

Rank- r latent models for cross-covariance*

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Abstract

We specify a class of Gaussian rank- r latent models for cross-covariance. We show by construction that any variance-covariance matrix for the observed variables induced by rank- r reduced-rank regression can be induced by a rank- r latent model.

1 Model specification

Basic terms are introduced which will be used to state the result.

1.1 Rank- r constraint models

Let p be the number of \mathbf{X} -variables and q the number of \mathbf{Y} -variables. The rank- r symmetric **constraint model** (equivalently, the rank- r reduced-rank-regression model) is the set of $(p + q) \times (p + q)$ positive semidefinite matrices satisfying a rank constraint on the cross-covariance matrix:

$$\left. \begin{aligned} \Sigma &= \begin{bmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{bmatrix}, \\ \text{where } \Sigma_{XY} &\text{ is } p \times q \text{ of rank } r. \end{aligned} \right\} \quad (1)$$

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1.2 Rank- r paired latent models

The rank- r symmetric **paired latent model** is the set of covariances over the latent r -vectors $\boldsymbol{\xi}$ and $\boldsymbol{\omega}$, the observed p -vector \mathbf{X} , the p -vector of errors $\boldsymbol{\epsilon}$, the observed q -vector \mathbf{Y} , and the q -vector of errors $\boldsymbol{\zeta}$, specified as follows.

$$\left. \begin{aligned}
 \mathbf{x} &= \mathbf{A}\boldsymbol{\xi} + \boldsymbol{\epsilon} \quad \text{and} \\
 \mathbf{y} &= \mathbf{B}\boldsymbol{\omega} + \boldsymbol{\zeta} \quad , \text{ where} \\
 \text{Var} \left(\boldsymbol{\xi}^T, \boldsymbol{\omega}^T \right)^T &= \begin{bmatrix} \mathbf{I}_r & \mathbf{R} \\ \mathbf{R}^T & \mathbf{I}_r \end{bmatrix} , \\
 \mathbf{R} &= \text{diag}(\rho_1, \dots, \rho_r) \quad , \\
 \text{Var}(\boldsymbol{\epsilon}) &= \boldsymbol{\Sigma}_{\boldsymbol{\epsilon}\boldsymbol{\epsilon}}, \quad p \times p, \\
 \text{Var}(\boldsymbol{\zeta}) &= \boldsymbol{\Sigma}_{\boldsymbol{\zeta}\boldsymbol{\zeta}}, \quad q \times q, \\
 \boldsymbol{\epsilon} \perp\!\!\!\perp \left(\boldsymbol{\xi}^T, \boldsymbol{\omega}^T \right)^T , \quad \boldsymbol{\epsilon} \perp\!\!\!\perp \boldsymbol{\zeta} , \quad \left(\boldsymbol{\xi}^T, \boldsymbol{\omega}^T \right)^T \perp\!\!\!\perp \boldsymbol{\zeta} , \\
 \mathbf{A} \in \mathbb{R}^{(p \times r)} , \quad \mathbf{B} \in \mathbb{R}^{(q \times r)} .
 \end{aligned} \right\} \quad (2)$$

Thus the parameters of the symmetric rank- r paired latent model are the correlations ρ_1, \dots, ρ_r and the matrices \mathbf{A} , \mathbf{B} , $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}\boldsymbol{\epsilon}}$, and $\boldsymbol{\Sigma}_{\boldsymbol{\zeta}\boldsymbol{\zeta}}$, subject to the feasibility constraints that $-1 \leq \rho_k \leq 1$ for all k and that $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}\boldsymbol{\epsilon}}$ and $\boldsymbol{\Sigma}_{\boldsymbol{\zeta}\boldsymbol{\zeta}}$ must be positive semidefinite. The observed variables \mathbf{X} and \mathbf{Y} are called **indicators**, and the columns of \mathbf{A} and \mathbf{B} are called **saliences** or **loadings**. A path diagram for this model may be seen in Figure 1 on page 3.

1.3 Rank- r single latent models

The rank- r symmetric **single latent model** is the set of distributions over the latent r -vector $\boldsymbol{\eta}$, the observed p -vector \mathbf{X} , the p -vector of errors $\boldsymbol{\epsilon}$, the observed

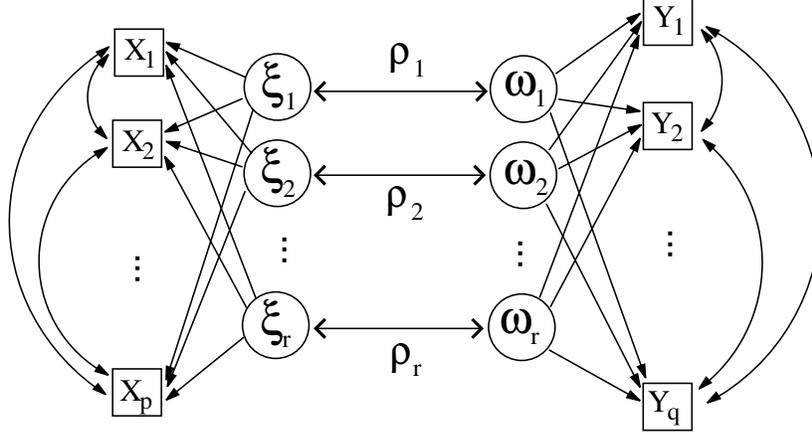


Figure 1: Path diagram representing a symmetric rank- r paired latent model. This model is defined in Section 1.2. In the parameterization guaranteed by Theorem 2.1, $\rho_1 = \dots = \rho_r = 1$ since $\xi_k \equiv \omega_k$ for all k .

q -vector \mathbf{Y} , and the q -vector of errors ζ , specified as follows.

$$\left. \begin{aligned}
 \mathbf{x} &= \mathbf{A}\boldsymbol{\eta} + \boldsymbol{\epsilon} \quad \text{and} \\
 \mathbf{y} &= \mathbf{B}\boldsymbol{\eta} + \boldsymbol{\zeta} \quad , \text{ where} \\
 \mathbf{Var}(\boldsymbol{\eta}) &= \mathbf{I}_r \quad , \\
 \mathbf{Var}(\boldsymbol{\epsilon}) &= \boldsymbol{\Sigma}_{\epsilon\epsilon}, \quad p \times p, \\
 \mathbf{Var}(\boldsymbol{\zeta}) &= \boldsymbol{\Sigma}_{\zeta\zeta}, \quad q \times q, \\
 \boldsymbol{\epsilon} \perp \boldsymbol{\eta} \quad , \quad \boldsymbol{\epsilon} \perp \boldsymbol{\zeta} \quad , \quad \boldsymbol{\eta} \perp \boldsymbol{\zeta} \quad , \\
 \mathbf{A} \in \mathbb{R}^{(p \times r)} \quad , \quad \mathbf{B} \in \mathbb{R}^{(q \times r)} \quad .
 \end{aligned} \right\} \quad (3)$$

Thus the parameters of the symmetric rank- r single latent model are the matrices \mathbf{A} , \mathbf{B} , $\boldsymbol{\Sigma}_{\epsilon\epsilon}$, and $\boldsymbol{\Sigma}_{\zeta\zeta}$, subject to the feasibility constraint that $\boldsymbol{\Sigma}_{\epsilon\epsilon}$ and $\boldsymbol{\Sigma}_{\zeta\zeta}$ must both be positive semidefinite. The reader will observe that the rank- r single latent model is a special case of the rank- r paired latent model where $\xi \equiv \omega$. A path diagram for a symmetric rank- r single latent model may be seen in Figure 2 on page 4.

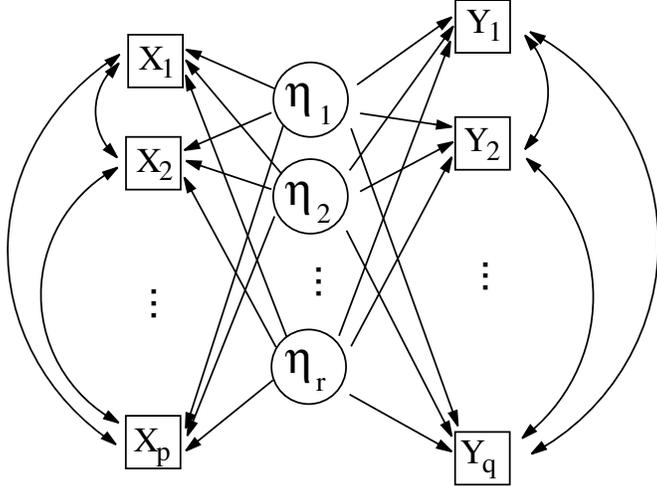


Figure 2: Path diagram representing a symmetric rank- r single latent model.

2 Maps between spaces of models

Every set of parameter values for the paired latent model induces a set of covariances over the observed variables as follows.

$$\left. \begin{aligned} \Sigma_{XX} &= \mathbf{A}\mathbf{A}^T + \Sigma_{\epsilon\epsilon}, \\ \Sigma_{YY} &= \mathbf{B}\mathbf{B}^T + \Sigma_{\zeta\zeta}, \\ \Sigma_{XY} &= \mathbf{A}\mathbf{R}\mathbf{B}^T. \end{aligned} \right\} \quad (4)$$

The equations (4) define a map from the space of rank- r paired latent models into the space of rank- r constraint models. The existence of such a map immediately raises the question whether every covariance in the rank- r constraint model can be obtained by a set of parameter values in the rank- r latent model—i.e., is the map onto. If such a set of parameter values exists, we say that it **parameterizes** or **is a latent parameterization of** the covariance matrix.

The answer to the question in the previous paragraph is yes. Every rank- r constraint model can be parameterized by a rank- r symmetric paired latent model. We show this by first proving a stronger result, i.e., that any rank- r constraint model can be parameterized by a symmetric rank- r single latent model. The result concerning paired latent models is obtained as a corollary.

2.1 A theorem regarding rank- r single latent models

We now state and prove the main result.

Theorem 2.1 *For each covariance matrix (1) in the rank- r constraint model there is at least one set of parameter values in the rank- r symmetric single latent model that induces it.*

Proof. Let \mathbf{X} and \mathbf{Y} be matrices such that

$$\begin{aligned}\Sigma_{XX} &= \mathbf{X}^T \mathbf{X} , \\ \Sigma_{XY} &= \mathbf{X}^T \mathbf{Y} , \text{ and} \\ \Sigma_{YY} &= \mathbf{Y}^T \mathbf{Y} .\end{aligned}$$

Such matrices are guaranteed to exist. For instance they may be obtained by partitioning the symmetric positive semidefinite square root of Σ . Let r_x be the rank of \mathbf{X} and r_y the rank of \mathbf{Y} . Without loss of generality suppose $r_x \leq r_y$. It can be shown that there are matrices \mathbf{U} and \mathbf{V} such that \mathbf{U} is a basis for the range (the column space) of \mathbf{X} , \mathbf{V} is a basis for the range of \mathbf{Y} , $\mathbf{U}^T \mathbf{U} = \mathbf{I}_{r_x}$, $\mathbf{V}^T \mathbf{V} = \mathbf{I}_{r_y}$, and

$$\mathbf{U}^T \mathbf{V} = [\mathbf{D} | \mathbf{0}] , \quad (5)$$

where $\mathbf{0}$ is an $r_x \times (r_y - r_x)$ matrix of zeroes, absent if $r_x = r_y$, \mathbf{D} is an $r_x \times r_x$ diagonal matrix satisfying

$$\mathbf{D} = \text{diag}(\cos(\theta_1), \dots, \cos(\theta_r), 0, \dots, 0) , \quad (6)$$

the last $(r_x - r)$ diagonal entries of (6) are zero if $r_x > r$, and

$$\cos(\theta_1) \geq \dots \geq \cos(\theta_r) > 0 .$$

The columns of \mathbf{U} and \mathbf{V} are **principal vectors**, and the θ_k are **principal angles**. These facts are reported as Theorem 9.1 and Corollary 9.11 in Afriat [1]. Golub and van Loan report an algorithm for computing \mathbf{U} and \mathbf{V} in the case when \mathbf{X} and \mathbf{Y} are of full rank (pages 603f [6]). Björck and Golub [5] discuss numerical methods, including the case where \mathbf{X} and \mathbf{Y} are rank-deficient. In a statistical context the $\cos(\theta_k)$ are known as **canonical correlations** and the principal vectors as **canonical correlation variables** or **canonical variates**. Mardia, Kent and Bibby develop these concepts within a statistical context for the case where Σ has full rank (Chapter 10, pages 281–299 [7]), as does T. W. Anderson [4]. The `cancor()` function in S-PLUS [8] may be used to compute canonical correlations. S-PLUS also computes two matrices, respectively $r_x \times r_x$ and $r_y \times r_y$, which may be used to compute \mathbf{U} and \mathbf{V} from \mathbf{X} and \mathbf{Y} provided \mathbf{X} and \mathbf{Y} have full rank.

Let n be the number of rows in \mathbf{X} . Then \mathbf{U} is $n \times r_x$ and \mathbf{V} is $n \times r_y$. Let \mathbf{E} be an $r_x \times p$ matrix and \mathbf{F} an $r_y \times q$ matrix such that

$$\mathbf{X} = \mathbf{U}\mathbf{E} , \quad \mathbf{Y} = \mathbf{V}\mathbf{F} . \quad (7)$$

Define the $p \times r_x$ matrix \mathbf{A} and the $q \times r_x$ matrix \mathbf{B} by

$$\begin{aligned}\mathbf{A} &= \mathbf{E}^T \sqrt{\mathbf{D}} , \\ \mathbf{B} &= \mathbf{F}^T \begin{bmatrix} \sqrt{\mathbf{D}} \\ \mathbf{0}^T \end{bmatrix} ,\end{aligned}$$

where \mathbf{D} and $\mathbf{0}$ have the same value as in (5). Then by (5)

$$\begin{aligned}\mathbf{A}\mathbf{B}^T &= \mathbf{E}^T\mathbf{U}^T\mathbf{V}\mathbf{F} \\ &= \mathbf{X}^T\mathbf{Y}.\end{aligned}$$

Then

$$\begin{aligned}\boldsymbol{\Sigma}_{XX} - \mathbf{A}\mathbf{A}^T &= \mathbf{X}^T\mathbf{X} - \mathbf{E}^T\mathbf{D}\mathbf{E} \\ &= \mathbf{E}^T\mathbf{U}^T\mathbf{U}\mathbf{E} - \mathbf{E}^T\mathbf{D}\mathbf{E} \\ &= \mathbf{E}^T(\mathbf{I}_{r_x} - \mathbf{D})\mathbf{E} \\ &= \mathbf{E}^T \text{diag}(1 - \cos(\theta_1), \dots, 1 - \cos(\theta_r), 1, \dots, 1)\mathbf{E},\end{aligned}\quad (8)$$

a positive semidefinite matrix. By a similar argument

$$\begin{aligned}\boldsymbol{\Sigma}_{YY} - \mathbf{B}\mathbf{B}^T &= \mathbf{F}^T \left(\mathbf{I}_q - \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \right) \mathbf{F} \\ &= \mathbf{F}^T \text{diag}(1 - \cos(\theta_1), \dots, 1 - \cos(\theta_r), 1, \dots, 1)\mathbf{F},\end{aligned}\quad (9)$$

also positive semidefinite. Define the $p \times p$ matrix $\boldsymbol{\Sigma}_{\epsilon\epsilon}$ and the $q \times q$ matrix $\boldsymbol{\Sigma}_{\zeta\zeta}$ by

$$\begin{aligned}\boldsymbol{\Sigma}_{\epsilon\epsilon} &= \boldsymbol{\Sigma}_{XX} - \mathbf{A}\mathbf{A}^T, \\ \boldsymbol{\Sigma}_{\zeta\zeta} &= \boldsymbol{\Sigma}_{YY} - \mathbf{B}\mathbf{B}^T.\end{aligned}$$

The values of \mathbf{A} , \mathbf{B} , $\boldsymbol{\Sigma}_{\epsilon\epsilon}$, and $\boldsymbol{\Sigma}_{\zeta\zeta}$ satisfy the definition of a rank- r single latent model, stated in (3), and they induce $\boldsymbol{\Sigma}$. \square

Corollary 2.2 *The values of both $\boldsymbol{\Sigma}_{\epsilon\epsilon}$ and $\boldsymbol{\Sigma}_{\zeta\zeta}$, derived in the proof of Theorem 2.1, are strictly positive definite if and only if $\boldsymbol{\Sigma}$ is strictly positive definite.*

Proof. $\boldsymbol{\Sigma}$ is strictly positive definite if and only if the columns of the combined matrix $[\mathbf{X}|\mathbf{Y}]$ are linearly independent. This condition holds if and only if the following three conditions hold.

1. The columns of \mathbf{X} are linearly independent of the columns of \mathbf{Y} , so that the first principal angle satisfies $\cos(\theta_1) < 1$ (the first canonical correlation is less than one in absolute value). Note that this is the only way that

$$\text{diag}(1 - \cos(\theta_1), \dots, 1 - \cos(\theta_r), 1, \dots, 1)$$

can have full rank.

2. The following equivalent conditions hold.

- The columns of \mathbf{X} are linearly independent.
- $r_x = p$.
- $\text{rank}(\mathbf{E}) = p$.

3. The following equivalent conditions hold.

- The columns of \mathbf{Y} are linearly independent.
- $r_y = q$.
- $\text{rank}(\mathbf{F}) = q$.

Thus if Σ is strictly positive definite, both (9) and (8) are of full rank, that is, strictly positive definite.

Suppose on the other hand that (9) and (8) are of full rank. The matrix at (9) is $p \times p$, the product of a $p \times r_x$ matrix, an $r_x \times r_x$ matrix, and an $r_x \times p$ matrix. Since $r_x \leq p$, this matrix can be of full rank only if $r_x = p$. Furthermore it can be of full rank only if the middle matrix is of full rank, which requires $\rho_1 < 0$. Similarly if (8) is of full rank it follows that $r_y = q$ and $\rho_1 < 0$. Thus Σ is of full rank. \square

Remark on Corollary 2.2. Corollary 2.2 notwithstanding, for a given strictly positive definite covariance matrix in the constraint model there may be parameterizations, different from those derived in the proof of Theorem 2.1, with singular within-block covariance. For instance, Wegelin et al. [10] show in the rank-one case that a parameterization is always possible in which the within-block-error covariance matrices are singular for both blocks.

Corollary 2.3 *Each rank- r constraint model can be parameterized by at least one rank- r paired latent model.*

Proof. Let η be the latent variable of the single latent model be given by Theorem 2.1, and let $\xi \equiv \omega \equiv \eta$.

Remark on Corollary 2.3. The correlations between ξ_k and ω_k , written ρ_k , are not to be confused with the canonical correlations which appear in the proof of Theorem 2.1. The correlation between the latents in the paired latent parameterization guaranteed by Theorem 2.1 is unity: $\text{Cor}(\xi_k, \omega_k) = 1$ for all k . The canonical correlation which appears in the proof of Theorem 2.1, on the other hand, is only unity if Σ is singular. In the example on page 7, for instance, the canonical correlation is about 0.57.

3 Example

Consider the following symmetric strictly positive definite matrix, and let $p = 2$, $q = 3$. This is a distribution in the rank-one constraint model.

$$\Sigma = \begin{bmatrix} 9 & 0 & 1 & 2 & 3 \\ 0 & 5 & 0.5 & 1 & 1.5 \\ 1 & 0.5 & 7 & 0 & 0 \\ 2 & 1 & 0 & 7 & 0 \\ 3 & 1.5 & 0 & 0 & 7 \end{bmatrix}.$$

Following the proof of Theorem 2.1, we obtain

$$\mathbf{U} = \begin{bmatrix} 0.79431 & 0.56228 \\ 0.5326 & -0.82666 \\ 0.07811 & -0.0058 \\ 0.15622 & -0.0116 \\ 0.23433 & -0.0174 \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 0.2615 & 0 & 0 \\ 0.15284 & 0 & 0 \\ 0.25471 & -0.9443 & 0.19202 \\ 0.50941 & -0.02053 & -0.8449 \\ 0.76412 & 0.32845 & 0.49926 \end{bmatrix},$$

$$\mathbf{D} = \begin{bmatrix} 0.56765 & 0 \\ 0 & 0 \end{bmatrix},$$

$$\mathbf{U}_1 = \begin{bmatrix} 0.75342 & 0 \\ 0 & 0 \end{bmatrix},$$

$$\mathbf{E} = \begin{bmatrix} 2.49136 & 1.24568 \\ 1.67126 & -1.85695 \end{bmatrix},$$

$$\mathbf{F} = \begin{bmatrix} 0.70711 & 1.41421 & 2.12132 \\ -2.49838 & -0.05431 & 0.869 \\ 0.50805 & -2.23541 & 1.32092 \end{bmatrix},$$

$$\mathbf{A} = \begin{bmatrix} 1.87705 & 0 \\ 0.93853 & 0 \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} 0.53275 & 0 \\ 1.0655 & 0 \\ 1.59825 & 0 \end{bmatrix}.$$

We check that

$$\mathbf{AB}^T = \begin{bmatrix} 1 & 2 & 3 \\ 0.5 & 1 & 1.5 \end{bmatrix} = \boldsymbol{\Sigma}_{XY}.$$

Then the within-block covariances are

$$\boldsymbol{\Sigma}_{\epsilon\epsilon} = \begin{bmatrix} 5.47668 & -1.76166 \\ -1.76166 & 4.11917 \end{bmatrix},$$

full rank with least eigenvalue 2.9, and

$$\boldsymbol{\Sigma}_{\zeta\zeta} = \begin{bmatrix} 6.71618 & -0.56765 & -0.85147 \\ -0.56765 & 5.86471 & -1.70294 \\ -0.85147 & -1.70294 & 4.44559 \end{bmatrix},$$

also full rank with least eigenvalue 3.03.

4 Discussion

Likelihood and the equivalence of model spaces. Three spaces of covariance matrices over the observed variables \mathbf{X} and \mathbf{Y} are of interest in the current work. They are:

1. Those corresponding to the rank-constraint model.
2. Those induced by the symmetric paired latent model.
3. Those induced by the symmetric single latent model.

It follows from definitions and from Equations (4) on page 4 that $\text{Set 3} \subset \text{Set 2} \subset \text{Set 1}$. Theorem 2.1, however, implies that $\text{Set 1} \subset \text{Set 3}$. Hence $\text{Set 1} = \text{Set 2} = \text{Set 3}$, a fact which we state as the following corollary.

Corollary 4.1 *The sets of covariance matrices over the observed variables induced by the rank- r symmetric paired latent correlation model and the rank- r symmetric single latent model are equal to the set of covariance matrices belonging to the rank- r constraint model.*

Thus all single and paired latent parameterizations within an equivalence class have the same likelihood under the multivariate normal model for $(\mathbf{X}^T, \mathbf{Y}^T)^T$, and consequently there is no way using only data to distinguish between the three models. Furthermore it may be shown that the rank-one constraint model is covariance equivalent to reduced-rank regression (RRR). Maximum-likelihood estimation procedures, and asymptotics, available for RRR (see Anderson [2] [3] [4]) and Ryan et al. [9]) are thus available for the paired and single latent models.

Future work: Characterization of feasible sets, and identifiability.

Wegelin et al. [10] have extended the current results for the rank-one case. They characterize the sets of parameter values for the single and paired latent models which induce a given covariance matrix in the rank-one constraint model. Two constants, α_{\min} and α_{\max} , functions of the covariance Σ , are sufficient to characterize each set. Furthermore a natural convention is presented by which the rank-one paired latent model can be made identifiable. The convention is that the correlation between the latent variables attains its minimum feasible value, $\frac{\alpha_{\min}}{\alpha_{\max}}$.

It would be interesting to see whether the results for the rank-one case can be extended to rank r ; that is, answers to the following questions would be interesting.

- How is the feasible set characterized for rank r ? Is it always a “corner” in $\mathbb{R}^{(2r)}$, as is the case when $r = 1$? Is there any way to visualize it?
- Are there constants, analogous to α_{\min} and α_{\max} , which characterize the feasible set for rank r ?

- Is there a single point in the feasible set which minimizes a reasonable criterion related to the correlations between the r pairs of latent variables? In particular, can the r correlations be simultaneously minimized, or does the minimization of, for instance, $\mathbf{Cor}(\boldsymbol{\xi}_1, \boldsymbol{\omega}_1)$ imply that $\mathbf{Cor}(\boldsymbol{\xi}_2, \boldsymbol{\omega}_2)$ is not minimized? In other words, are these parameters variation independent?

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