

Estimation in the multivariate linear normal models with linearly structured covariance matrices

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Basic model

We consider the extended growth curve model as defined in von Rosen (1989):

$$\mathbf{X} = \sum_{i=1}^m \mathbf{A}_i \mathbf{B}_i \mathbf{C}_i + \mathbf{E} \quad (1)$$

where the sample matrix $\mathbf{X} : p \times n$, the mean parameter matrices $\mathbf{B}_i : q_i \times k_i$, the within individual design matrices $\mathbf{A}_i : p \times q_i$ and the between individual design matrices $\mathbf{C}_i : k_i \times n$ are such that $\mathcal{C}(\mathbf{C}'_i) \subseteq \mathcal{C}(\mathbf{C}'_{i-1})$, $i = 2, 3, \dots, m$.

The columns of \mathbf{E} are assumed to be independently distributed as a p -variate normal distribution with mean zero and a dispersion matrix Σ .

Maximum likelihood estimators

The maximum likelihood method is one of several approaches used to find estimators of parameters in the EGC model.

One can find an exhaustive description of how to get those estimators in Kollo and von Rosen (2005).

Hereafter we give some important results from which the main idea of our discussion is derived starting with the theorem stated and proved in von Rosen (1989).

Maximum likelihood estimators

Let $\widehat{\mathbf{B}}_i$'s be the maximum likelihood estimators of \mathbf{B}_i 's in the EGC model. Then

$$\mathbf{P}_r \sum_{i=r}^m \mathbf{A}_i \widehat{\mathbf{B}}_i \mathbf{C}_i = \sum_{i=r}^m (\mathbf{I} - \mathbf{T}_i) \mathbf{X} \mathbf{C}'_i (\mathbf{C}_i \mathbf{C}'_i)^{-1} \mathbf{C}_i,$$

where,

$$\mathbf{P}_r = \mathbf{T}_{r-1} \mathbf{T}_{r-2} \times \cdots \times \mathbf{T}_0, \quad \mathbf{T}_0 = \mathbf{I}, \quad r = 1, 2, \dots, m+1,$$
$$\mathbf{T}_i = \mathbf{I} - \mathbf{P}_i \mathbf{A}_i (\mathbf{A}'_i \mathbf{P}'_i \mathbf{S}_i^{-1} \mathbf{P}_i \mathbf{A}_i)^{-1} \mathbf{A}'_i \mathbf{P}'_i \mathbf{S}_i^{-1}, \quad i = 1, 2, \dots, m,$$

$$\mathbf{S}_i = \sum_{j=1}^i \mathbf{K}_j, \quad i = 1, 2, \dots, m,$$

$$\mathbf{K}_j = \mathbf{P}_j \mathbf{X} (\mathbf{C}'_{j-1} (\mathbf{C}_{j-1} \mathbf{C}'_{j-1})^{-1} \mathbf{C}_{j-1} - \mathbf{C}'_j (\mathbf{C}_j \mathbf{C}'_j)^{-1} \mathbf{C}_j) \mathbf{X}' \mathbf{P}'_j, \quad \mathbf{C}_0 = \mathbf{I}.$$

Maximum likelihood estimators

When $r = 1$, we get the estimated mean structure, i.e.,

$$\widehat{E[\mathbf{X}]} = \sum_{i=1}^m \mathbf{A}_i \widehat{\mathbf{B}}_i \mathbf{C}_i = \sum_{i=1}^m (\mathbf{I} - \mathbf{T}_i) \mathbf{X} \mathbf{C}_i' (\mathbf{C}_i \mathbf{C}_i')^{-1} \mathbf{C}_i \quad (2)$$

or equivalently

$$\widehat{E[\mathbf{X}]} = \sum_{i=1}^m \mathbf{P}_i \mathbf{A}_i (\mathbf{A}_i' \mathbf{P}_i' \mathbf{S}_i^{-1} \mathbf{P}_i \mathbf{A}_i)^{-1} \mathbf{A}_i' \mathbf{P}_i' \mathbf{S}_i^{-1} \mathbf{X} \mathbf{C}_i' (\mathbf{C}_i \mathbf{C}_i')^{-1} \mathbf{C}_i. \quad (3)$$

Maximum likelihood estimators

To shorten matrix expressions put

$$\mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i} = \mathbf{P}_i \mathbf{A}_i (\mathbf{A}_i' \mathbf{P}_i' \mathbf{S}_i^{-1} \mathbf{P}_i \mathbf{A}_i)^{-1} \mathbf{A}_i' \mathbf{P}_i' \mathbf{S}_i^{-1} \quad \text{and} \quad \mathbf{P}_{\mathbf{C}'_i} = \mathbf{C}'_i (\mathbf{C}_i \mathbf{C}'_i)^{-1} \mathbf{C}_i.$$

Thus, (3) becomes

$$\widehat{E[\mathbf{X}]} = \sum_{i=1}^m \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i} \mathbf{X} \mathbf{P}_{\mathbf{C}'_i}. \quad (4)$$

Noticing that the matrix $\mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i}$ and $\mathbf{P}_{\mathbf{C}'_i}$ are projector matrices, we see that estimators of the mean structure is based on a projection of the observations on the space generated by the design matrices.

Naturally, the estimators of the variance parameters are based on a projection of the observations on the residual space, that is the orthogonal complement to the design space.

Main idea and space decomposition

If Σ would have been known, we would have from least squares theory the best linear estimator (BLUE) given by

$$\widetilde{E}[\mathbf{X}] = \sum_{i=1}^m \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \Sigma} \mathbf{X} \mathbf{P}_{\mathbf{C}'_i}, \quad (5)$$

where \mathbf{S}_i in \mathbf{P}_i is replaced with Σ .

We see that in the projections, if Σ is unknown, the parameter has been replaced with \mathbf{S}_i 's, which according to their expressions are not maximum likelihood estimators. However, \mathbf{S}_i 's define consistent estimators of Σ in the sense that $n^{-1}\mathbf{S}_i \rightarrow \Sigma$ in probability.

Main idea and space decomposition

Applying the vec-operator on both sides of (4) we get

$$\text{vec}(\widehat{E[\mathbf{X}]}) = \sum_{i=1}^m (\mathbf{P}_{\mathbf{C}'_i} \otimes \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i}) \text{vec} \mathbf{X}.$$

where \otimes denotes the Kronecker product.

Note that the matrix $\mathbf{P} = \sum_{i=1}^m \mathbf{P}_{\mathbf{C}'_i} \otimes \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i}$ is a projector and its column space is the design space

$$\mathcal{C}(\mathbf{P}) = \sum_{i=1}^m \mathcal{C}(\mathbf{C}'_i) \otimes \mathcal{C}_{\mathbf{S}_i}(\mathbf{P}_i \mathbf{A}_i) \quad (6)$$

where now \otimes denotes a tensor product of linear spaces and the subscript \mathbf{S}_i in $\mathcal{C}_{\mathbf{S}_i}(\mathbf{P}_i \mathbf{A}_i)$ indicates that the inner products are defined via the positive definite matrices \mathbf{S}_i^{-1} .

Main idea and space decomposition

Therefore $\mathcal{C}(\mathbf{P})$ is used to estimate the mean structure whereas $\mathcal{C}(\mathbf{P})^\perp$ is used to create residuals, where $^\perp$ denotes the orthogonal complement.

To estimate $\mathbf{\Sigma}$, the general idea is to use the variation in the residuals. For our purposes we decompose the residual space into $m + 1$ orthogonal subspaces.

On one hand, the conditions $\mathcal{C}(\mathbf{C}'_i) \subseteq \mathcal{C}(\mathbf{C}'_{i-1})$, $i = 2, 3, \dots, m$, imply that $\mathcal{C}(\mathbf{C}'_1)$ can be decomposed as a sum of orthogonal subspaces as follows:

$$\begin{aligned} \mathcal{C}(\mathbf{C}'_1) = & [\mathcal{C}(\mathbf{C}'_1) \cap \mathcal{C}(\mathbf{C}'_2)^\perp] \oplus [\mathcal{C}(\mathbf{C}'_2) \cap \mathcal{C}(\mathbf{C}'_3)^\perp] \oplus \dots \\ & \oplus [\mathcal{C}(\mathbf{C}'_{m-1}) \cap \mathcal{C}(\mathbf{C}'_m)^\perp] \oplus \mathcal{C}(\mathbf{C}'_m) \end{aligned}$$

where \oplus denotes the direct sum of linear spaces.

Main idea and space decomposition

On the other hand, the subspaces

$$\mathcal{V}_i = \mathcal{C}_{\mathbf{S}_i}(\mathbf{P}_i \mathbf{A}_i), \quad i = 1, 2, \dots, m,$$

are orthogonal.

Now, put

$$\begin{aligned} \mathcal{W}_0 &= \mathcal{C}(\mathbf{C}'_1)^\perp, \quad \mathcal{W}_r = \mathcal{C}(\mathbf{C}'_r) \cap \mathcal{C}(\mathbf{C}'_{r+1})^\perp, \quad r = 1, \dots, m-1, \\ \mathcal{W}_m &= \mathcal{C}(\mathbf{C}'_m), \quad \text{and } \mathcal{V}_0 = \bigoplus_{i=1}^m \mathcal{V}_i \oplus \left(\bigoplus_{i=1}^m \mathcal{V}_i\right)^\perp. \end{aligned}$$

With these notations, the residual space is decomposed as

$$\mathcal{C}(\mathbf{P})^\perp = I_0 \boxplus I_1 \boxplus \dots \boxplus I_m$$

where \boxplus denotes the orthogonal direct sum of tensor spaces,

$$I_r = \mathcal{W}_r \otimes \left(\bigoplus_{i=1}^r \mathcal{V}_i\right)^\perp, \quad r = 0, 1, 2, \dots, m,$$

in which by convenience $\left(\bigoplus_{i=1}^0 \mathcal{V}_i\right)^\perp = \emptyset^\perp = \mathcal{V}_0$.

Main idea and space decomposition

The residuals obtained by projecting data to these subspaces are

$$\mathbf{R}_r = (\mathbf{I} - \sum_{i=1}^r \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i}) \mathbf{X} (\mathbf{P}_{\mathbf{C}'_r} - \mathbf{P}_{\mathbf{C}'_{r+1}}), \quad r = 0, 1, 2, 3, \dots, m,$$

where we use for convenience $\sum_{i=k+1}^k \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \mathbf{S}_i} = \mathbf{0}$, $\mathbf{C}_0 = \mathbf{I}$ and $\mathbf{C}_{m+1} = \mathbf{0}$.

Thus a natural estimator of $\mathbf{\Sigma}$ is obtained from the sum of squared residuals, i.e.,

$$n \hat{\mathbf{\Sigma}} = \mathbf{R}_0 \mathbf{R}'_0 + \mathbf{R}_1 \mathbf{R}'_1 + \dots + \mathbf{R}_m \mathbf{R}'_m.$$

Estimators when the covariance matrix is linearly structured

Now we consider the EGC model when the covariance matrix Σ is linearly structured (e.g.: Uniform, compound symmetry, banded, Toeplitz). This Σ will be denoted $\Sigma^{(s)}$ so that $\mathbf{E} \sim N_{p,n}(\mathbf{0}, \Sigma^{(s)}, \mathbf{I}_n)$.

By $\text{vec}\Sigma(K)$ we mean the patterned vectorization of the linearly structured matrix $\Sigma^{(s)}$, that is the columnwise vectorization of $\Sigma^{(s)}$ where all 0's and repeated elements (by modulus) have been disregarded. Then there exists a transformation matrix \mathbf{T} such that

$$\text{vec}\Sigma(K) = \mathbf{T}\text{vec}\Sigma^{(s)} \quad \text{or} \quad \text{vec}\Sigma^{(s)} = \mathbf{T}^+\text{vec}\Sigma(K), \quad (7)$$

where \mathbf{T}^+ denotes the Moore-Penrose generalized inverse of \mathbf{T} .

Estimators when the covariance matrix is linearly structured

The estimation procedure that we propose will rely on the decomposition of the spaces as we did for the unstructured case, the only difference being that, for the structured case, we do not replace $\Sigma^{(s)}$ with \mathbf{S}_i 's because now $\Sigma^{(s)}$ is structured.

The idea was first used by Ohlson and von Rosen (2010) for the classical growth curve model.

Estimators when the covariance matrix is linearly structured

Here we use

$$\begin{aligned}\mathbf{P}_r &= \mathbf{T}_{r-1}\mathbf{T}_{r-2} \times \cdots \times \mathbf{T}_0, \quad \mathbf{T}_0 = \mathbf{I}, \quad r = 1, 2, \dots, m+1, \\ \mathbf{T}_i &= \mathbf{I} - \mathbf{P}_{\mathbf{P}_i\mathbf{A}_i, \Sigma^{(s)}}, \quad i = 1, 2, \dots, m, \\ \mathcal{V}_i &= \mathcal{C}_{\Sigma^{(s)}}(\mathbf{P}_i\mathbf{A}_i), \quad i = 1, 2, \dots, m.\end{aligned}$$

The corresponding residuals will be denoted

$$\mathbf{H}_r = \left(\mathbf{I} - \sum_{i=1}^r \mathbf{P}_{\mathbf{P}_i\mathbf{A}_i, \Sigma^{(s)}}\right)\mathbf{X}(\mathbf{P}_{\mathbf{C}'_r} - \mathbf{P}_{\mathbf{C}'_{r+1}}), \quad r = 0, 1, 2, 3, \dots, m.$$

Estimators when the covariance matrix is linearly structured

If $\Sigma^{(s)}$ would have been known, we would have a BLUE of the mean

$$\widetilde{E[\mathbf{X}]} = \sum_{i=1}^m \widetilde{\mathbf{M}}_i,$$

where $\widetilde{\mathbf{M}}_i = \mathbf{P}_{\mathbf{P}_i \mathbf{A}_i, \Sigma^{(s)}} \mathbf{X} \mathbf{P}_{\mathbf{C}'_i}$, that is a projection of observations on $\mathcal{C}(\mathbf{C}'_i) \otimes \mathcal{V}_i$.

Estimators when the covariance matrix is linearly structured

To get more insight on what is going on, we are going to illustrate the space decomposition for $m = 3$. In this case the BLUE of the mean is

$$\widehat{E[\mathbf{X}]} = \widetilde{\mathbf{M}}_1 + \widetilde{\mathbf{M}}_2 + \widetilde{\mathbf{M}}_3,$$

where

$$\widetilde{\mathbf{M}}_1 = \mathbf{P}_{\mathbf{A}_1, \Sigma^{(s)}} \mathbf{X} \mathbf{P}_{\mathbf{C}'_1},$$

$$\widetilde{\mathbf{M}}_2 = \mathbf{P}_{\mathcal{T}_1 \mathbf{A}_2, \Sigma^{(s)}} \mathbf{X} \mathbf{P}_{\mathbf{C}'_2}, \quad \mathcal{T}_1 = \mathbf{I} - \mathbf{P}_{\mathbf{A}_1, \Sigma^{(s)}} = \mathbf{T}_1,$$

$$\widetilde{\mathbf{M}}_3 = \mathbf{P}_{\mathcal{T}_2 \mathbf{A}_3, \Sigma^{(s)}} \mathbf{X} \mathbf{P}_{\mathbf{C}'_3}, \quad \mathcal{T}_2 = \mathbf{I} - \mathbf{P}_{\mathbf{A}_1, \Sigma^{(s)}} - \mathbf{P}_{\mathcal{T}_1 \mathbf{A}_2, \Sigma^{(s)}} = \mathbf{T}_2 \mathbf{T}_1.$$

Estimators when the covariance matrix is linearly structured

From here we see that the estimated mean is obtained by projecting observations on some subspaces.

The matrices $\mathbf{P}_{\mathbf{A}_1, \Sigma(s)}$, $\mathbf{P}_{\mathcal{T}_1 \mathbf{A}_2, \Sigma(s)}$ and $\mathbf{P}_{\mathcal{T}_2 \mathbf{A}_3, \Sigma(s)}$ are projector matrices on the subspaces

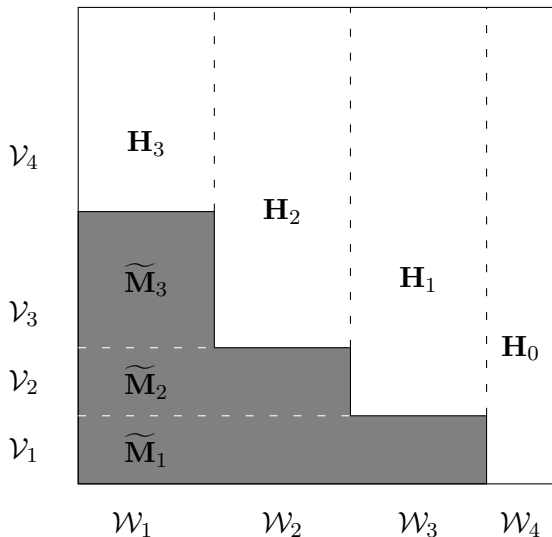
$$\mathcal{V}_1 = \mathcal{C}_{\Sigma(s)}(\mathbf{A}_1),$$

$$\mathcal{V}_2 = \mathcal{C}_{\Sigma(s)}(\mathbf{A}_1 : \mathbf{A}_2) \cap \mathcal{C}_{\Sigma(s)}(\mathbf{A}_1)^\perp \text{ and}$$

$$\mathcal{V}_3 = \mathcal{C}_{\Sigma(s)}(\mathbf{A}_1 : \mathbf{A}_2 : \mathbf{A}_3) \cap \mathcal{C}_{\Sigma(s)}(\mathbf{A}_1 : \mathbf{A}_2)^\perp$$

respectively.

Estimators when the covariance matrix is linearly structured



Estimators when the covariance matrix is linearly structured

In practice $\Sigma^{(s)}$ is not known and should be estimated. As for the unstructured case, it is natural to use the sum of squared residuals when finding inner product estimate.

We will sequentially estimate the inner product in the spaces \mathcal{V}_i , $i = 1, 2, \dots, m$.

While finding the inner product estimate in the space \mathcal{V}_1 it is natural to use $\mathbf{Q}_0 = \mathbf{H}_0\mathbf{H}_0'$ and apply the general least squares approach by minimizing $\text{tr} \{(\mathbf{Q}_0 - (n - r_1)\Sigma^{(s)})(\cdot)'\}$ with respect to $\Sigma^{(s)}$, where the notation $(\mathbf{Y})(\cdot)'$ stands for $(\mathbf{Y})(\mathbf{Y})'$. That is

$$\widehat{\Sigma}_1^{(s)} = \min \text{tr} \left\{ (\mathbf{Q}_0 - (n - r_1)\Sigma^{(s)})(\cdot)' \right\}.$$

Estimators when the covariance matrix is linearly structured

Assuming that $\widehat{\Sigma}_1^{(s)}$ is positive definite (which always holds for large n), we can use $\widehat{\Sigma}_1^{(s)}$ to define the inner product in the space \mathcal{V}_1 , and therefore we consider $\mathcal{C}_{\widehat{\Sigma}_1^{(s)}}(\mathbf{A}_1)$ instead of $\mathcal{C}_{\Sigma^{(s)}}(\mathbf{A}_1)$.

By the same time an estimator of \mathbf{M}_1 , and also that of \mathbf{H}_1 are found by projecting observations on $\mathcal{C}(\mathbf{C}'_1) \otimes \mathcal{V}_1$ and $(\mathcal{C}(\mathbf{C}'_1) \cap \mathcal{C}(\mathbf{C}'_2)^\perp) \otimes \mathcal{V}_1^\perp$ respectively, i.e.,

$$\begin{aligned}\widehat{\mathbf{M}}_1 &= \mathbf{P}_{\mathbf{A}_1, \widehat{\Sigma}_1^{(s)}} \mathbf{X} \mathbf{P}_{\mathbf{C}'_1}, \\ \widehat{\mathbf{H}}_1 &= (\mathbf{I} - \mathbf{P}_{\mathbf{A}_1, \widehat{\Sigma}_1^{(s)}}) \mathbf{X} (\mathbf{P}_{\mathbf{C}'_1} - \mathbf{P}_{\mathbf{C}'_2}).\end{aligned}\tag{8}$$

A second estimator of $\Sigma^{(s)}$ is obtained using the sum of \mathbf{Q}_0 and $\widehat{\mathbf{H}}_1 \widehat{\mathbf{H}}'_1$ and so on.

Estimators when the covariance matrix is linearly structured

After the r^{th} stage we have the following quantities.

$$\mathbf{W}_i = \mathbf{X}(\mathbf{P}_{\mathbf{C}'_i} - \mathbf{P}_{\mathbf{C}'_{i+1}})\mathbf{X}' \sim W_p(\boldsymbol{\Sigma}^{(s)}, r_i - r_{i+1}),$$
$$i = 0, 1, 2, \dots, r,$$

$$\hat{\mathbf{P}}_j = \hat{\mathbf{T}}_{j-1}\hat{\mathbf{T}}_{j-2} \times \cdots \times \hat{\mathbf{T}}_0, \quad \hat{\mathbf{T}}_0 = \mathbf{I}, \quad j = 1, 2, \dots, i,$$

$$\hat{\mathbf{T}}_i = \mathbf{I} - \mathbf{P}_{\hat{\mathbf{P}}_i \mathbf{A}_i, \boldsymbol{\Sigma}^{(s)}}, \quad i = 0, 2, \dots, r,$$

$$\hat{\mathcal{T}}_i = \mathbf{I} - \sum_{j=1}^i \mathbf{P}_{\hat{\mathbf{P}}_j \mathbf{A}_j, \hat{\boldsymbol{\Sigma}}_j^{(s)}}, \quad i = 0, 1, 2, 3, \dots, r,$$

$$\hat{\mathbf{H}}_i \hat{\mathbf{H}}_i' = \hat{\mathcal{T}}_i \mathbf{W}_i \hat{\mathcal{T}}_i', \quad i = 0, 1, 2, 3, \dots, r,$$

$$\hat{\mathbf{Q}}_r = \sum_{i=0}^r \hat{\mathbf{H}}_i \hat{\mathbf{H}}_i' = \sum_{i=0}^r \hat{\mathcal{T}}_i \mathbf{W}_i \hat{\mathcal{T}}_i', \quad r = 0, 1, 2, 3, \dots, m,$$

$$\hat{\mathcal{T}}_r \mathbf{W}_r \hat{\mathcal{T}}_r' | \hat{\mathbf{Q}}_{r-1} \sim W_p(\hat{\mathcal{T}}_r \boldsymbol{\Sigma}^{(s)} \hat{\mathcal{T}}_r', r_r - r_{r+1}).$$

Estimators when the covariance matrix is linearly structured

Theorem: Let $\widehat{\mathbf{Q}}_r$ be defined as in (10) and let

$$\widehat{\mathbf{Y}}_r = \sum_{i=0}^r (r_i - r_{i+1}) \widehat{\mathcal{T}}_i \otimes \widehat{\mathcal{T}}_i, \quad r = 0, 1, 2, \dots, m.$$

Then, the minimizers of

$$f_r(\boldsymbol{\Sigma}^{(s)}) = \text{tr} \left\{ \left(\widehat{\mathbf{Q}}_r - \sum_{i=0}^r (r_i - r_{i+1}) \widehat{\mathcal{T}}_i \boldsymbol{\Sigma}^{(s)} \widehat{\mathcal{T}}_i' \right) ()' \right\}, \quad r = 0, 1, 2, \dots, m,$$

are given by

$$\text{vec} \widehat{\boldsymbol{\Sigma}}_{r+1}^{(s)} = \mathbf{T}^+ \left((\mathbf{T}^+)' \widehat{\mathbf{Y}}_r' \widehat{\mathbf{Y}}_r \mathbf{T}^+ \right)^- (\mathbf{T}^+)' \widehat{\mathbf{Y}}_r' \text{vec} \widehat{\mathbf{Q}}_r.$$

Estimators when the covariance matrix is linearly structured

Theorem [Main result]: Let the EGC model be given by (1). Then





- (i) A consistent estimator of the structured covariance matrix $\Sigma^{(s)}$ is given by

$$\text{vec}\widehat{\Sigma}_{m+1}^{(s)} = \mathbf{T}^+ \left((\mathbf{T}^+)' \widehat{\mathbf{Y}}_m' \widehat{\mathbf{Y}}_m \mathbf{T}^+ \right)^- (\mathbf{T}^+)' \widehat{\mathbf{Y}}_m' \text{vec}\widehat{\mathbf{Q}}_m. \quad (9)$$

- (ii) An unbiased estimator of the mean is given by

$$\widehat{E}[\mathbf{X}] = \sum_{i=1}^m (\mathbf{I} - \widehat{\mathcal{T}}_i) \mathbf{X} \mathbf{C}_i' (\mathbf{C}_i \mathbf{C}_i')^- \mathbf{C}_i. \quad (10)$$

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Thank you!