Cross Entropy Approximation of Structured Covariance Matrices

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\textbf{Abstract:} We apply two variations of the principle of Minimum Cross Entropy (the Kullback information measure) to fit parameterized probability density models to observed data densities. For an array beamforming problem with $P$ incident narrowband point sources, $N > P$ sensors, and colored noise, both approaches yield eigenvector fitting methods similar to that of the MUSIC algorithm\cite{1}. Furthermore, the corresponding cross-entropies are related to the MDL model order selection criterion\cite{2}.

\textbf{Key words and phrases:} Array Beamforming, Eigenvector methods, Kullback Information Measure, Minimum Cross Entropy, Stochastic Estimation, Structured Covariance

1. Introduction

Many existing high resolution methods for spectral analysis and for optimal beamforming utilize covariance matrices estimated from observed data. Often, an underlying structure for the covariance matrix is known in advance, and our goal is to estimate the covariance matrix with this structure which best fits the observed data. Previous literature has suggested a variety of methods of optimally estimating structured covariance matrices from data\cite{3,4,5}. In this paper, we will apply the minimum cross entropy (CE)\cite{6,7} and minimum reverse cross-entropy (RCE)\cite{6} principles to estimate the covariance matrix. These principles have proved to be quite powerful in a wide variety of signal processing applications\cite{8,9} and have been justified as being ”optimal” under suitable assumptions. In section 2, we apply the CE and RCE procedures to the problem of estimating structured covariance matrices, and in section 3 we demonstrate the utility of the idea for a beamforming application.
2. Problem Statement

Let \( \mathbf{x} \) be an \( N \)-dimensional real or complex random vector. Assume that a Gaussian probability density for \( \mathbf{x} \) is either known a prior, or has been estimated by some procedure from observed data:

\[
p(\mathbf{x}) = N(\mathbf{m}, R)
\]

where \( \mathbf{m} \) is the expected value of \( \mathbf{x} \) and \( R \) is the covariance matrix, \( R = E[\mathbf{x}\mathbf{x}^H] \), and where \( \mathbf{x}^H \) is the Hermitian (complex conjugate transpose) of \( \mathbf{x} \). Suppose we wish to approximate this \( p(\mathbf{x}) \) with a parameterized probability density function (PDF):

\[
q_{\theta}(\mathbf{x}) = N(m_\theta, R_\theta)
\]

where \( \theta \) denotes the unknown parameters \( \theta \) in the model \( q_{\theta}(\mathbf{x}) \) which are to be estimated. Conceptually, we wish to choose \( \theta \) to make \( q_{\theta}(\mathbf{x}) \) optimally match \( p(\mathbf{x}) \). An appropriate objective function is the Kullback information measure[6], otherwise known as the Minimum Cross-Entropy principle[7]. Because this measure is asymmetric, we can apply it in two different ways to this problem. Following[8,9,10] we call these the "Cross-Entropy" and "Reverse Cross-Entropy" methods:

\[
CE : \quad \hat{q}_{\theta} \leftarrow \min_{\theta} H(q_{\theta}, p)
\]

\[
RCE : \quad \hat{q}_{\theta} \leftarrow \min_{\theta} H(p, q_{\theta})
\]

where:

\[
H(p_1, p_2) = \int p_1(\mathbf{x}) \log \frac{p_1(\mathbf{x})}{p_2(\mathbf{x})} d\mathbf{x}
\]

Kullback[6] has argued that \( H(p_1, p_2) \) measures the mean amount of information for discriminating in favor of the hypothesis that \( p_1 \) is the correct density of \( \mathbf{x} \) rather than \( p_2 \). Shore and Johnson[7] have argued that minimizing \( H(p_1, p_2) \) over \( p_1 \) is the only consistent estimation procedure for estimating a PDF given an a priori density estimate \( p_2(\mathbf{x}) \) combined with new structural information about the density, such as one or more of its moments. The measure \( H(p_1, p_2) \) has several pleasing mathematical properties: it is convex in \( p_1 \), and convex in \( p_2 \), and attains
its minimum value of zero when \( p_1(x) = p_2(x) \) almost everywhere. Another useful property is that estimating \( \theta \) from either (3) or (4) is straightforward. Substitute (1) and (2) into the CE and RCE formulas to obtain:

\[
\text{CE : } H(q_\theta, p) = \xi \left\{ \text{tr} \left( R^{-1} R_\theta \right) - N \log |R^{-1} R_\theta| + (m_\theta - m)^H R^{-1} (m_\theta - m) \right\}
\]

\[
\text{RCE : } H(p, q_\theta) = \xi \left\{ \text{tr} \left( R^{-1} R_\theta \right) - N \log |R^{-1} R_\theta| + (m_\theta - m)^H R^{-1} (m_\theta - m) \right\}
\]

where \( \xi = 1/2 \) when \( x \) is real and \( \xi = 1 \) when \( x \) is complex.

To simplify the remainder of the discussion, assume that the mean is known, \( m_\theta = m \), so that we can focus on the estimation of the covariance matrix and compare the results with those by Burg and Gray [4] and Gray, Anderson, Sim[5]. The two estimation problems reduce to minimizing:

\[
\text{CE : } H(q_\theta, p) = \xi \left\{ \text{tr} \left( R^{-1} R_\theta \right) - N \log |R^{-1} R_\theta| \right\} \quad (6)
\]

\[
\text{RCE : } H(p, q_\theta) = \xi \left\{ \text{tr} \left( R^{-1} R_\theta \right) - N \log |R^{-1} R_\theta| \right\} \quad (7)
\]

Setting the gradients of the above two objective functions with respect to \( \theta \) to zero, we obtain the necessary conditions that \( \hat{\theta} \) be the optimal solution:

\[
\text{CE: } \left. \text{tr} \left\{ (R^{-1} - R_\theta^{-1}) \frac{\partial R_\theta}{\partial \theta} \right\} \right|_{\theta = \hat{\theta}} = 0 \quad (8)
\]

\[
\text{RCE: } \left. \text{tr} \left\{ (R - R_\theta) \frac{\partial R_\theta^{-1}}{\partial \theta} \right\} \right|_{\theta = \hat{\theta}} = 0 \quad (9)
\]

for all \( i \), where \( \theta_i \) is the \( i^{th} \) element of \( \theta \). When \( R_\theta \) is invertible and differentiable in \( \theta \):

\[
\frac{\partial R_\theta^{-1}}{\partial \theta_i} = -R_\theta^{-1} \frac{\partial R_\theta}{\partial \theta_i} R_\theta^{-1} \quad (10)
\]

Substituting this into the RCE formula gives an alternate set of necessary conditions for the optimal RCE solution:

\[
\text{RCE: } \left. \text{tr} \left\{ (R_\theta^{-1} RR_\theta^{-1} - R_\theta^{-1}) \frac{\partial R_\theta}{\partial \theta} \right\} \right|_{\theta = \hat{\theta}} = 0 \quad (11)
\]
3. Application to Array Beamforming

In this section we will apply the CE and RCE methods to fitting a low rank plus noise covariance matrix to data. Such problems arise in a variety of contexts, including narrowband sensor array processing and harmonic retrieval. We focus on the former problem. Let \( x[n] = (x_1[n], \ldots, x_N[n])^T \) be a vector of sensor measurements at time \( n \), where \( N \) is the total number of sensors in the array. Assume that the signal is narrowband (perhaps because the sensor data has been preprocessed through a Fast Fourier Transform of each sensor’s data). Let our initial PDF estimate for the data be given by \( p(x[n]) = N(0, R) \), where \( R \) is any non-parameterized estimate of the signal covariance, such as
\[
R = \frac{1}{K} \sum_{k=1}^{K} x[k] x^H[k]
\]
where \( K \) snapshots of array data are used.

Now suppose we wish to model the data \( x[n] \) as:
\[
x[n] = \sum_{i=1}^{P} s_i[n] u_i + \sigma w[n]
\] (12)

where \( s_1[n], \ldots, s_P[n] \) are \( P \) source signals, \( P < N \), arriving from unknown directions \( u_1, \ldots, u_P \), with additive noise \( w[n] \) with gain \( \sigma \). Suppose that signals \( s_i[n] \) are statistically independent, real or complex zero mean Gaussian random variables with covariance \( \Lambda_i > 0 \), and that the noise samples \( w[n] \) are statistically independent, real or complex zero mean Gaussian random variables with covariance \( W \).

\[
p(s_i[n]) = N(0, \Lambda_i)
\] (13)
\[
p(w[n]) = N(0, W)
\] (14)

Thus the parameterized model PDF of \( x[n] \) is Gaussian:
\[
q_\theta(x[n]) = N(0, R_\theta)
\] (15)

where:
\[
R_\theta = \sum_{i=1}^{P} \Lambda_i u_i u_i^H + \sigma^2 W
\] (16)

We will assume that the noise covariance \( W \) is known, but that all the other
parameters $\theta = (\Lambda_1, ..., \Lambda_P, u_1, ... u_P, \sigma)^T$ must be estimated. For convenience, define:

$$R_\theta = U \Lambda U^H + \sigma^2 W$$

where:

$$U = \begin{bmatrix} u_1 & u_2 & ... & u_P \end{bmatrix} \quad \text{and} \quad \Lambda = \begin{bmatrix} \Lambda_1 & 0 & \cdots & 0 \\ 0 & \Lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Lambda_P \end{bmatrix}$$

Suppose there are no a priori constraints on the matrix $U$, and that the only constraints on $\Lambda$ are that $\Lambda_i > 0$. This would typically be true if the array were uncalibrated, or subject to heavy unknown multipath distortion. (Note that because we assume an uncalibrated array, we will not be able to directly derive information about the direction of arrival.) Appendices A and B apply the CE and RCE criteria to this model. They show that the solution to these two problems are quite similar, and can be found by the following algorithm:

**CE and RCE BEAMFORMING ALGORITHMS**

1. Find the generalized eigenvector $u_i$ and eigenvalue $\lambda_i$ solutions to:

$$\lambda_i R_{\theta}^{-1} u_i = W^{-1} u_i$$

with normalization constraint $u_i^H W^{-1} u_j = \delta_{i,j}$.

2. Sort the eigenvectors and eigenvalues so that $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N$. Then the optimal structured covariance matrix approximation $\hat{R}_\theta$ to $R$ is:

$$\hat{R}_\theta = \left( \begin{array}{ccc} u_1 & u_2 & \cdots & u_P \end{array} \right) \begin{pmatrix} \lambda_1 - \hat{\sigma}^2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ 0 & \cdots & \lambda_P - \hat{\sigma}^2 \end{pmatrix} \begin{pmatrix} u_1^H \\ u_2^H \\ \vdots \\ u_P^H \end{pmatrix} + \hat{\sigma}^2 W$$
where:

\[
\begin{cases}
\frac{1}{\hat{\sigma}^2} = \frac{1}{N-P} \sum_{i=P+1}^{N} \frac{1}{\lambda_i} \quad \text{for CE} \\
\hat{\sigma}^2 = \frac{1}{N-P} \sum_{i=P+1}^{N} \lambda_i \quad \text{for RCE}
\end{cases}
\] (21)

3. The cross entropy for the optimal model is:

CE: \[ H(\hat{q}_\theta, p) = \xi \sum_{i=P+1}^{N} \log \left( \frac{\lambda_i}{\hat{\sigma}_i^2} \right) \] (22)

RCE: \[ H(p, \hat{q}_\theta) = \xi \sum_{i=P+1}^{N} \log \left( \frac{\hat{\sigma}_i^2}{\lambda_i} \right) \] (23)

The estimates of \( \hat{R}_\theta \) and \( \hat{\sigma}^2 \) will be unique if and only if \( \lambda_P > \lambda_{P+1} \). (The estimate of \( U \) will not be unique.)

An interesting alternative form for the cross-entropy formulas can be found by substituting the value of \( \hat{\sigma}^2 \) from (21) into (22):

CE: \[ H(\hat{q}_\theta, p) = \xi (N-P) \log \left( \frac{\left[ \frac{1}{\lambda_{P+1}}, \ldots, \frac{1}{\lambda_N} \right]_{\text{avg}} \right.}{\left[ \frac{1}{\lambda_{P+1}}, \ldots, \frac{1}{\lambda_N} \right]_{\text{geo}}} \] (24)

RCE: \[ H(p, \hat{q}_\theta) = \xi (N-P) \log \left( \frac{\left[ \lambda_{P+1}, \ldots, \lambda_N \right]_{\text{avg}}}{\left[ \lambda_{P+1}, \ldots, \lambda_N \right]_{\text{geo}}} \right) \] (25)

where:

\[
[\beta_{P+1}, \ldots, \beta_N]_{\text{avg}} = \frac{1}{N-P} \sum_{i=P+1}^{N} \beta_i \\
[\beta_{P+1}, \ldots, \beta_N]_{\text{geo}} = (\beta_{P+1} \beta_{P+2} \cdots \beta_N)^{1/(N-P)}
\] (26) (27)

The cross-entropies are proportional to the log of the ratio of the arithmetic mean to the geometric mean of the eigenvalues (or their inverses) that are not used in building \( U \). The cross-entropy will therefore be positive, and will attain their minimum value of zero only if the geometric average of \( \lambda_{P+1}, \ldots, \lambda_N \) (or their inverses) equals their arithmetic mean. This will only occur if these \( N-P \)
smallest generalized eigenvalues are all equal.

Note the similarity of the RCE formula to the MDL order determination algorithm suggested by Wax and Kailath[2]. The RCE criterion is also strongly related to the Maximum Likelihood problem of estimating the structured covariance matrix given observations \( \mathbf{x}_1, \ldots, \mathbf{x}_K \):

\[
\hat{R}_\theta \leftarrow \max_\theta \log p(\mathbf{x}_1, \ldots, \mathbf{x}_K | \theta)
\]  \hspace{1cm} (28)

where:

\[
p(\mathbf{x}_1, \ldots, \mathbf{x}_K | \theta) = \prod_{i=1}^{K} p(\mathbf{x}_i | \theta)
\]  \hspace{1cm} (29)

and:

\[
p(\mathbf{x}_i | \theta) = N(0, R)
\]  \hspace{1cm} (30)

This is because:

\[
H(p, q_\theta) = \frac{1}{K} \log p(\mathbf{x}_1, \ldots, \mathbf{x}_K | \theta) - \xi(N + \log |R|)
\]  \hspace{1cm} (31)

Since the second term in (31) does not depend on \( \theta \), the RCE estimate of \( R_\theta \) will be identical to the ML estimate.

For the special case when the background noise is white Gaussian noise, \( W = I \), the \( \mathbf{u}_i \) must satisfy:

\[
R\mathbf{u}_i = \lambda_i \mathbf{u}_i
\]  \hspace{1cm} (32)

and thus the \( \mathbf{u}_i \) are the eigenvectors of the observed data correlation matrix \( R \). This special case is thus quite similar to that used in the MUSIC algorithm[1] and other similar beamforming algorithms.

If subroutines for computing generalized eigenvectors are not available, we can use subroutines for computing eigenvectors of symmetric positive definite matrices as follows. Factor \( W = W^{1/2}W^{H/2} \) where \( W^{1/2} \) is any square root of \( W \) and \( W^{H/2} \) is its Hermitian. Then to compute the \( \mathbf{u}_i \):

1. From the whitened data correlation matrix:

\[
\tilde{R} = W^{-1/2}RW^{-H/2}
\]  \hspace{1cm} (33)
where $W^{-1/2}$ is the inverse of $W^{1/2}$. Note that $\tilde{R}$ is symmetric and positive definite.

2. Solve for the eigenvectors $t_j$ and corresponding eigenvalues $\lambda_i$ of $\tilde{R}$.

$$\tilde{R} t_j = \lambda_i t_j$$

(34)

where $t_j^T t_i = \delta_{i,j}$. Sort these so that the eigenvalues are in descending order.

3. Then:

$$u_i = W^{1/2} t_i$$

(35)

It is also interesting to consider the effect of using the structured covariance matrix estimate when forming either a classical or optimal beamformer. Let $w_0$ be the ideal array response for a signal in a particular direction. The classical beamformer estimates the signal $s[n]$ from the array data as $s[n] = w_0^T x[n]$. The expected received power from this direction is then $E[s^2[n]] = w_0^T R \theta w_0$.

Now suppose that $w_0$ is in the space spanned by the columns of $R^{-1}U$, i.e. $w_0 = R^{-1}U \alpha$ for some vector $\alpha$. It is shown in Appendix A that $R^{-1}U = R^{-1}$. Therefore:

$$w_0^H R \theta w_0 = \alpha^H U^H R^{-H} R \theta R^{-1} U \alpha$$

$$= \alpha^H U^H R^{-H} U \alpha$$

$$= w_0^H R w_0$$

(36)

In this case, replacing $R$ with the structured covariance estimate $R_\theta$ in the classical beamformer makes no difference. However, if $w_0$ is not in the subspace spanned by $R^{-1}u_1, ..., R^{-1}u_P$, then $R^{-1}w_0 \neq R^{-1}w_0$, and using the structured covariance estimate in the classical beamformer will yield a different beam pattern.

A similar statement holds for the optimum minimum variance beamformer, $s[n] = w^T x[n]$, which uses a window $w$ designed such that the expected response energy $w^T R_\theta w$ is minimized subject to the constraint that the response to a plane wave from the direction of interest is unity, $w^T w_0 = 1$. The solution is
\( w = (w_0^T R_\theta^{-1} w_0)^{-1} R_\theta^{-1} w_0 \). Note that if \( w_0 \) is in the subspace spanned by the columns of \( U \), then there exists some vector \( \alpha \) such that \( w_0 = U \alpha \). Since \( R_\theta^{-1} U = R^{-1} U \),

\[
R_\theta^{-1} w_0 = R_\theta^{-1} U \alpha = R^{-1} U \alpha = R^{-1} w_0
\]

which in turn implies:

\[
w = (w_0^T R_\theta^{-1} w_0)^{-1} R_\theta^{-1} w_0 = (w_0^T R^{-1} w_0)^{-1} R^{-1} w_0
\]

In this case, replacing \( R \) with the structured covariance estimate \( R_\theta \) in the optimal beamformer makes no difference. However, if \( w_0 \) is not in the subspace spanned by the columns of \( U \), then \( R_\theta^{-1} w_0 \neq R^{-1} w_0 \), and using the structured covariance estimate in the optimal beamformer will yield a different beam pattern. These results are contrary to the suggestion implied in [5] that replacing \( R \) with \( R_\theta \) in an optimal beamformer should make no difference.

4. Conclusion

In this paper, we have derived the optimal solution for correlation matrix estimation by the CE and RCE principles. The two methods give identical results in the problem of estimating the sum of a low rank signal matrix plus noise matrix, differing only in the value of the noise level estimate. The RCE method gives the same results as the Maximum Likelihood approach, and when the noise is white, both methods are similar to MUSIC. It is interesting that the cross-entropy approach thus provides a unifying framework for deriving spectral estimation algorithm including Bartlett, MLM[8], MEM[10], and now MUSIC.
A Derivation of CE Beamforming Algorithm

In this appendix we derive the optimal structured covariance estimate using the CE principle. First, to simplify the effort, let us define: $V = U \Lambda^{1/2}$, where $\Lambda^{1/2} = \text{diag}(\Lambda_1^{1/2}, ..., \Lambda_N^{1/2})$. Then:

$$R_\theta = VV^H + \sigma^2 W$$  \hspace{1cm} (39)

Substitute this into the CE entropy expression (6), and set the derivatives with respect to the real and imaginary part of every element of the $V$ matrix, and with respect to $\sigma^2$, to zero. Arranging these derivatives in complex matrix form gives:

$$(R^{-1} - R_\theta^{-1})V = 0$$  \hspace{1cm} (40)

$$\text{tr}\{(R^{-1} - R_\theta^{-1})W\} = 0$$  \hspace{1cm} (41)

Using the Woodward lemma:

$$R_\theta^{-1} = \frac{1}{\sigma^2} W^{-1} - \frac{1}{\sigma^2} W^{-1}V \left[V^H \frac{1}{\sigma^2} W^{-1}V + I\right]^{-1} V^H \frac{1}{\sigma^2} W^{-1}$$  \hspace{1cm} (42)

Substituting into (40) and simplifying gives:

$$R^{-1}V = \frac{1}{\sigma^2} W^{-1}V \left[V^H \frac{1}{\sigma^2} W^{-1}V + I\right]^{-1}$$  \hspace{1cm} (43)

This equation has many possible solutions. Let $V$ refer to any one of these. Then let $\Psi = V^H W^{-1}V$. Diagonalize $\Psi$ by factoring it: $\Psi = Q\Phi Q^H$, where $\Phi$ is diagonal and $Q$ is orthonormal, $Q^H Q = I$. Define $\tilde{V} = VQ$. Note that $\tilde{V}$ is also a solution to (43). In fact,

$$R^{-1}\tilde{V} = \frac{1}{\sigma^2} W^{-1}\tilde{V} \left[\frac{1}{\sigma^2} \Phi + I\right]^{-1}$$  \hspace{1cm} (44)

and:

$$\tilde{V}^H W^{-1}\tilde{V} = \Phi$$  \hspace{1cm} (45)
Let the $P$ columns of $\tilde{V}$ be $\tilde{v}_1, ..., \tilde{v}_P$, and let the $P$ diagonal elements of $\Phi$ be $\phi_1, ..., \phi_P$. Then:

$$\lambda_i R^{-1} \tilde{v}_i = W^{-1} \tilde{v}_i$$  \hspace{1cm} (46)

where:

$$\lambda_i = \phi_i + \sigma^2$$  \hspace{1cm} (47)

The columns of $\tilde{V}$ must therefore either be zero, or else must be generalized eigenvector solutions to (46). Because $R$ and $W$ are conjugate symmetric and positive definite, there are always $N$ linearly independent generalized eigenvector solutions $\tilde{v}_1, ..., \tilde{v}_N$ to (46), with corresponding generalized eigenvalues $\lambda_1, ..., \lambda_N$ which are positive. Assume without loss of generality that the first $P_0$ columns of $\tilde{V}$ are non-zero, where $P_0 \leq P$. These first $P_0$ columns must be selected from among the $N$ possible generalized eigenvectors, in a manner we will determine later. Also note that it is not necessary to estimate $Q$ or $V$ directly, since we can construct $R_\theta$ directly from $\tilde{V}$:

$$R_\theta = VV^H + \sigma^2 W$$

$$= VQ^HQV^H + \sigma^2 W$$

$$= \tilde{V} \tilde{V}^H + \sigma^2 W$$  \hspace{1cm} (48)

Now to solve for $\sigma^2$. Substitute (42) into (41), and simplify by exploiting the facts that $tr(AB) = tr(BA)$ and $tr(C + D) = tr(C) + tr(D)$ and $tr(\alpha C) = \alpha tr(C)$ where $A, B$ are matrices, $C, D$ are square matrices, and $\alpha$ is a scalar.
where we used (45) in the fourth line, and (47) in the fifth. This can be further simplified by noticing that if $\tilde{v}_i$ is any generalized eigenvector solution to (46), then:

$$W R^{-1} \tilde{v}_i = W \left( \frac{1}{\lambda_i} W^{-1} \tilde{v}_i \right) = \frac{1}{\lambda_i} \tilde{v}_i$$

(50)

Therefore, the $\tilde{v}_i$ are eigenvectors of $WR^{-1}$ with eigenvalues $1/\lambda_i$. Thus:

$$tr \{ WR^{-1} \} = \sum_{i=1}^{N} \frac{1}{\lambda_i}$$

(51)

Substituting back into (49), then solving for $\sigma^2$ gives:

$$\sigma^2 = \frac{N - P_0}{\sum_{i=1}^{N} \frac{1}{\lambda_i}}$$

(52)

Now substitute the solution for $\tilde{V}$ and for $\sigma^2$ into (48), and then substitute this back into the formula (6) for the cross-entropy. The algebra is simplified by
noting that if \( \tilde{v}_i \) is any generalized eigenvector solution to (46), then:

\[
R_\theta R_\theta^{-1} \tilde{v}_i = (\tilde{V}\tilde{V}^H + \sigma^2 W) \left( \frac{1}{\lambda_i} W^{-1} \tilde{v}_i \right)
\]

\[
= \frac{1}{\lambda_i} (\tilde{V}\tilde{V}^H W^{-1} \tilde{v}_i + \sigma^2 \tilde{v}_i)
\]

\[
= \begin{cases} 
\frac{1}{\lambda_i} (\phi_i + \sigma^2) \tilde{v}_i & \text{for } i = 1, ..., P_0 \\
\frac{1}{\lambda_i} \sigma^2 \tilde{v}_i & \text{for } i = P_0 + 1, ..., N
\end{cases}
\]

\[
= \begin{cases} 
\tilde{v}_i & \text{for } i = 1, ..., P_0 \\
\frac{\sigma^2}{\lambda_i} \tilde{v}_i & \text{for } i = P_0 + 1, ..., N
\end{cases}
\]

Therefore, the \( \tilde{v}_i \) are all eigenvectors of \( R_\theta R_\theta^{-1} \). The first \( P_0 \) eigenvalues are equal to 1, and the remainder are equal to \( \sigma^2/\lambda_{i+1}, ..., \sigma^2/\lambda_N \). Putting all this together, the cross-entropy at this solution has the value:

\[
H(q_\theta, p) = \xi \left\{ tr\{R_\theta R_\theta^{-1}\} - N - \log |R_\theta R_\theta^{-1}| \right\}
\]

\[
= \xi \left\{ P_0 + \sigma^2 \sum_{i=P_0+1}^N \frac{1}{\lambda_i} - N - \log \prod_{i=P_0+1}^N \frac{\sigma^2}{\lambda_i} \right\}
\]

\[
= \xi \sum_{i=P_0+1}^N \log \left( \frac{\lambda_i}{\sigma^2} \right)
\]

(54)

Substituting the value of \( \sigma^2 \) from (52) gives the alternate form:

\[
H(q_\theta, p) = \xi (N - P_0) \log \left[ \frac{\sum_{i=P_0+1}^N \frac{1}{\lambda_i}}{\prod_{i=P_0+1}^N \frac{1}{\lambda_i}^{1/(N-P_0)}} \right]
\]

(55)

Now to return to the issue of which of the \( N \) possible generalized eigenvector solutions should be used for the \( P_0 \) non-zero columns of \( \tilde{V} \). Let us call the selected \( P_0 \) eigenvectors \( \tilde{v}_1, ..., \tilde{v}_{P_0} \) the "signal eigenvectors", and let us call the remainder the "noise eigenvectors". The signal eigenvectors satisfy \( \tilde{v}_i \neq 0 \); since \( W^{-1} > 0 \), then \( \phi_i = \tilde{v}_i^H W^{-1} \tilde{v}_i > 0 \) and thus \( \lambda_i = \phi_i + \sigma^2 > \sigma^2 \) for \( i = \)}
We show that these signal eigenvalues must be the largest eigenvalue solutions to (46). Suppose this were not true, so that the global optimum solution corresponded to an $R_\theta$ such that one of the signal eigenvalues, say $\lambda_{P_0}$, was smaller than the largest of the noise eigenvalues, say $\lambda_{F_{b+1}}$. Thus $\sigma^2 < \lambda_{F_b} < \lambda_{F_{b+1}}$. But then, as we will see, swapping these eigensolutions, making $\tilde{v}_{P_0+1}$ a signal eigenvector and $\tilde{v}_{P_0}$ a noise eigenvector will further decrease the cross-entropy, contradicting our assumption of global optimality. To show this, let $H(\lambda_{P_0+1}, \lambda_{P_0+2},..., \lambda_N)$ represent the cross-entropy with a model $R_\theta$ built using non-zero solutions $\tilde{v}_1, ..., \tilde{v}_{P_0-1}, \tilde{v}_{P_0}$, and let $H(\lambda_{P_0}, \lambda_{P_0+2},..., \lambda_N)$ represent the cross-entropy with a model $R_\theta$ built using non-zero solutions $\tilde{v}_1, ..., \tilde{v}_{P_0-1}, \tilde{v}_{P_0+1}$. Then because the cross-entropy formula (55) is an analytic function of the $\lambda_i$, by the mean value theorem:

$$H(\lambda_{P_0+1}, \lambda_{P_0+2},..., \lambda_N) - H(\lambda_{P_0}, \lambda_{P_0+2},..., \lambda_N) = \frac{\partial H}{\partial \lambda}(\lambda, \lambda_{P_0+2},..., \lambda_N)|_{\lambda=\bar{\lambda}}(\lambda_{P_0+1} - \lambda_{P_0})$$

(56)

where $\bar{\lambda}$ is some value in the range $\lambda_{P_0} < \bar{\lambda} < \lambda_{P_0+1}$. But:

$$\frac{\partial H}{\partial \lambda} = \xi \frac{1}{\lambda^2} \left( \lambda - \frac{N - P_0}{\frac{1}{\lambda} + \sum_{i=P_0+2}^{N} \frac{1}{\lambda_i}} \right)$$

$$> 0$$

(57)

for all $\lambda_{P_0} < \lambda < \lambda_{P_0+1}$, where the last line is true because:

$$\lambda > \lambda_{P_0}$$

$$> \sigma^2$$

$$= \frac{N - P_0}{\sum_{i=P_0+1}^{N} \frac{1}{\lambda_i}}$$

$$> \frac{N - P_0}{\frac{1}{\lambda} + \sum_{i=P_0+2}^{N} \frac{1}{\lambda_i}}$$

(58)

Since $\lambda_{P_0+1} - \lambda_{P_0} > 0$, the change in (56) must be positive. Therefore, swapping
\( \tilde{v}_{P_0} \) and \( \tilde{v}_{P_0+1} \) reduces the cross-entropy, and our assumed global optimum solution cannot be globally optimum. The \( P_0 \) signal eigenvalues must therefore be the largest eigenvalue solutions to (46), and the non-zero \( P_0 \) columns of \( \tilde{V} \) must be the corresponding general eigenvectors.

Finally, we must show that we should always choose \( P_0 = P \) eigenvectors. Without loss of generality, let us sort all the eigenvalues \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N \). Let \( H_i \) represent the minimum cross-entropy with \( i \) non-zero columns in \( \tilde{V} \). Then using (55):

\[
H_{P_0} - H_{P_0+1} = \xi (N - P_0) \log \left[ \frac{1}{\lambda_{P_0+1}} \left( \frac{1}{(N-P_0)} + \frac{1 - (N-P_0)}{\lambda_{P_0+1}} \right) \right] \\
\geq 0
\]

where \( \frac{1}{\lambda} = \frac{1}{N-P_0-1} \sum_{i=P_0+2}^{N} \frac{1}{\lambda_i} \) and where we used the inequality \( \rho \alpha + (1-\rho) \beta \geq \alpha^\rho \beta^{1-\rho} \) for any \( 0 \leq \rho \leq 1 \) in the last line. Thus the cross-entropy decreases as \( P_0 \) varies from 0 to \( P \), so the best choice for \( P_0 \) must be \( P_0 = P \).

The proof that \( R_\theta \) is unique when \( \lambda_P > \lambda_{P+1} \) is messy but straightforward. The key issue is that the space spanned by the signal eigenvectors is uniquely determined. If there are multiple signal eigenvalues, then the eigenvectors themselves may not be uniquely determined, and thus \( \tilde{V} \) may not be uniquely determined.

We get the formulas in the text by defining \( U = \tilde{V} \Phi^{-1/2} \).
B Derivation of RCE Algorithm

In this appendix we give the solution to the RCE problem. The derivation is quite similar to that for the CE problem, and therefore we present this quickly. With our Gaussian models, the RCE cross-entropy has the value:

\[
RCE: \quad H(p, q_\theta) = \xi \left\{ \text{tr} (R_\theta^{-1}R) - N - \log |R_\theta^{-1}R| \right\} \quad (60)
\]

Differentiating with respect to the real and imaginary parts of \( V \) and setting these to zero, as before, gives:

\[
\left( R_\theta^{-1}RR_\theta^{-1} - R_\theta^{-1} \right) V = 0 \quad (61)
\]

Multiplying both sides by \( R^{-1}R_\theta \) gives:

\[
(R_\theta^{-1} - R^{-1})V = 0 \quad (62)
\]

which is exactly the same equations which the solution for \( V \) in the CE problem must satisfy, (40). Therefore, we can construct \( R_\theta \) from (48), where the columns of \( \tilde{V} \) must be solutions to the generalized eigenvector problem (46).

Now differentiating (60) with respect to \( \sigma^2 \) and setting it to zero gives:

\[
\text{tr}\{(R_\theta^{-1}RR_\theta^{-1} - R_\theta^{-1})W\} = 0 \quad (63)
\]

Combining this with (61) gives:

\[
0 = \text{tr}\{(R_\theta^{-1}RR_\theta^{-1} - R_\theta^{-1})(\tilde{V}\tilde{V}^H + \sigma^2W)\}
= \text{tr}\{(R_\theta^{-1}RR_\theta^{-1} - R_\theta^{-1})R_\theta\}
= \text{tr}\{R_\theta^{-1}R - I\} \quad (64)
\]

which implies that:

\[
\text{tr}\{R_\theta^{-1}R\} = N \quad (65)
\]

But (53) implies that \( R_\theta^{-1}R \) has \( P_0 \) eigenvalues equal to 1, and the rest have values \( \lambda_{P_0+1}/\sigma^2, ..., \lambda_N/\sigma^2 \). Since the trace of a matrix is just the sum of its
eigenvalues:

\[ P_0 + \frac{1}{\sigma^2} \sum_{i=P_0+1}^{N} \lambda_i = N \]  

(66)

which gives:

\[ \sigma^2 = \frac{1}{(N - P_0)} \sum_{i=P_0+1}^{N} \lambda_i \]  

(67)

Using the facts that the trace of a matrix is the sum of the eigenvalues, and the determinant is the product of the eigenvalues:

\[
H(p,q,\theta) = \xi \{ tr \{ R^{-1} \theta R \} - N - \log | R^{-1} \theta R | \} \\
= \xi \sum_{i=P_0+1}^{N} \log \frac{\sigma^2}{\lambda_i}
\]

(68)

The proofs that we must choose \( \lambda_1, ..., \lambda_{P_0} \) to be the largest eigenvalues, that we should choose \( P_0 = P \), and that the solution \( R_\theta \) is unique if \( \lambda_P > \lambda_{P+1} \), are similar to the proofs for the CE algorithm.
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