MML Probabilistic Principal Component Analysis

A Preprint

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Abstract

Principal component analysis (PCA) is perhaps the most widely method for data dimensionality reduction. A key question in PCA decomposition of data is deciding how many factors to retain. This manuscript describes a new approach to automatically selecting the number of principal components based on the Bayesian minimum message length method of inductive inference. We also derive a new estimate of the isotropic residual variance and demonstrate, via numerical experiments, that it improves on the usual maximum likelihood approach.

Keywords minimum message length · factor analysis · model selection

1 Introduction

The principal component analysis (PCA) model \cite{Jolliffe2002,JolliffeCadima2016} postulates that \( N \) independent realisations of \( K \)-dimensional data \( x_i \in \mathbb{R}^K \), \( i = 1, \ldots, N \) are described as

\[
x_i = v_i a_1 + \cdots + v_i a_J + \epsilon_i = \sum_{j=1}^{J} v_{ij} a_j + \epsilon_i, \quad \epsilon \sim N_K(0, \sigma^2 I_K),
\]

where \( \{a_1, \ldots, a_J\} \) are the \( J( < K) \) latent (unobserved) factor loadings with each factor loading \( a_j \in \mathbb{R}^K \), and \( v_j \sim N(0, I_N) \) are the factor scores distributed as per the standard normal distribution. It is assumed that the residuals follow an isotropic zero mean normal distribution with the variance-covariance matrix \( \sigma^2 I_K \). Without loss of generality, we assume that the data has been centered to the mean. We can write this PCA model in matrix notation as follows

\[
x_i = Av_i + \epsilon, \quad A \in \mathbb{R}^{K \times J}, \quad v_i \in \mathbb{R}^J, \quad \epsilon \sim N_K(0, \sigma^2 I_K),
\]

where \( i = (1, \ldots, N) \), \( A = (a_1, \ldots, a_J) \) and \( V = (v_1, \ldots, v_N) \in \mathbb{R}^{J \times N} \). Integrating out the factor scores yields the multivariate Gaussian marginal distribution of the data

\[
x_i \sim N_K(0_K, \Sigma_0), \quad \Sigma = AA' + \sigma^2 I_K.
\]

The probabilistic principal component model as described suffers from identifiability constraints \cite{AndersonRubin1956,LawleyMaxwell1971}. A key reason for this is that the latent factors affect the likelihood function only through their outer product \( AA' \), which implies that an estimate of the factors can only be determined up to a rotation. To ensure the model is not over parametrised, the maximum number of latent factors to be estimated cannot exceed

\[
J_{\text{MAX}} \leq K + \frac{1}{2} \left( 1 - \sqrt{8k + 1} \right),
\]

see \cite{Beal2003} (pp. 108) for details. For example, when \( K = 4, 5, 6 \) we have \( J_{\text{MAX}} = 1, 2, 3 \), respectively. \cite{TippingBishop1999a} showed how to interpret standard PCA model in a probabilistic framework and obtained maximum likelihood estimates of the latent factors and residual variance.
This manuscript examines estimation of the probabilistic PCA model under the Bayesian minimum message length (MML) inductive inference framework. Although single and multiple factor analysis has been examined within the MML framework by Wallace and Freeman [1992] and Wallace [1998] respectively, this manuscript departs from the earlier work in the following:

- We consider the marginal distribution of the data [3] rather than the model [1] analysed by Wallace [1998].
- Using polar decomposition, we write the factor load matrix A as a product of an orthogonal matrix and a diagonal matrix representing the direction and length of the loadings, respectively. Unlike the earlier MML approaches, we parameterize the orthogonal matrix via Givens rotations to explicitly capture orthogonality constraints.
- We use matrix polar decomposition to develop a prior distribution for the latent factors A that is a product of a matrix variate Cauchy distribution and a uniform distribution over the corresponding Stiefel manifold.
- We obtain analytic MML estimates of the parameters and find a polynomial whose roots yield the MML estimate of the residual variance.

2 Maximum likelihood estimation

This section summarises the results of Tipping and Bishop [1999a]. The negative log-likelihood of the data under the probabilistic PCA model is

\[ \ell(\theta) = \frac{NK}{2} \log(2\pi) + \frac{N}{2} \log |\Sigma| + \frac{N}{2} \text{tr} (\Sigma^{-1} S_x) \]  \hspace{1cm} (5)

where \( S_x = \frac{1}{N} \sum x_i x_i' \) is the sample variance-covariance matrix. We have the observed data \( X \) and wish to estimate the number of latent factors \( J \) and all parameters \( \theta = \{A, \sigma^2\} \). Differentiating the negative log-likelihood with respect to the factor loads

\[ \partial \ell(\theta) = N \text{tr} A' \Sigma^{-1} (\partial A) - N \text{tr} (A' \Sigma^{-1} S_x \Sigma^{-1} (\partial A)) \]

and setting the derivatives to zero we get

\[ S_x \Sigma^{-1} A = A \]

Consider the singular value decomposition \( A = ULV' \), where \( U \in \mathbb{R}^{K \times J}, L = \text{diag}(l_1, \ldots, l_J) \) and \( V \in \mathbb{R}^{J \times J} \) is an orthogonal matrix. Noting that \( \Sigma^{-1} A = UL(L^2 + \sigma^2 I_J)^{-1}V' \), we have

\[ S_x U = U(L^2 + \sigma^2 I_J) \]
\[ S_x u_j = (l_j^2 + \sigma^2) u_j, \quad (j = 1, \ldots, J), \]

which is an example of the eigenvalue problem. That is, \( U \) is a \((K \times J)\) matrix whose columns are the top \( J \) eigenvectors of the sample covariance matrix \( S_x \) corresponding to the \( J \) largest eigenvalues

\[ \delta_j = l_j^2 + \sigma^2, \quad j = 1, \ldots, J, \]  \hspace{1cm} (6)

where \( \hat{l}_j = (\delta_j - \sigma^2)^{\frac{1}{2}} \) is the \( j \)-th largest singular value of \( A \). Without loss of generality we assume that \( \delta_1 > \delta_2 > \ldots > \delta_K > 0 \) throughout the manuscript. This implies that the maximum likelihood estimate is

\[ \hat{A}_{ML} = U(\Delta - \sigma^2 I_J)^{\frac{1}{2}} O, \quad \Delta = \text{diag}(\delta_1, \ldots, \delta_J) \]  \hspace{1cm} (7)

where \( O \) is an arbitrary (orthogonal) rotation matrix and \( \Delta \) is a diagonal matrix with the \( J \)-th largest eigenvalues of \( S_x \). Substituting the maximum likelihood estimate of the factor loads into the negative log-likelihood we have

\[ \ell(\sigma, \hat{A}_{ML}) = \frac{NK}{2} \log(2\pi) + \frac{N}{2} \sum_{i=1}^J \log \delta_j + \frac{N(K-J)}{2} \log \sigma^2 + \frac{NJ}{2} + \frac{N}{2\sigma^2} \sum_{j=J+1}^K \delta_j. \]  \hspace{1cm} (8)

The concentrated negative log-likelihood is minimised by

\[ \hat{\sigma}_{ML}^2 = \frac{1}{K-J} \sum_{j=J+1}^K \delta_j \]  \hspace{1cm} (9)

which is the sum of the \((K-J)\) smallest eigenvalues of the sample variance-covariance matrix. Tipping and Bishop [1999a] show that these estimates minimise the negative log-likelihood and discuss other saddle points of the log-likelihood function.
3 Minimum message length analysis of the PCA model

Introduced in the late 1960s by Wallace and Boulton, the minimum message length (MML) principle [Wallace and Boulton, 1968] [Wallace and Freeman, 1987] [Wallace and Dowe, 1999] [Wallace, 2005] is a framework for inductive inference rooted in information theory. The key idea underlying MML is that both parameter estimation and model selection problems can be interpreted as examples of data compression. Given data \( y \in \mathbb{R}^n \), the MML principle provides a method for computing the minimum length of a message that describes this data. In the MML approach, this message length is the single necessary inferential quantity. For the MML message to be decodable by a receiver, we require that the message encodes both a model for the data as well as the data itself. Formally, a MML message comprises two parts:

1. the assertion: describes the structure of the model, including all model parameters \( \theta \in \Theta \subseteq \mathbb{R}^p \). Let \( I(\theta) \) denote the codelength of the assertion.
2. the detail: describes the data \( y \) using the model \( p(y|\theta) \) nominated in the assertion. Let \( I(y|\theta) \) denote the codelength of the detail.

The total length of the MML message, \( I(y, \theta) \), measured in units of information (for example, bits) is the sum of the lengths of the assertion and the detail:

\[
I(D, \theta) = I(\theta) + I(y|\theta). \tag{10}
\]

The length of the assertion measures the complexity of the model, with longer assertions able to state more parameters with high accuracy or describe more complicated model structures. In contrast, a short assertion may encode the model parameters imprecisely and describe only simple models. The length of the detail tells us how well the model stated in the assertion is able to fit or describe the data. A complex model, that is one with a long assertion, will have lots of explanatory power and be able to encode more data strings using fewer bits compared to a simple model. MML seeks the model \( \hat{\theta}(y) = \arg \min_{\theta \in \Theta} \{ I(y, \theta) \} \) that minimises the length of the two-part message message. The key point is that minimising the two part message requires balancing the complexity of the model (assertion) with how well the model describes the data (detail). Ideally, we wish to find the simplest model that fits the observed data well enough; essentially, a formalisation of the famous razor of Occam. An advantage of MML is that the message length, measured in (say) bits, is a universal gauge that allows comparison across models with different model structures and numbers of parameters. As long as we can compute the MML codelengths of models, we can compare them. In this fashion, an MML practitioner is able to compare, for example, a linear regression model [Schmidt and Makalic, 2009], to a finite mixture model [Wallace and Patrick, 1993] to a decision tree [Wallace and Patrick, 1993] via their codelengths for some observed data set.

The exact solution to (11) is known as Strict MML [Wallace and Boulton, 1975] [Wallace, 2005], and is deemed to be the “gold standard” codelength. The high computational complexity of Strict MML, renders it’s applications, outside of simple models with one dimensional sufficient statistic ([Dowty, 2015], Farr and Wallace, 2002), mostly of interest from a theoretical standpoint only. Although there exist several approximations to the Strict MML codelength, the MML87 approximation [Wallace and Freeman, 1987] [Wallace, 2005] is perhaps the most widely applied. Under suitable regularity conditions [Wallace, 2005] (pp. 226), the MML87 codelength approximation for data \( x \) is

\[
I_{87}(x, \theta) = -\log \pi(\theta) + \frac{1}{2} \log |J_\theta(\theta)| + \frac{P}{2} \log \kappa_P + \frac{P}{2} - \log p(x|\theta) \tag{12}
\]

where \( \pi(\theta) \) is the prior distribution for the parameters \( \theta \), \( |J_\theta(\theta)| \) is the determinant of the expected Fisher information matrix, \( p(x|\theta) \) is the likelihood function of the model and \( \kappa_P \) is a quantization constant [Conway and Sloane, 1998], [Agrell and Eriksson, 1998]. For small \( P \) we have

\[
\kappa_1 = \frac{1}{2}, \quad \kappa_2 = \frac{5}{30\sqrt{3}}, \quad \kappa_3 = \frac{19}{192 \times 21^{1/3}}, \tag{13}
\]

while, for large \( P \), \( \kappa_P \) is well-approximated by [Wallace, 2005]:

\[
\frac{P}{2} (\log \kappa_P + 1) \approx -\frac{P}{2} \log 2\pi + \frac{1}{2} \log p \pi - \gamma, \tag{14}
\]

where \( \gamma \approx 0.5772 \) is the Euler–Mascheroni constant.
For many sufficiently well-behaved models, the MML87 code length is virtually identical to the Strict MML code length while being simpler to compute, requiring only the prior distribution for the model parameters and the determinant of the expected Fisher information matrix. Additionally, for large sample sizes $n \to \infty$, it is easy to show that the MML87 code length is asymptotically equivalent to the well-known Bayesian information criterion (BIC) [Schwarz 1978]

$$I_{87}(\mathbf{y}, \boldsymbol{\theta}) = -\log p(\mathbf{y}|\boldsymbol{\theta}) + \frac{p}{2} + O(1),$$

where the $O(1)$ term depends on the prior distribution, the Fisher information and the number of parameters $p$. The MML87 code length results in estimates that are invariant under (smooth) one-to-one reparameterization, just like the maximum likelihood estimate. MML87 has been applied to a wide range of statistical models including decision trees [Wallace and Patrick 1993], causal inference [Wallace and Korb 1999], factor analysis [Wallace and Freeman, 1992] and mixture models [Wallace and Doane 2000].

### 3.1 Orthogonality constraints

As discussed in Section 1, it is well-known that the PCA model is not identifiable given the data. A key reason for this is that the latent vectors affect the likelihood only through their outer product $\mathbf{A} \mathbf{A}' = \sum_{j=1}^{J} \mathbf{a}_j \mathbf{a}_j'$. However, there are infinitely many sets of vectors that could generate the same matrix. To resolve this ambiguity, it is a convention to estimate the factor load vectors to be mutually orthogonal; that is,

$$\mathbf{A}' \mathbf{A} = \mathbf{\alpha} = \text{diag}(\alpha_1^2, \ldots, \alpha_J^2), \quad \alpha_j = (\mathbf{a}_j' \mathbf{a}_j)^{\frac{1}{2}}, \quad (j = 1, \ldots, J),$$

where $\alpha_j$ denote the length of the $j$-th load vector. We enforce orthogonality constraints by parameterizing the matrix $\mathbf{A}$ in terms of Givens rotations [Pourzanjani et al., 2021]. Specifically, we can write $\mathbf{A}$ as

$$\mathbf{A} = \left[ R_{12}(\phi_{1.2}) \cdots R_{1.K}(\phi_{1.K}) R_{2.3}(\phi_{2.3}) \cdots R_{2.K}(\phi_{2.K}) \cdots R_{J,J+1}(\phi_{J,J+1}) \cdots R_{J,K}(\phi_{J,K}) \right] \mathbf{I}_{K,J} \mathbf{\alpha}$$

where $\mathbf{I}_{K,J}$ is the first $J$ columns of a $K \times K$ identity matrix and $R_{i,j}(\phi_{i,j})$ is a $(K \times K)$ rotation matrix that is equal to the identity matrix except for the $(i, i)$ and $(j, j)$ positions which are replaced by $\cos(\phi_{i,j})$, and the $(i, j)$ and $(j, i)$ positions which are replaced by $-\sin(\phi_{i,j})$ and $\sin(\phi_{i,j})$ respectively. Thus $\mathbf{R} \in \mathbb{R}^{K \times K}$ and $\mathbf{\alpha} \in \mathbb{R}^{J \times J}$ denote the orientations and lengths of the factor load vectors, respectively. For example, when $K = J = 2$, we have

$$\mathbf{A} = \begin{pmatrix} \cos(\phi_{1.2}) & -\sin(\phi_{1.2}) \\ \sin(\phi_{1.2}) & \cos(\phi_{1.2}) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}.$$  

This parametrization explicitly takes into account that the estimated factor loads are pairwise orthogonal. The model parameters are now

- the lengths of the latent factors $\mathbf{\alpha} = (\alpha_1, \ldots, \alpha_J) \in \mathbb{R}_+^J$,
- the orientation of the factor load vectors as captured by the $D = JK - J(J + 1)/2$ angles $\phi = (\phi_{1.2}, \ldots, \phi_{1.K}, \phi_{2.3}, \ldots, \phi_{2.K}, \ldots, \phi_{J,J+1}, \ldots, \phi_{J,K})$
- and the residual variance $\sigma^2 > 0$.

### 3.2 Fisher information

Following lengthy and tedious algebra, the expected Fisher information matrix is seen to be block diagonal with determinant

$$|\mathbf{J}(\mathbf{\alpha}, \sigma, \phi)| = N^P |\mathbf{J}(\mathbf{\alpha}, \sigma)| |\mathbf{J}(\phi)|$$

$$|\mathbf{J}(\mathbf{\alpha}, \sigma)| = \frac{2^{J+1}(K-J)}{\sigma^2} \prod_{j=1}^{J} \frac{\alpha_j^2}{(\alpha_j^2 + \sigma^2)^2}$$

$$|\mathbf{J}(\phi)| = |\mathbf{J}_{\mathbf{A} \to \phi}|^2 \left( \prod_{i=1}^{J} \frac{\alpha_i^4}{\sigma^2} \right)^{K-J} \left( \frac{1}{(\alpha_i^2 + \sigma^2)^{K-i}} \right) \prod_{j<k} (\alpha_j^2 - \alpha_k^2)^2$$

where $|\mathbf{J}_{\mathbf{A} \to \phi}|$ is the transformation of measure under the Givens representation [Pourzanjani et al., 2021]

$$|\mathbf{J}_{\mathbf{A} \to \phi}| = \prod_{i=1}^{J} \prod_{j=i+1}^{K} (\cos(\phi_{i,j}))^{j-i-1},$$
and $P = (D + J + 1)$ is the total number of free parameters. Combining all the terms we have

$$
|J(\alpha, \sigma, \phi)| = N^P \left( \frac{2^{J+1}(K-J)}{\sigma^2} \right) |J_A| \cdot \alpha_i^2 \left( \prod_{i=1}^{J} \left( \frac{\alpha_i^2}{\sigma^2} \right) \right) \left( \frac{\alpha_i^4}{\sigma^2} \right)^{K-J-1} \prod_{j<k} (\alpha_j^2 - \alpha_k^2)^2
$$

$$
= \frac{N^P 2^{J+1}(K-J)}{\sigma^{2J(K-J)+1}} \prod_{i=1}^{J} \left( \frac{\alpha_i^4}{\sigma^2} \right)^{K-J+2} \prod_{j<k} (\alpha_j^2 - \alpha_k^2)^2.
$$

(23)

### 3.3 Prior information

The prior distribution for the residual standard deviation $\Sigma^{1/2}$ is chosen to be the scale-invariant density

$$
\pi_\sigma(\sigma) \propto \sigma^{-1},
$$

defined over some suitable range.

The prior distribution for the matrix of factor loads $A \in \mathbb{R}^{K \times J}$ is not immediately obvious as the estimates of the factor loads are enforced to be mutually orthogonal. Ideally, we would like a prior distribution that is uniform over the direction of the $J$ factors, while the distribution of the lengths of these vectors should be heavy tailed to allow for a wide range of lengths. We follow a similar approach to [Wallace, 1998] and assume a prior distribution over the unknown latent vectors that is then transformed to account for the estimated factors being mutually orthogonal. Further, as in [Wallace, 1998], we shall consider a prior distribution for the scaled factors

$$
b_j = A_j / \sigma, \quad \beta_j = (b_j^T b_j)^{1/2}, \quad (j = 1, \ldots, J)
$$

where the residual variance is used as a default scale. Let $\hat{B} \in \mathbb{R}^{K \times J}$ denote the matrix containing the $J$ true (unknown) scaled factors. We assume $\hat{B}$ to follow a matrix variate Cauchy distribution [Bandekar and Nagar, 2003] with probability density function

$$
\pi_{\hat{B}}(\hat{B}) = \frac{1}{\pi^{KJ/2} \Gamma(J/2)^{-\frac{J+1}{2}}} \left| I_K + \hat{B} \hat{B}^T \right|^{-(K+J)/2}.
$$

(25)

This is a reasonable choice as the matrix variate Cauchy is spherically symmetric and has appropriate heavy tails. Further, our choice of the prior distribution implies that $B' \in \mathbb{R}^{J \times K}$ follows a matrix variate Cauchy distribution with density

$$
\pi_B(B') = \frac{1}{\pi^{KJ/2} \Gamma(J/2)^{-\frac{J+1}{2}}} \left| I_J + B' B' \right|^{-(K+J)/2}.
$$

(26)

Consider the unique matrix polar decomposition

$$
\hat{B}' = W_B^\frac{1}{2} H_B, \quad W_B = B' \hat{B}, \quad H_B = (\hat{B}' \hat{B})^{-\frac{1}{2}}
$$

(27)

where $H_B$ is defined over the Stiefel manifold $\mathcal{V}_J(\mathbb{R}^K)$ and $W_B$ is a symmetric positive definite matrix. We may think of the matrix $H_B$ as the orientation matrix, while the matrix $W_B$ determines the squared lengths of the true scaled latent vectors. If $B'$ follows a matrix variate Cauchy distribution, it is known that $H_B$ is distributed uniformly over the Stiefel manifold with density function [Bandekar and Nagar, 2003]:

$$
\pi_H(H_B) = \frac{1}{\text{Vol}(\mathcal{V}_J(\mathbb{R}^K))}, \quad \text{Vol}(\mathcal{V}_J(\mathbb{R}^K)) = 2^{J/2} \pi^{KJ/2} \Gamma(J/2),
$$

(28)

where $\Gamma_p(y)$ is the multivariate Gamma function

$$
\Gamma_J(y) = \pi^{J(J-1)/4} \prod_{j=1}^{J} \Gamma(y + (1 - j)/2).
$$

Further, the random variable $W_B$ representing the squared lengths of the true scaled factors is independent of $H_B$ with probability density function [Bandekar and Nagar, 2003]

$$
\pi_W(W_B) \propto \det(W_B)^{(K-J-1)/2} \det(I_K + W_B)^{-(K+J)/2}.
$$

(29)

which is a matrix variate beta type II distribution $W_B \sim B_{(K/2, J/2)}^{(K-J-1)/2}$ with parameters $(K/2, J/2)$ (see [Gupta and Nagar, 1999], pp. 166, for further details); this is also known as the matrix variate $F$ distribution. Recall that the estimated (scaled) factor load vectors obey

$$
S_B = \hat{B} \hat{B}' = \sum_{j=1}^{J} \hat{\beta}_j \hat{\beta}_j' = \sum_{j=1}^{J} \beta_j \beta_j' = BB', \quad \beta_j' \beta_k' \neq 0.
$$

(30)
where \( S_B \) is a \((K \times K)\) symmetric matrix of rank \( J \). The distribution of the squared scaled lengths \( \beta^2 \) of the estimated latent factors can then be taken as the joint distribution of the \( J \) eigenvalues of \( S_B \) which is (see Appendix F)

\[
\pi_{\beta^2}(\beta^2_1, \ldots, \beta^2_J) = \frac{\pi^{J/2}}{\Gamma_J(J/2)\Gamma_J(2, J/2)} \prod_{j=1}^{J} \beta_j^{(K-J)(1 + \beta^2_j)^{-1}} \prod_{j<k} |\beta_j^2 - \beta_k^2|,
\]

where \( \pi_{\beta^2}(a, b) \) denote the multivariate beta function

\[
\pi_{\beta^2}(a, b) = \frac{\Gamma_J(a) \Gamma_J(b)}{\Gamma_J(a + b)}.
\]

This implies that the prior distribution of the lengths of the scaled latent factors is

\[
\pi_{\beta}(\beta_1, \ldots, \beta_J) = \frac{2^J \pi^{J^2/2}}{\Gamma_J(J/2)\Gamma_J(K/2, J/2)} \prod_{j=1}^{J} \beta_j^{(K-J)(1 + \beta_j^2)^{-1}} \prod_{j<k} |\beta_j^2 - \beta_k^2|.
\]

Finally, the prior distribution for the lengths of the (unscaled) latent factors is

\[
\pi_{\alpha}(\alpha_1, \ldots, \alpha_J) = \frac{2^J \pi^{J^2/2} \sigma^{J^2}}{\Gamma_J(J/2)\Gamma_J(K/2, J/2)} \prod_{j=1}^{J} \alpha_j^{(K-J)(\sigma^2 + \alpha_j^2)^{-1}} \prod_{j<k} |\alpha_j^2 - \alpha_k^2|.
\]

The complete prior distribution over all model parameters is

\[
\pi(\alpha, \sigma, \phi) = \pi_{\sigma}(\Sigma^{1/2}) \pi_{\alpha}(\alpha_1, \ldots, \alpha_J) |J_{A \rightarrow \phi}| J!,
\]

where the term \( J! \) is included because the labelling of the latent factors is arbitrary and \( |J_{A \rightarrow \phi}| \) is the transformation of measure from the matrix parametrization \( A \) to the orthogonality-preserving parameterization based on Givens rotations.

### 3.4 Codelength

Omitting constants, the MML codelength [Wallace and Freeman, 1987] for the probabilistic PCA model is

\[
\mathcal{I} \propto \frac{N}{2} \log |\Sigma| + \frac{N}{2} \text{tr} (\Sigma^{-1} S_x) - KJ \log(\sigma) + \frac{1}{2} \sum_{j=1}^{J} \log \left[ \alpha_j^{2(K-J+1)} (\alpha_j^2 + \sigma^2)^{(J-1)} \right]
\]

where \( S_x = \frac{1}{N} \sum_i x_i x_i^T \) is the sample variance-covariance matrix. To obtain MML estimates, we start with the Lagrangian of the factor orientations

\[
\psi(R) = \log |\Sigma| + \text{tr} (\Sigma^{-1} S_x) - \text{tr} L(R R^T - I),
\]

where \( L \) is a \( J \times J \) symmetric matrix of Lagrange multipliers. Clearly, minimising \( \psi(R) \) is equivalent to minimising the codelength with respect to \( R \). The first differential of the Lagrangian is

\[
\partial \psi(R) = 2\text{tr} \left[ \alpha A' (\Sigma^{-1} - \Sigma^{-1} S_x \Sigma^{-1}) (dR) \right] - 2\text{tr} (LR' (dR)),
\]

which implies the following first order conditions

\[
\alpha A' (\Sigma^{-1} - \Sigma^{-1} S_x \Sigma^{-1}) = 0 \quad \text{(34)}
\]

\[
LR' = 0 \quad \text{(35)}
\]

\[
R' R = I_J \quad \text{(36)}
\]

From (35) we have that \( L = 0 \) and from (34)

\[
S_x R = \text{R diag} (\sigma^2 + \alpha^2_1, \ldots, \sigma^2 + \alpha^2_J)
\]

\[
S_x r_j = r_j (\sigma^2 + \alpha^2_j), \quad (j = 1, \ldots, J).
\]

We see that, at the codelength minimum, the MML estimate of the factor orientations is the matrix \( R \) whose columns are the top \( J \) eigenvectors of the variance–covariance matrix \( S_x \) with eigenvalues \( \delta_j = (\sigma^2 + \alpha^2_j) \), for \( j = 1, \ldots, J \).
This is identical to the corresponding maximum likelihood estimate. The concentrated codelength, as a function of $\sigma^2$ is

$$\mathcal{I}(\sigma) \propto \frac{N}{2} \log \left( (\sigma^2)^{-J} \prod_{j=1}^{J} (\alpha_j^2 + \sigma^2) \right) + \frac{N}{2\sigma^2} \left( \sum_{j=1}^{K} \delta_j \right) - \frac{N}{2\sigma^2} \sum_{j=1}^{J} \alpha_j^2$$

$$- KJ \log(\sigma) + \frac{1}{2} \sum_{j=1}^{J} \log \left[ \alpha_j^{2(K-J+1)} (\alpha_j^2 + \sigma^2)^{(J-1)} \right]$$

$$= \frac{N(K-J)-KJ}{2} \log(\sigma^2) + \frac{N}{2\sigma^2} \left( \sum_{j=1}^{K} \delta_j \right) - \frac{N}{2\sigma^2} \sum_{j=1}^{J} (\delta_j - \sigma^2) + \frac{(K+J-1)}{2} \sum_{j=1}^{J} \log (\delta_j - \sigma^2)$$

(37)

The following theorem shows how to obtain the MML estimate of the residual variance from the concentrated message length.

**Theorem 1.** Let $\tau = \sigma^2$. The concentrated codelength (37) has $(J+1)$ stationary points whose location are the roots of the $n = (J+1)$-degree polynomial

$$a_n \tau^n + a_{n-1} \tau^{n-1} + \cdots + a_1 \tau + a_0, \quad (0 < \tau < \delta_J)$$

with coefficients

$$a_0 = -\hat{\tau}_{\text{ML}} e_J,$$

$$a_j = (-1)^{j+1} \left[ \hat{\tau}_{\text{ML}} e_{J-j} + \left( 1 - \frac{(j-1)(J-1)}{N(K-J)} - \frac{K(J-J+1)}{N(K-J)} \right) e_{J-j+1} \right], \quad (1 \leq j \leq J)$$

$$a_n = (-1)^J \left[ 1 - \frac{J(J-1)}{N(K-J)} \right]$$

where $\hat{\tau}_{\text{ML}}$ is the maximum likelihood estimate of the residual variance and $e_i$ denote elementary symmetric polynomials $e_i(\delta_1, \ldots, \delta_J)$ in $J$ variables $(\delta_1, \ldots, \delta_J)$. For example, for $J = 3$, we have the following four elementary symmetric polynomials

$$e_0(\delta_1, \delta_2, \delta_3) = 1,$$

$$e_1(\delta_1, \delta_2, \delta_3) = \delta_1 + \delta_2 + \delta_3,$$

$$e_2(\delta_1, \delta_2, \delta_3) = \delta_1 \delta_2 + \delta_1 \delta_3 + \delta_2 \delta_3,$$

$$e_3(\delta_1, \delta_2, \delta_3) = \delta_1 \delta_2 \delta_3.$$

**MML estimate of the residual variance** $\hat{\sigma}^2_{\text{MML}}$ is the stationary point in the domain $0 < \tau < \delta_J$ that yields the shortest codelength. MML estimates of the factor lengths can be obtained from $\hat{\delta}_j = (\delta_j - \hat{\sigma}^2_{\text{MML}})^{\frac{1}{2}}$ for all $j = 1, \ldots, J$.

Importantly, all $(J+1)$ elementary symmetric polynomials can be efficiently computed in $O(J \log^2 J)$ time by Fast Fourier Transform polynomial multiplication, following an algorithm widely attributed to Ben-Or.

**Example 1:** For a single latent factor ($J = 1$), the stationary points of the concentrated codelength are the roots of the quadratic polynomial in $\tau$:

$$-\delta_1 \hat{\tau}_{\text{ML}} + (\hat{\tau}_{\text{ML}} + c \delta_1) \tau - \tau^2 = 0, \quad c = 1 - \frac{K}{N(K-1)},$$

(38)

given by

$$\frac{1}{2} \left( \hat{\tau}_{\text{ML}} + c \delta_1 \pm \Delta^{\frac{1}{2}} \right), \quad \Delta = c^2 \delta_1^2 + 2(c-2)\delta_1 \hat{\tau}_{\text{ML}} + \hat{\tau}_{\text{ML}}^2.$$

The quadratic polynomial has no real roots if:

$$- \frac{c + 2\sqrt{1-c} - 2}{c^2} < \frac{\delta_1}{\hat{\tau}_{\text{ML}}} < - \frac{c + 2\sqrt{1-c} + 2}{c^2}$$

(39)
in which case the MML solution is the uncorrelated multivariate Gaussian model. For example, when \( N = 25 \) and \( K = 4 \), the quadratic will have no real roots if
\[
0.219 < \frac{\delta_1}{\delta_2 + \delta_3 + \delta_4} < 0.564.
\]
In the limit as \( N \to \infty \), we have
\[
\lim_{N \to \infty} \pm \frac{c + 2\sqrt{1-c} - 2}{c^2} = 1.
\]
so that both the lower and upper bound in (39) approach 1.

**Example 2:** For a PCA model with two latent factors \((J = 2)\), the stationary points of the concentrated code length are the roots of the cubic polynomial in \(\tau\):
\[
-\delta_1 \delta_2 \hat{\sigma}_{\text{ML}} + ((\delta_1 + \delta_2) \hat{\sigma}_{\text{ML}} + c_1 \delta_1 \delta_2) \tau - (\hat{\sigma}_{\text{ML}} + (c_0 + c_1) (\delta_1 + \delta_2)) \tau^2 + (2c_0 + c_1) \tau^3
\]
where the constants
\[
c_0 = \frac{K - 1}{N(K - 2)}, \quad c_1 = 1 - \frac{2K}{N(K - 2)},
\]
depend only on \(N\) and \(K\).

### 4 Experiments

#### 4.1 Parameter estimation

This section compares the newly derived MML parameter estimates for the probabilistic PCA model to the standard approach based on the maximum likelihood estimator. Since MML and maximum likelihood estimates of the factor lengths (for a given \(\sigma^2\)) and factor orientations are identical, the key difference between the two approaches is in the estimation of the residual variance. Our simulation experiments are loosely based on Section 6 in [Wallace, 1998]. We conducted \(10^5\) simulations for each combination of the sample size \(N \in \{25, 50, 100\}\), the dimensionality of the data \(K \in \{5, 8, 16\}\) and the number of estimated latent factors \(J \in \{1, 2, 4\}\). As both maximum likelihood and MML are scale invariant, the residual variance was set to \(\sigma^2 = 1\) and the factors lengths were \(\alpha_j = 1 (j = 1, \ldots, J)\) for each simulation run, without loss of generality. The factor directions were randomly sampled from a unit \(K\)-sphere.

We used the three performance metrics discussed in [Wallace, 1998] to evaluate the estimators:
\[
S_1 = \log \hat{\sigma}, \quad S_2 = (\log \hat{\sigma})^2,
\]
and the Kullback–Leibler (KL) divergence [Kullback and Leibler, 1951] between two multivariate Gaussian distributions
\[
\text{KL}(\Sigma_0, \Sigma_1) = \frac{1}{2} \left( \text{tr}(\Sigma_1^{-1} \Sigma_0) + \log \left( \frac{\Sigma_1}{\Sigma_0} \right) - K \right).
\]
which only depends on the variance-covariance matrices of the two models. The first metric \(S_1\) is a measure of bias, while \(S_2\) measures error in any direction. Both \(S_1\) and \(S_2\) are zero for exact estimates as the true residual variance was \(\sigma^2 = 1\) in all experiments. The error measures were specifically chosen as they do not depend on the number of estimated latent vectors \(J\). Simulation results averaged over \(10^5\) iterations are shown in Table 1.

The MML estimate of the residual variance was found to be superior to the usual maximum likelihood estimate for all tested combinations of sample sizes, data dimensionality and the number of latent vectors. Maximum likelihood appeared to underestimate the residual variance more strongly compared to the minimum message length estimate. The differences in the performances of the two estimates were most pronounced when the sample size and data dimensionality was small \((N \leq 50, K = 5)\).

#### 4.2 Model selection

We have also compared the performance of MML model selection against the highly popular Bayesian information criterion (BIC) and Laplace’s method for approximating the marginal distribution of the data [Minka, 2000], referred to as ‘Bayes’ henceforth. Using numerical experiments, [Minka, 2000] demonstrated that approximating Bayesian evidence is superior to methods like cross validation. The simulation setup was identical to Section 4.1 except the sample size was \(N \in \{50, 100\}\), the dimensionality of the data \(K = 10\) and the number of estimated latent factors \(J \in \{1, 2, 4\}\). Simulation results, averaged over \(10^5\) iterations, are shown in Table 2. As expected, both MML and the Bayes method have similar performance and both improve significantly over the popular BIC criterion.
While any reasonable Bayesian approach to the PCA model with sensible priors is expected to yield similar performance to our MML codelength, MML also provides the practitioner with point estimates for all model parameters. Unlike, say, the maximum a posteriori estimate, the MML estimates are invariant to reparametrisation of the model and are obtained by simply minimising the codelength. Importantly, the MML codelength is a universal yardstick that allows comparison of models across different model structures (e.g., generalized linear model [Schmidt and Makalic, 2013] vs a decision tree [Wallace and Patrick, 1993]) and numbers of parameters. This means that we can use our MML codelength to discriminate between multivariate Gaussian models with specific covariance structures. For example,
Table 2: Model selection simulation results for minimum message length (MML), Bayesian information criterion (BIC) and Laplace’s method for estimating Bayesian evidence averaged over $10^5$ simulations. In all experiments, data dimensionality was $K = 10$.

| $N$ | $J$ | Method | KL Divergence | Model Selection (%) |
|-----|-----|--------|---------------|---------------------|
|     |     |        | $< J$ | $= J$ | $> J$ |
| 1   | 0.060 | MML | 99.55 | 0.45 |
|     | 0.063 | BIC | 100.00 | 0.00 |
|     | 0.066 | Bayes | 97.19 | 2.81 |
| 50  | 0.126 | MML | 70.40 | 28.32 | 1.27 |
|     | 0.129 | BIC | 52.52 | 45.17 | 2.31 |
|     | 0.198 | Bayes | 81.00 | 5.78 | 13.22 |
| 4   | 0.257 | MML | 99.99 | 0.01 | 0.00 |
|     | 0.209 | BIC | 91.09 | 7.92 | 0.98 |

we can use the MML codelength to test the hypothesis that the covariance matrix is spherical versus a more general covariance structure (e.g., the PCA model).

Additionally, the MML codelength derived in this manuscript allows the PCA model to be incorporated into other component-based models with all the advantages of MML (i.e., automatic model selection and improved parameter estimation). For example, we could incorporate the MML PCA codelength into a finite mixture model to create mixtures of probabilistic principal component analyzers, similar to [Edwards and Dowe, Tipping and Bishop, 1999b]. Alternatively, we can use the MML PCA model in the leaves of a decision tree, similar to the Max-Cut model in [Bodine and Hochbaum, 2022].

Appendix A. Joint eigenvalue distribution for the central $F$ matrix

A $(p \times p)$ random symmetric positive definite matrix has a matrix variate beta type II distribution with parameters $(a, b)$ if it has the probability density function

$$f(V) = \frac{\Gamma_p(a + b)}{\Gamma_p(a) \Gamma_p(b)} \det(V)^{(a-(p+1)/2) \det(I_p + V)^{-(a+b)}}$$

where $a > (p - 1)/2$ and $b > (p - 1)/2$. We write $V \sim B_{p}^{II}(a, b)$ to denote this distribution, which is also known as the matrix variate $F$ distribution. Let $B_p(a, b)$ denote the multivariate beta function

$$B_p(a, b) = \frac{\Gamma_p(a) \Gamma_p(b)}{\Gamma_p(a + b)}.$$ (41)

Consider the random variable $V \sim B_{p}^{II}(\nu_1/2, \nu_2/2)$ and the transformation $V = H\Lambda H'$ from $V$ to its eigenvalues $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_p)$ and eigenvectors $H$, where $H \in O(p)$ is in the orthogonal group with the $j$-th column being the normalized eigenvector of $V$ corresponding to the eigenvalue $\lambda_j$. The joint distribution of the $p$ eigenvalues $\Lambda$ of $V$ is ([Muirhead, 1982], Theorem 3.2.17, pp. 104)

$$\pi_{\Lambda}(\lambda_1, \ldots, \lambda_p) = \frac{\pi p^{p/2}}{\Gamma_p(p/2)} \prod_{i<j} |\lambda_i - \lambda_j| \int_{O(p)} f(H\Lambda H')(dH).$$ (42)
The integral can be evaluated as follows

\[
\int_{O(p)} f(HA'H)(dH) = \frac{1}{B_p(n_1/2, n_2/2)} \prod_{j=1}^{p} \lambda_j^{(n_1-p-1)/2} (1 + \lambda_j)^{-(n_1+n_2)/2} \int_{O(p)} (dH)
\]

\[
= \frac{1}{B_p(n_1/2, n_2/2)} \prod_{j=1}^{p} \lambda_j^{(n_1-p-1)/2} (1 + \lambda_j)^{-(n_1+n_2)/2}
\]

(43)

where (see [Muirhead, 1982], pp. 104)

\[
\int_{O(p)} (dH) = 1.
\]

(44)

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