsic dimension is then the dimension of the resulting subspace. Such methods can be divided into three subfamilies.

- *Projection methods*: The lower dimensional subspace can be estimated by minimizing some projection errors. Examples of such approaches include PCA [13] sometimes associated with Cattell's scree test [9] and its non linear extensions based either on autoassociative models [14], [10] or Mercer kernels [21]. Multidimensional scaling type algorithms aim at finding the projection which (locally) preserve the distances among data. Recent methods include LLE [20] and ISOMAP [23].
- *Fractal-based methods*: These techniques rely on the assumption that the dataset is generated by a dynamic system. Their goal is to estimate the dimension of the attractor associated to this dynamic system. For instance, [15] addresses this problem through the estimation of the box-counting dimension and some heuristic methods are introduced in [8]. Most of these methods are designed for low-dimensional datasets since their complexity grows exponentially with the dimension.
- *Model-based methods*: The use of a parametric model permits to derive a maximum likelihood (ML) estimator of the intrinsic dimension. For instance, in [16], the number of points in a small sphere is modeled by a Poisson process. We also refer to [17] for a bias correction of the previous ML estimator. In a similar spirit, [11] uses a polynomial regression based on a uniformity assumption. Minka [18] proposed a penalized likelihood criterion dedicated to the PPCA model and based on the Bayesian Information Criterion (BIC) [22]. The underlying idea is that the likelihood is an increasing function of the complexity and thus of the dimensionality as well. This remark motivates the authors to use a penalized likelihood criterion.

In our work, a constrained version of PPCA is introduced, called isotropic PPCA, and it is demonstrated that the ML criterion is asymptotically optimal in this case, the complexity

of the model being not an increasing function of the dimensionality. The ML criterion is compared in different situations on simulated and real data to two classical model selection criteria, AIC [1] and BIC [22], to the empirical scree-test of Cattell [9], and to the model-based methods [16] and [11].

This paper is organized as follows. Section 2 introduces an isotropic version of probabilistic PCA and considers the estimation of its parameters. Section 3 focuses on the intrinsic dimension estimation and demonstrates that the maximum likelihood method can be used for this task in the context of the isotropic PPCA model. Section 4 illustrates on simulations and real datasets the behavior of the proposed approach in different situations and Section 5 proposes some concluding remarks.

2 Isotropic Probabilistic PCA

In this section, after having reminded the Probabilistic PCA (PPCA) model, it is reformulated using an eigenvalue decomposition. An isotropic version of PPCA is then introduced and inference aspects are addressed.

2.1 Factor Analysis, Probabilistic PCA and Extreme Component Analysis

The Factor Analysis model [2], [3] links linearly a p-dimensional random vector y to a d-dimensional Gaussian vector x of latent variables:

$$y = Hx + \mu + \varepsilon.$$

The $p \times d$ factor matrix H relates the two random vectors and $\mu \in \mathbb{R}^p$ is a nonrandom position parameter. When $d < p$, the latent vector x provides a parsimonious representation of y. Without loss of generality, it can be assumed that $x \sim \mathcal{N}(0, I_d)$. If, moreover, the noise ε is supposed to be Gaussian $\varepsilon \sim \mathcal{N}(0, \Psi)$, where Ψ is a $p \times p$ variance matrix, and independent from x, then we end up with a Gaussian distribution for the observations y, *i.e.* $y \sim \mathcal{N}(\mu, \Sigma)$ where:

$$\Sigma = HH^t + \Psi. \tag{1}$$

In such a case, the model parameters can be estimated by maximum likelihood even though an iterative procedure is involved. To overcome this practical difficulty, one can assume an isotropic noise $\Psi = bI_p$ with $b > 0$. This model is referred to as the Probabilistic PCA model [25]. The variance matrix of y can be simplified in:

$$\Sigma = HH^t + bI_p.$$

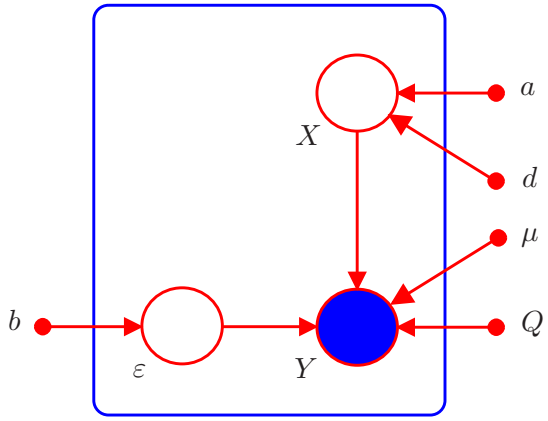


Fig. 1. Graphical representation of the isotropic PPCA model.

In contrast to the general Factor Analysis model, all parameters μ, b and H benefit from closed form estimators. Assuming without loss of generality that the columns of H are orthogonal, *i.e.* H^tH is diagonal, the eigenvalues of Σ are $\|h_1\|^2 + b, \ldots, \|h_d\|^2 + b$ and b. Consequently, the d eigenvalues associated to the latent subspace are always larger than the eigenvalues associated to the noise subspace. In contrast, in the Probabilistic Minor Component Analysis (PMCA) [29] method, the converse assumption is made. Finally, the two approaches are unified in the Extreme Component Analysis (XCA) method [28] where the noise ε is supposed to be orthogonal to the columns of H. This assumption yields $\Psi = b(I - H(H^tH)^{-1}H^t)$ in (1) and thus the eigenvalues of Σ are $\|h_1\|^2, \ldots, \|h_d\|^2$ and b. Since no assumption is made on their relative magnitudes, PPCA and PMCA may be interpreted as particular cases of XCA.

2.2 Isotropic Probabilistic PCA

Similarly, it may be of interest to consider an isotropic factor matrix. In this case, the matrix H can be rewritten as $H = \sqrt{a-b}V$ with $a > b$ and where V is a $p \times d$ matrix such that $V^tV = I_d$. Thus, the variance matrix of the observation y is given by:

$$\Sigma = (a-b)VV^t + bI_p.$$

An alternative, and more intuitive, parametrization of Σ can be obtained using its eigenvalue decomposition:

$$\Sigma = Q\Delta Q^t,$$

where Q is an orthogonal matrix containing the eigenvectors of Σ and Δ is a diagonal matrix containing the eigenvalues of Σ. Naturally, it is possible to express the eigenvector matrix Q

regarding the transformation matrix V as follows: $Q = [V, U]$ where U is a $p \times (p-d)$ matrix such that Q is orthogonal. Therefore, the matrix Δ associated with the isotropic PPCA model has the following form:

$$\Delta = \begin{pmatrix} \boxed{\begin{matrix} a & & 0 \\ & \ddots & \\ 0 & & a \end{matrix}} & \mathbf{0} \\ \mathbf{0} & \boxed{\begin{matrix} b & & 0 \\ & \ddots & \\ & & \ddots \\ 0 & & b \end{matrix}} \end{pmatrix} \begin{matrix} \left.\vphantom{\begin{matrix} a \\ \\ a \end{matrix}}\right\} d \\ \left.\vphantom{\begin{matrix} b \\ \\ \\ b \end{matrix}}\right\} (p-d) \end{matrix}$$

with $a > b$. Let us emphasize that, since H is supposed to have only two different eigenvalues, the assumption $a > b$ is made without loss of generality and thus this model can also be interpreted as an isotropic XCA model.

The isotropic PPCA model is parametrized by μ, Q, a, b and d. A graphical representation of the isotropic PPCA model is given by Figure 1. As it can be observed on Figure 2 which illustrates the model in a 3-dimensional space, such a modelling assumes that the distribution is spherical and modelled by a within the d-dimensional latent subspace where the data actually live. The d-dimensional latent subspace is spanned by the d first columns of Q which control the orientation of the subspace whereas μ locates the subspace in the original space. The isotropic PPCA model supposes as well that the variance of noise can be modelled outside the latent subspace with an unique parameter b. Finally, it should also be noticed that the mixture model introduced in [5] is in fact a mixture of isotropic PPCA applied to discriminant analysis, *i.e.* each class is modelled by a specific isotropic PPCA model.

2.3 Inference for isotropic PPCA

Before focusing on the estimation of the intrinsic dimension d, the inference on model parameters for the isotropic PPCA model is considered. In the case of the isotropic PPCA model, the parameters to be estimated are μ, a, b, U and V. As in the classical Gaussian framework, the maximum likelihood strategy is retained for parameter estimation. Denoting by n the number of observations, the log-likelihood associated with the isotropic PPCA model is:

$$-\frac{2}{n}\log(L) = d\log(a) + (p-d)\log(b) + \frac{1}{a}\sum_{j=1}^{d} v_j^t W v_j + \frac{1}{b}\sum_{j=1}^{p-d} u_j^t W u_j, \tag{2}$$

where W is the empirical variance matrix:

$$W = \frac{1}{n}\sum_{\ell=1}^{n}(x_\ell - \hat{\mu})(x_\ell - \hat{\mu})^t, \ \hat{\mu} = \frac{1}{n}\sum_{\ell=1}^{n} x_\ell.$$

The estimation of the matrices U and V is similar to the estimation of H in the context of the actual PPCA model (see [24] for further details). For a given value of d, the ML estimator of the

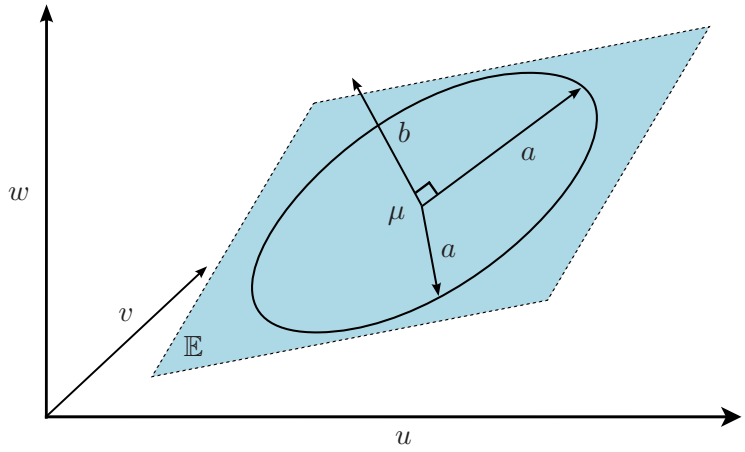


Fig. 2. The isotropic PPCA model: a controls the variance in the latent subspace $\mathbb{E}$ spanned by the d first columns of Q, μ locates the subspace in the original space and b controls the variance outside $\mathbb{E}$.

transformation matrix V is the matrix containing the eigenvectors associated with the d largest eigenvalues of the empirical variance matrix W. Similarly, the ML estimator of U is the matrix containing the eigenvectors associated with the $p-d$ smallest eigenvalues of W. Using this eigenvalue decomposition of W in (2), we obtain

$$-\frac{2}{n}\log(L) = d\log(a) + (p-d)\log(b) + \frac{1}{a}\sum_{j=1}^{d}\lambda_j + \frac{1}{b}\sum_{j=d+1}^{p}\lambda_j, \tag{3}$$

where λ_j is the jth eigenvalue of W. It follows that

$$\hat{a} = \frac{1}{d}\sum_{j=1}^{d}\lambda_j \text{ and } \hat{b} = \frac{1}{(p-d)}\sum_{j=d+1}^{p}\lambda_j.$$

As one can observe, maximum likelihood provides intuitive estimates of model parameters. Particularly, ML estimates of parameters a and b are respectively means of the largest and smallest eigenvalues of the empirical covariance matrix. From a numerical point of view, such estimates should be more robust than eigenvalue estimates when the number of observations is small compared to the data dimension p. Furthermore, it is not necessary in practice to compute the $(p-d)$ smallest eigenvalues of W since $\hat{b}$ can be computed as $\hat{b} = \left(\mathrm{tr}(W) - da\right)/(p-d)$.

3 Estimation of the intrinsic dimension by maximum likelihood

In this section, we focus on the estimation of the intrinsic dimension d^*. First the following proposition is proved.

Proposition: The maximum likelihood of d^* is asymptotically unique and consistent.

Proof: Since d is an integer parameter, it is possible to compute the likelihood for each value of $d =$

$1, ..., p-1$ and to select the value associated to the largest likelihood. From Equation (3), the maximized log-likelihood of the isotropic PPCA model can be written at the optimum $\hat{\theta} = (\hat{\mu}, \hat{a}, \hat{b}, \hat{U}, \hat{V})$ as

$$-\frac{2}{n}\log(L(\hat{\theta}, d)) = d\log(\hat{a}) + (p-d)\log(\hat{b}) + \frac{\mathrm{tr}(W)}{\hat{b}} + \left(\frac{1}{\hat{a}} - \frac{1}{\hat{b}}\right)\sum_{j=1}^{d}\lambda_j.$$

Since $\hat{a} = \frac{1}{d}\sum_{j=1}^{d}\lambda_j$, $\hat{b} = \frac{1}{(p-d)}\sum_{j=d+1}^{p}\lambda_j$ and $\mathrm{tr}(W) = \sum_{j=1}^{p}\lambda_j$, the log-likelihood reduces to:

$$-\frac{2}{n}\log(L(\hat{\theta}, d)) = d\log(\hat{a}) + (p-d)\log(\hat{b}) + p.$$

Consequently, the maximization of the likelihood is equivalent to the minimization of $\phi_n(d) = d\log(\hat{a}) + (p-d)\log(\hat{b})$. Asymptotically, as the number of (independent) observations n tends to infinity, $\hat{\lambda}_j$ converges almost surely (a.s.) to a if $j \leq d^*$ and $\hat{\lambda}_j$ converges a.s. to b if $j > d^*$, see Lemma 2.1 [26]. Two cases can arise.

Situation $d \leq d^*$: In this case, $\hat{a} \to a$ and $\hat{b} \to \frac{1}{p-d}\left[(d^*-d)a + (p-d^*)b\right]$ a.s. when $n \to \infty$. Consequently, $\phi_n(d) \to \phi(d)$ a.s. where we have defined

$$\phi(d) = d\log(a) + (p-d)\log\left(\frac{(d^*-d)}{(p-d)}a + \frac{(p-d^*)}{(p-d)}b\right),$$

or equivalently

$$\frac{\phi(d) - p\log(a)}{p-d^*} = \frac{(p-d)}{(p-d^*)}\log\left(1 + \frac{(p-d^*)}{(p-d)}\left(\frac{b}{a} - 1\right)\right) = \delta\log\left(1 + \frac{\gamma}{\delta}\right),$$

with $\delta = \frac{(p-d)}{(p-d^*)}$ and $\gamma = \frac{b}{a} - 1$. Thus, the study of $\phi(d)$ reduces to the study of $\psi(\delta) = \delta\log\left(1 + \frac{\gamma}{\delta}\right)$ where $\delta \geq 1$ and $\gamma \leq 0$. Since ψ is a strictly increasing function on $[1, +\infty)$ for all $\gamma \leq 0$, its minimum is reached for $\delta = 1$ and therefore the minimum of ϕ on $[1, d^*]$ is reached for $d = d^*$.

Situation $d \geq d^*$: Here, $\hat{a} \to \frac{1}{d}\left(d^*a + (d-d^*)b\right)$ and $\hat{b} \to b$ a.s. when $n \to \infty$. It leads to $\phi_n(d) \to \phi(d)$ a.s. where

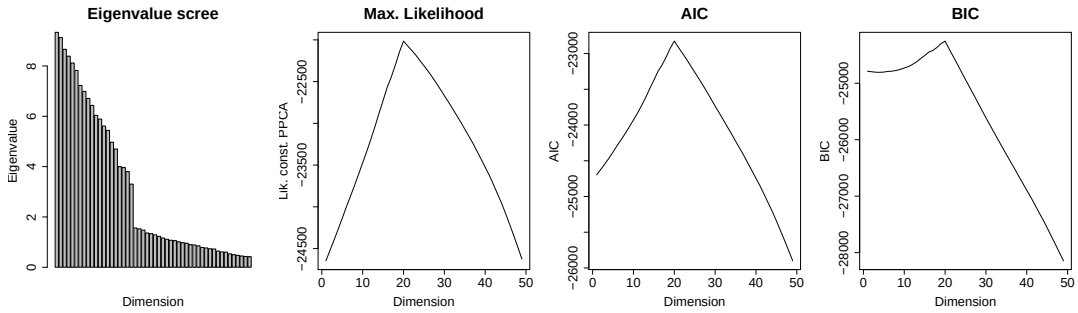
$$\phi(d) = d\log\left(\frac{d^*}{d}a + \frac{d-d^*}{d}b\right) + (p-d)\log(b).$$

Similarly to the first situation, we can write

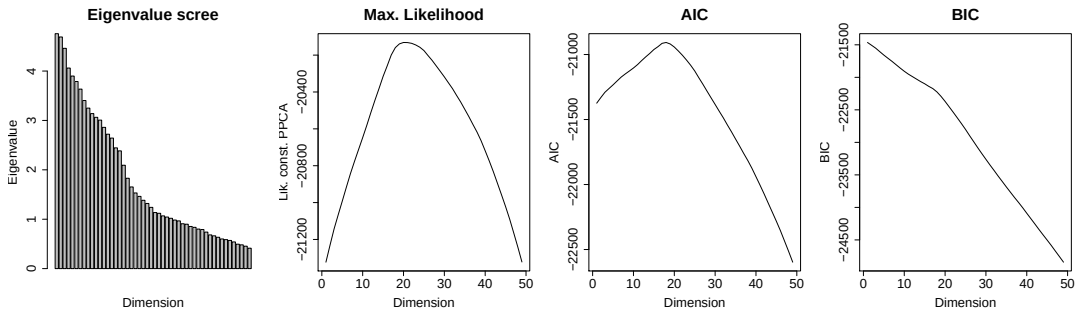
$$\frac{\phi(d) - p\log(b)}{d^*} = \frac{d}{d^*}\log\left(1 + \frac{d^*}{d}\left(\frac{a}{b} - 1\right)\right) = \delta\log\left(1 + \frac{\gamma}{\delta}\right),$$

with $\delta = \frac{d}{d^*}$ and $\gamma = \frac{a}{b} - 1$. Again, the study of $\phi(d)$ reduces to the study of $\psi(\delta) = \delta\log\left(1 + \frac{\gamma}{\delta}\right)$ where $\delta \geq 1$ and $\gamma \geq 0$. Remarking that ψ is a strictly increasing function on $[1, +\infty)$ for all $\gamma \geq 0$, its minimum is reached for $\delta = 1$ and therefore the minimum of ϕ on $[d^*, p]$ is reached for $d = d^*$. As a conclusion, we have proved that the likelihood associated with the model has asymptotically a unique maximum for the actual intrinsic dimension d^* of the data. □

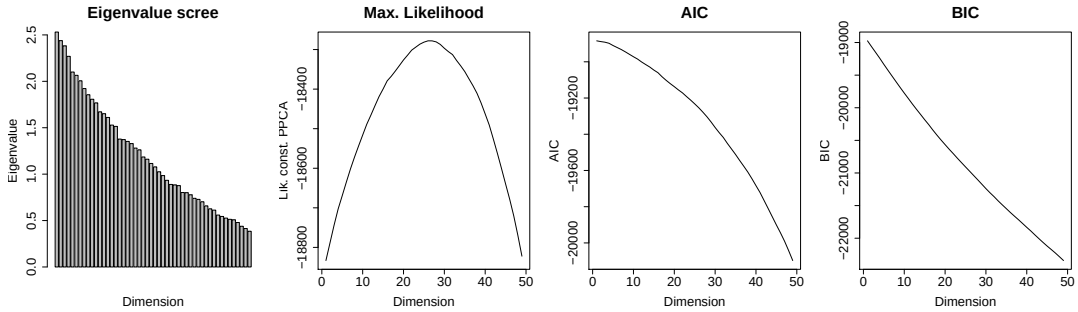
From this proposition, it is deduced that the maximum likelihood criterion can be used to estimate d^* in the context of the isotropic PPCA model. Usually, as for instance for the general PPCA model, model selection criteria using the maximum likelihood need an additional penalty term because the maximum likelihood of a model is asymptotically a non decreasing function of the number of model parameters. However, for isotropic PPCA, the proposition states that the likelihood is asymptotically maximum for the intrinsic dimension d^* of the data. Therefore ML criterion is a good candidate to



$\alpha = 5$ and $\beta = 4$



$\alpha = 5$ and $\beta = 2$



$\alpha = 5$ and $\beta = 1$

Fig. 3. Dimension selection on data simulated according to the isotropic PPCA model with ML, AIC and BIC. The data were simulated with $p = 50$, $b = 1$ and the actual intrinsic dimension is $d^* = 20$.

estimate the intrinsic dimension of a dataset in the isotropic PPCA framework. Other criteria of the form ML + pen(n) where pen(n) is a penalty such that pen(n)/n tends to 0 as n tends to infinity are other consistent criteria to estimate this intrinsic dimension. In the following such criteria as AIC and BIC are compared with ML on an experimental ground.

4 Numerical Experiments

This section presents numerical experiments on simulated and real datasets in order to highlight the main features of different intrinsic dimension estimation methods in the context of the isotropic PPCA model. The maximum likelihood criterion, for which we have demonstrated the asymptotic

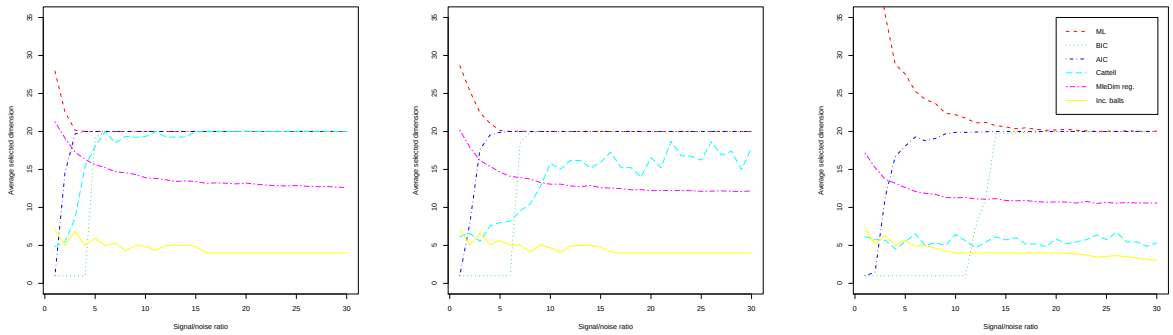
consistency, is compared in the following to two penalized likelihood criteria (AIC and BIC), an empirical criterion (Cattell's scree-test), the MleDim method of [16] and the incising balls (Inc. balls) algorithm [11]. For the sake of simplicity, the following experiments will be set up according to two parameters: $\alpha = n/p$ and $\beta = d^*a/[(p-d^*)b]$. The parameter α controls the estimation conditions through the ratio between the number of observations and the dimension of the observation space. The second parameter, β, controls the signal to noise ratio through the condition number a/b of the variance matrix. We remind that AIC and BIC respectively penalize the log-likelihood by the quantities $\nu(\mathcal{M})$ and $\nu(\mathcal{M})\log(n)/2$ where $\nu(\mathcal{M})$ is the number of independent parameters (complexity) of the used model $\mathcal{M}$. The scree-test of Cattell is an empirical method which compares the differences between consecutive eigenvalues with a fixed threshold for finding a breakdown point in the eigenvalue scree. We refer respectively to [16] and [11] for details on the MleDim and Inc. balls algorithms. Finally, for all the following experiments, the parameters p, b and d^* will remain fixed to the values $p = 50$, $b = 1$ and $d^* = 20$.

4.1 An introductory example

The first experiment aims to show the behavior of the three likelihood-based criteria (ML, AIC and BIC) according to the signal to noise ratio β for a fixed value of α. The simulated model for this experiment is the isotropic PPCA model. The parameter α has been set to 5 which means that the estimation conditions are favorable. Figure 3 shows the eigenvalue scree (left panels) and the behavior of the three likelihood-based criteria (from left to right, ML, AIC and BIC) for different values of β. The first row of Figure 3 considers an easy situation where the eigenvalue scree has a clear breakdown point between relevant and irrelevant dimensions and all criteria succeed in finding the correct intrinsic dimension $d^* = 20$. The second row presents a slightly more difficult situation for which ML and AIC still succeed in determining d^* whereas BIC penalizes too much the likelihood and fails in determining d^*. Finally, the last row focuses on a difficult situation where there is no elbow in the eigenvalue scree. In this case, AIC and BIC fail in estimating d^* by proposing $\hat{d} = 1$. Conversely, ML slightly overestimates the actual value of d^* by proposing $\hat{d} = 28$. It should be noticed that, in the dimension reduction framework, slightly overestimating the intrinsic dimension is preferable to underestimating it because all relevant dimensions are still retained.

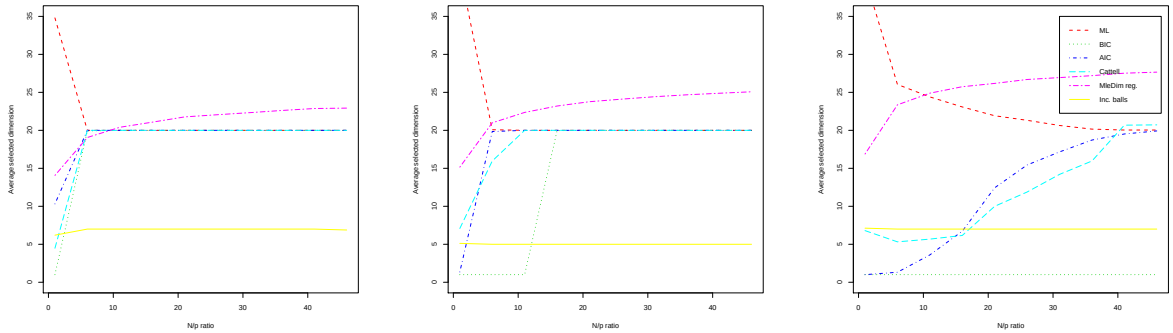
4.2 Influence of the signal to noise ratio

The second experiment focuses on the influence of the signal to noise ratio (parameter β) on the intrinsic dimension estimation with the five studied dimension selection methods and this for different values of $\alpha = n/p$. In order not to favour the likelihood-based methods, ML, AIC and BIC, the simulated model used in this numerical experiment will not be the isotropic PPCA model but a uniform model with d^* dimensions of variance $a/12$ and $(p-d^*)$ dimensions of variance $b/12$ is used. The results have been averaged from 50 independent simulated datasets. Figure 4 shows the behavior of the criteria ML, AIC, BIC, the scree-test of Cattell, MleDim and Inc. balls according to



$\alpha = 3$ and $\beta = 1, ..., 30$ $\alpha = 2$ and $\beta = 1, ..., 30$ $\alpha = 1$ and $\beta = 1, ..., 30$

Fig. 4. Average selected dimension according to the signal to noise ratio β for different values of α with ML, AIC, BIC and the scree-test of Cattell. The data were simulated according to an uniform distribution (see text for details) with $p = 50$ and the actual intrinsic dimension is $d^* = 20$.



$\beta = 3$ and $\alpha = 1, ..., 50$ $\beta = 2$ and $\alpha = 1, ..., 50$ $\beta = 1$ and $\alpha = 1, ..., 50$

Fig. 5. Average selected dimension according to the ratio $\alpha = n/p$ for different values of β with ML, AIC, BIC and the scree-test of Cattell. The data were simulated according to an uniform distribution (see text for details) with $p = 50$ and the actual intrinsic dimension is $d^* = 20$.

β for three values of $\alpha = 1, 2, 3$. The left panel of Figure 4 considers a situation where the n/p ratio is quite favorable to the estimation ($\alpha = 3$). Consequently, all likelihood-based criteria and the scree-test of Cattell succeed on average in estimating the actual intrinsic dimension $d^* = 20$ for a large range of values of β. Surprisingly, Inc. balls and MleDim underestimate the intrinsic dimension in this quite comfortable situation and Inc. balls appears to provide poor estimates of d^*. Naturally, for all methods, the task of estimating d^* becomes difficult when β is close to 1. In this case, AIC and ML are clearly more efficient than the other criteria and ML should be recommended since it slightly overestimates d^* whereas AIC underestimates it. The center panel of Figure 4 focuses on a more difficult estimation situation ($\alpha = 2$) and a similar behavior can be observed for all the criteria except

for the empirical criterion of Cattell which is clearly less efficient than ML, AIC and BIC. Finally, the right panel of Figure 4 considers a difficult situation ($\alpha = 1$) where the number of observations is small compared to the number of parameters to be estimated. It first appears that the scree-test of Cattell, MleDim and Inc. balls fail for all values of β and should not be used in such a case. Secondly, BIC turns out to perform poorly for values of β smaller than 15. For values of β between 5 and 15, AIC and ML outperform other criteria even though ML tends to dramatically overestimate d^*. When the number of observations is small compared to the dimension of the observation space, it is desirable to slightly penalize the maximum likelihood and the AIC criterion could be preferred to the ML criterion to select the intrinsic dimension of a dataset.

4.3 Influence of the n/p ratio

We now focus on the influence of the n/p ratio (parameter α) on the intrinsic dimension estimation with the six studied criteria for different values of the signal to noise parameter β. Again, the results have been averaged from 50 independent simulated datasets. Figure 5 shows the behavior of the criteria ML, AIC, BIC, the scree-test of Cattell, MleDim and Inc. balls according to α for three values of $\beta = 1, 2, 3$. On the one hand, the left and center panels of Figure 5 consider situations where the signal to noise ratio is relatively good with a clear breakdown point in the eigenvalue scree. In such situations, the criteria ML, AIC, BIC and Cattell are efficient for a large range of α values whereas, as previously, MleDim and Inc. balls respectively overestimate and underestimate the actual intrinsic dimension. It should be noticed that the scree-test of Cattell and BIC appear again to be less efficient than AIC and ML. On the other hand, the right panel of Figure 5 focuses on a difficult situation: there is no clear breakdown point in the eigenvalue scree and the n/p ratio varies from a comfortable situation ($\alpha = 50$) to a critical one ($\alpha = 1$). It can be observed that, in this case, BIC, MleDim and Inc. balls fail in estimating d^* whatever the α value is. The scree-test of Cattell and AIC tend to largely underestimate d^* whereas ML only slightly overestimates it. We can therefore recommend to use the ML criterion for selecting the intrinsic dimension of a dataset when the signal to noise ratio is low. This study demonstrates as well that the task of estimating the intrinsic dimension of a dataset is extremely difficult when α and β are both close to 1.

4.4 Application to supervised classification

Finally, in order to compare and assess the different dimension selection methods on real datasets, we chose to consider the supervised classification task. Supervised classification offers indeed the ability to numerically evaluate the performance of the studied methods on real data (for which the actual intrinsic dimension is unknown) through the correct classification rate. We selected seven datasets on the UCI Machine Learning Repository (*http://archive.ics.uci.edu/ml/*): Abalone, Glass, Satellite, Sonar, USPS, Wine and Yeast datasets. The USPS dataset has been modified to focus on discriminating the three most difficult classes to be classify, namely the classes of the digits 3, 5 and 8. This dataset has been called USPS 358. The second and the third columns of Table 1 give respectively the number of

Dataset	n	p	ML	BIC	AIC	Cattell	MleDim
Abalone	4177	8	**0.5319** (2.0)	**0.5319** (2.0)	**0.5319** (2.0)	0.5049 (1.0)	**0.5318** (1.9)
Glass	214	9	**0.4987** (5.7)	**0.4916** (4.7)	**0.5003** (5.2)	0.4733 (3.0)	0.4663 (3.4)
Satellite	6435	36	**0.8207** (7.8)	**0.8205** (7.4)	**0.8205** (7.7)	0.7647 (2.0)	**0.8213** (8.0)
Sonar	208	60	**0.6355** (6.4)	0.5654 (3.1)	0.5849 (3.8)	0.5278 (1.8)	**0.6237** (5.0)
USPS 358	2248	256	0.9062 (85.5)	0.9100 (15.0)	**0.9175** (50.5)	0.7637 (2.6)	0.9094 (11.9)
Wine	178	13	**0.7277** (2.6)	**0.7110** (2.2)	**0.7138** (2.3)	0.6813 (1.0)	0.6813 (1.0)
Yeast	1479	8	**0.5107** (4.5)	**0.5359** (3.7)	**0.5204** (4.2)	**0.5190** (3.7)	0.4599 (5.3)
Significant wins	-	-	**6**	5	**6**	1	3

TABLE 1

Classification results on real datasets (UCI): reported values are average correct classification rate computed on validation sets and the values in bracket are the average selected dimensions. The results which are not in bold are significantly less than other results.

observations and the number of dimensions of the seven datasets. In order to evaluate the ability of the studied dimension selection methods, the following experimental setup has been used. Each dataset was randomly split into a learning set of 10% of the observations and a validation set made of the remaining observations for simulating a difficult classification situation. The intrinsic dimension d was then selected with each dimension selection method before designing the classifier using linear discriminant analysis (LDA) on the d first principal components (classical PCA). The correct classification rate was computed afterward on the validation set. The results have been averaged from 50 repetitions of the experimental setup. This experimental setup has been applied to the previous dimension selection methods except the Inc. balls algorithm which gave very disappointing results in the previous experiments. Table 1 reports the average correct classification rate of each dimension selection method for the seven datasets. The average selected dimensions are also given into brackets. The results which are not in bold are significantly worse than other results. Finally, the last rows of Table 1 summarizes the number of significant wins of each dimension selection method for the classification task. It appears that the likelihood-based methods ML, BIC and AIC perform better than Cattell and MleDim to classify real data. It can be also noticed that ML turns out to be particularly efficient when the n/p ratio is small (Sonar and Wine datasets) which reinforces our previous conclusions.

5 Discussion

The present work focused on the estimation of the intrinsic dimension d which controls in PPCA the number of parameters to be estimated. This problem can be regarded as a model selection problem. From this point of view, it can be thought of as surprising to propose the maximum likelihood (ML)

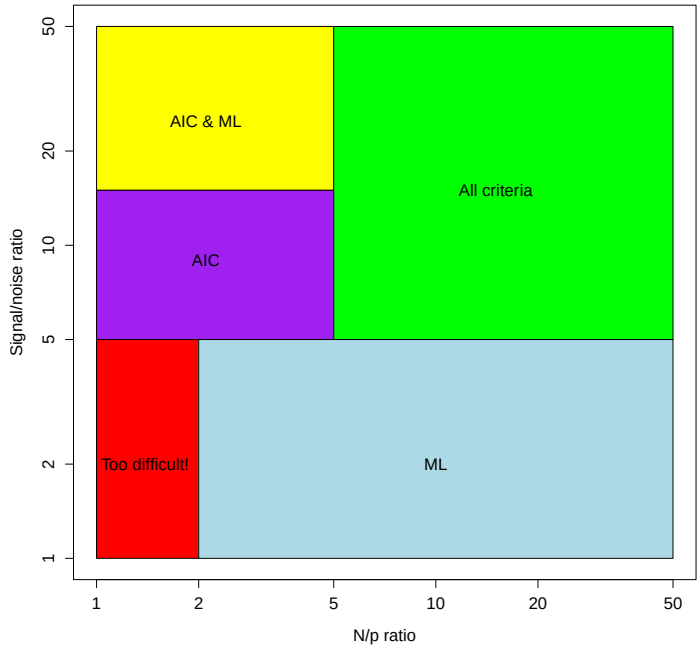


Fig. 6. Recommended criteria for intrinsic dimension selection according to the n/p and signal to noise ratios in the context of the isotropic PPCA model.

as a model selection criterion since in most situations this criterion could be expected to increase with the model complexity. The reason why ML can be used to estimate d^* for the isotropic PPCA model is the perfect duality between the subspace spanned by the eigenvectors associated with the d largest eigenvalues of W and the supplementary noise subspace with dimension $(p-d)$. Because of the symmetry between a and b occurring in the isotropic PPCA model, the number of parameters to be estimated is a function of $\min(\tau(d), \tau(p-d))$ where $\tau(d) = d(p-(d+1)/2)$ is the number of parameters to be estimated for variance matrix Σ. Consequently, the complexity of the isotropic PPCA model does not increase strictly with d: it increases between 1 and the actual intrinsic dimension d^* and decreases between d^* and $(p-1)$. It is therefore not surprising that the ML criterion is able to find the actual intrinsic dimension of the data without requiring an additional complexity penalty.

The theoretical result of Section 3 ensures that the ML criterion is consistent to estimate the actual intrinsic dimension of the isotropic PPCA model. In practice, the sample size n is finite and can be small in regard to p. Thus, it could happen that the sample variability leads to a ML criterion whose maximum is attained for a larger dimension than the actual intrinsic dimension d^*. In such cases and especially for small n, a slight penalty term, as the AIC penalty term, could be desirable to select a proper intrinsic dimension. Figure 6 displays a summary of the recommendations that could be given from our experience. As it can be seen on this figure, it appear that AIC can outperform ML criterion when $n/p < 5$ for a moderate signal to noise ratio. Finally, when n is not very large, it could be

recommended to compare the dimensions selected by AIC and ML and to choose d on an empirical ground when the AIC and ML selected dimensions differ. And, in that purpose, the recommendations provided by Figure 6 could be helpful.

Finally, the theoretical result exhibited in this work should have interesting applications in methods related to or based on the isotropic probabilistic PCA model. On the one hand, the intrinsic dimension selection approach proposed in this work could be used to approximately determine the intrinsic dimension in PPCA, PMCA and XCA. Indeed, although the maximum likelihood estimate is not asymptotically consistent for the PPCA, PMCA and XCA models, it could provide a first approximation of the intrinsic dimension for those models. On the other hand, the isotropic PPCA model has been used in [5], in a supervised classification framework, for modelling and classifying the data of K classes in different subspaces with specific intrinsic dimensions d_k^*, $k = 1, ..., K$, estimated through an empirical strategy. In such a context, the BEC criterion [4] could be also used since it is a penalized-likelihood criterion taking into account the classification goal. Alternatively, the asymptotic optimality of the ML criterion for the isotropic PPCA model should allow this classification method to efficiently determine the intrinsic dimension d_k^* of each class using the ML criterion avoiding numerical problems when α or/and β go close to 1.

REFERENCES

[1] H. Akaike. A new look at the statistical model identification. *IEEE Transactions on Automatic Control*, 19(6):716–723, 1974.

[2] D. J. Bartholomew. *Latent Variable Models and Factor Analysis*. Charles Griffin & Co. Ltd, London, 1987.

[3] A. Basilevsky. *Statistical Factor Analysis and Related Methods*. Wiley, New York, 1994.

[4] G. Bouchard and G. Celeux. Selection of generative models in classification. *IEEE transactions on Pattern Analysis and Machine Intelligence*, 28(4):544–554, 2006.

[5] C. Bouveyron, S. Girard, and C. Schmid. High Dimensional Discriminant Analysis. *Communications in Statistics: Theory and Methods*, 36(14):2607–2623, 2007.

[6] J. Bruske and G. Sommer. Intrinsic dimensionality estimation with optimally topology preserving maps. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 20(5):572–575, 1998.

[7] F. Camastra. Data dimensionality estimation methods: a survey. *Pattern Recognition*, 36:2945–2954, 2003.

[8] F. Camastra and A. Vinciarelli. Estimating the intrinsic dimension of data with a fractal-based method. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 24(10):1404–1407, 2002.

[9] R. Cattell. The scree test for the number of factors. *Multivariate Behavioral Research*, 1(2):245–276, 1966.

[10] B. Chalmond and S. Girard. Nonlinear modeling of scattered multivariate data and its application to shape change. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 21(5):422–432, 1999.

[11] M. Fan, H. Qiao, and B. Zhang. Intrinsic dimension estimation of manifolds by incising balls. *Pattern Recognition*, 42(5):780–787, 2009.

[12] K. Fukunaga and D.R. Olsen. An algorithm for finding intrinsic dimensionality of data. *IEEE Transactions on Computers*, 20(2):176–183, 1971.

[13] I. Jolliffe. *Principal Component Analysis*. Springer-Verlag, New York, 1986.

[14] J. Karhunen and J. Joutsensalo. Representation and separation of signals using nonlinear PCA type learning. *Neural Networks*, 7(1):113–127, 1994.

[15] B. Kegl. Intrinsic Dimension Estimation Using Packing Numbers. In *15th Annual Conference on Neural Information Processing Systems*, 2002.

[16] E. Levina and P. Bickel. Maximum Likelihood Estimation of Intrinsic Dimension. In *17th Annual Conference on Neural Information Processing Systems*, 2005.

[17] D. MacKay and Z. Ghahramani. Comments on 'maximum likelihood estimation of intrinsic dimension' by E. Levina and P. Bickel, 2005. Technical report. `inference.phy.cam.ac.uk/mackay/dimension`.

[18] T. Minka. Automatic choice of dimensionality for PCA. In *13th Annual Conference on Neural Information Processing Systems*, 2000.

[19] E. Pettis, T. Bailey, A. Jain, and R. Dubes. An intrinsic dimensionality estimator from nearest-neighbor information. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 1:25–37, 1979.

[20] S. Roweis and L. Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.

[21] B. Schölkopf, A. Smola, and K-R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10(5):1299–1319, 1998.

[22] G. Schwarz. Estimating the dimension of a model. *The Annals of Statistics*, 6:461–464, 1978.

[23] J. Tenenbaum, V. De Silva, and J. Langford. A global geometric framework for non linear dimensionality reduction. *Science*, 290(5500):2319–2323, 2000.

[24] M. Tipping and C. Bishop. Mixtures of probabilistic principal component analyzers. *Neural Computation*, 11(2):443–482, 1999.

[25] M. Tipping and C. Bishop. Probabilistic Principal Component Analysis. *Journal of the Royal Statistical Society, Series B*, 3(61):611–6222, 1999.

[26] D. Tyler. Asymptotic Inference for Eigenvectors. *Annals of Statistics*, 9(4):725–736, 1981.

[27] P. Verveer and R. Duin. An evaluation of intrinsic dimensionality estimators. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 17(1):81–86, 1995.

[28] M. Welling, F. Agakov, and C. Williams. Extreme Components Analysis. In *16th Annual Conference on Neural Information Processing Systems*, 2003.

[29] C. Williams and F. Agakov. Products of Gaussians and Probabilistic Minor Component Analysis. *Neural Computation*, 14(5):1169–1182, 2002.