Envelope Models and Methods

Dimension Reduction for Efficient Estimation in Multivariate Statistics

R. Dennis Cook
School of Statistics
University of Minnesota
Minneapolis, MN 55455, U.S.A.

November 18, 2013

Contents

Chapter 6

Envelope formulation and estimation

In this chapter we describe a general principle for choosing the ingredients $\mathbf{M}$ and $\mathcal{S}$ in the envelope $\mathcal{E}_{\mathbf{M}}(\mathcal{S})$ to improve estimative efficiency in multivariate statistical studies. In Section 6.1 we give a general paradigm for enveloping a vector-valued parameter; matrix-values parameters are considered in Section 6.2. The rest of the chapter is devoted to methods for estimating an envelope.

6.1 Envelope formulation for vector-valued parameters

6.1.1 Envelope definition

Let $\widetilde{\boldsymbol{\theta}} \in \mathbb{R}^m$ denote an estimator of an unknown parameter vector $\boldsymbol{\theta} \in \mathbb{R}^m$ based on a sample of size n. For example, $\widetilde{\boldsymbol{\theta}}$ might be the estimator of the coefficient vector in a generalized linear model, a least squares estimator or a robust estimator in linear regression with a univariate response. The goal of an envelope in this context is to reduce the variation in $\widetilde{\boldsymbol{\theta}}$ without introducing worrisome bias.

Assume, as is often the case, that $\sqrt{n}(\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta})$ converges in distribution to a normal random vector with mean 0 and covariance matrix $\mathbf{V}(\boldsymbol{\theta}) > 0$ as $n \to \infty$. In the first applications of Chapters 1 and 2, $\mathbf{V}$ does not depend on the parameter being estimated, but $\mathbf{V}$ may depend on $\boldsymbol{\theta}$ more generally. The assumption of normality is used to insure that the covariance matrix $\mathbf{V}(\boldsymbol{\theta})$ adequately reflects the asymptotic uncertainty in $\widetilde{\boldsymbol{\theta}}$. This might not be so in non-normal cases and then a different approach might be necessary.

To accommodate the possible presence of nuisance parameters we decompose $\boldsymbol{\theta}$ as $\boldsymbol{\theta} = (\boldsymbol{\psi}^T, \boldsymbol{\phi}^T)^T$ where $\boldsymbol{\phi} \in \mathbb{R}^p$ is the parameter vector of interests and $\boldsymbol{\psi} \in \mathbb{R}^{m-p}$ is the nuisance parameter vector. Let $\mathbf{V}_{\boldsymbol{\phi}}(\boldsymbol{\theta})$ be the $p \times p$ lower right block of $\mathbf{V}(\boldsymbol{\theta})$, which is the asymptotic covariance matrix of $\widetilde{\boldsymbol{\phi}}$. Then we define the envelope as follows.

Definition 6.1 *The envelope for the parameter* $\boldsymbol{\phi} \in \mathbb{R}^p$ *with estimator* $\widetilde{\boldsymbol{\phi}}$ *is defined as* $\mathcal{E}_{\mathbf{V}_{\boldsymbol{\phi}}(\boldsymbol{\theta})}(\boldsymbol{\phi}) \subseteq \mathbb{R}^p$.

This definition links an envelope to a particular pre-specified method of estimation through the covariance matrix $\mathbf{V}_{\boldsymbol{\phi}}(\boldsymbol{\theta})$, while in previous chapters only maximum likelihood estimation was considered. The goal of an envelope is to improve that pre-specified estimator, depending on the original goals of the analysis. This may provide additional intuition for the discussion of non-normality in Section 2.8. Also, the matrix to be reduced – here $\mathbf{V}_{\boldsymbol{\phi}}(\boldsymbol{\theta})$ – is dictated by the pre-specified method of estimation, and it can depend on the parameter being estimated, in addition to perhaps other parameters.

Some insights into the interpretation and potential advantages of envelopes in this general context can be gained by considering the estimator $\widetilde{\boldsymbol{\theta}}$ of the whole parameter vector $\boldsymbol{\theta}$ with covariance matrix $\mathbf{V}(\boldsymbol{\theta})$, and assuming that the envelope $\mathcal{E}_{\mathbf{V}(\boldsymbol{\theta})}(\boldsymbol{\theta})$ is known. Since $\boldsymbol{\theta} \in \mathcal{E}_{\mathbf{V}(\boldsymbol{\theta})}(\boldsymbol{\theta})$, $\sqrt{n}\mathbf{P}_{\mathcal{E}}(\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta}) = \sqrt{n}(\mathbf{P}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta})$, where $\widehat{\boldsymbol{\theta}}_{\mathcal{E}} := \mathbf{P}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$ is an envelope estimator of $\boldsymbol{\theta}$ with known envelope. Straightforwardly, $\sqrt{n}(\mathbf{P}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta})$ converges to a normal random vector with mean $\boldsymbol{\theta}$ and variance $\mathbf{P}_{\mathcal{E}}\mathbf{V}\mathbf{P}_{\mathcal{E}}$, and $\sqrt{n}\mathbf{Q}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$ converges to a normal random vector with mean 0 and covariance $\mathbf{Q}_{\mathcal{E}}\mathbf{V}\mathbf{Q}_{\mathcal{E}}$. Since $\mathcal{E}_{\mathbf{V}(\boldsymbol{\theta})}(\boldsymbol{\theta})$ reduces $\mathbf{V}$, we have by Proposition 5.1 $\mathbf{V} = \mathbf{P}_{\mathcal{E}}\mathbf{V}\mathbf{P}_{\mathcal{E}} + \mathbf{Q}_{\mathcal{E}}\mathbf{V}\mathbf{Q}_{\mathcal{E}}$, so that $\mathbf{P}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$ and $\mathbf{Q}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$ are asymptotically independent. In sum, $\widetilde{\boldsymbol{\theta}} = \mathbf{P}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}} + \mathbf{Q}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}} = \widehat{\boldsymbol{\theta}}_{\mathcal{E}} + \mathbf{Q}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$. Since $\mathbf{Q}_{\mathcal{E}}\widetilde{\boldsymbol{\theta}}$ is an estimator of 0 and is asymptotically independent of $\widehat{\boldsymbol{\theta}}$, it represents the immaterial information in the original estimator $\widetilde{\boldsymbol{\theta}}$ that is eliminated by using the envelope estimator $\widehat{\boldsymbol{\theta}}$. Depending on the context, this general notion of immaterial information might be cast in terms of measured variates, as in Section 2.8.

6.1.2 Illustrations

In this section we describe relationships between the envelopes used in previous methodology and the envelopes resulting from Definition 6.1.

Enveloping a multivariate mean. As described in Chapter 1, consider the problem of estimating a multivariate mean based on a sample $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ of a random vector $\mathbf{Y}$ with mean 0 and variance $\boldsymbol{\Sigma}$. If our original estimator is $\widetilde{\boldsymbol{\theta}} = \bar{\mathbf{Y}}$, then $\mathbf{V} = n^{-1}\boldsymbol{\Sigma}$, and

Definition 6.1 leads us to consider $\mathcal{E}_{\mathbf{V}}(\boldsymbol{\mu}) = \mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\mu})$. Estimation in Chapter 1 was based normality, which is not required by Defintion 6.1.

Univariate linear regression. Consider the univariate linear regression model $Y = \alpha + \boldsymbol{\beta}^T\mathbf{X} + \epsilon$, where ϵ is independent of $\mathbf{X}$, and has mean 0 and variance σ^2. The ordinary least squares estimator of $\boldsymbol{\beta}$ has asymptotic variance $\mathbf{V}_{\boldsymbol{\beta}} = \sigma^2\boldsymbol{\Sigma}_{\mathbf{X}}^{-1}$. Direct application of Definition 6.1 then leads to the $\sigma^2\boldsymbol{\Sigma}_{\mathbf{X}}^{-1}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$. However, it follows from Corollary 5.2 that $\mathcal{E}_{\mathbf{V}_{\boldsymbol{\beta}}}(\boldsymbol{\beta}) = \mathcal{E}_{\boldsymbol{\Sigma}_{\mathbf{X}}}(\boldsymbol{\beta})$, the $\boldsymbol{\Sigma}_{\mathbf{X}}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$. This is the envelope estimated by the SIMPLS algorithm for partial least squares regression in an effort to improve upon the ordinary least squares estimator for the purpose of prediction, as discussed in Chapter 4.

Multivariate linear regression with a univariate predictor. The multivariate linear model, $\mathbf{Y} = \boldsymbol{\alpha} + \boldsymbol{\beta}X + \boldsymbol{\varepsilon}$ and $\mathrm{var}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma}$, with a univariate predictor X provides another illustration on the use of Definition 6.1. In Chapter 2 we based envelope estimation on the $\boldsymbol{\Sigma}$-envelope of $\mathcal{B} = \mathrm{span}(\boldsymbol{\beta})$, so the envelope is the smallest subspace $\mathcal{S}$ that satisfies the two conditions (a) $\mathbf{P}_{\mathcal{S}}\boldsymbol{\beta} = \boldsymbol{\beta}$ and (b) $\boldsymbol{\Sigma} = \mathbf{P}_{\mathcal{S}}\boldsymbol{\Sigma}\mathbf{P}_{\mathcal{S}} + \mathbf{Q}_{\mathcal{S}}\boldsymbol{\Sigma}\mathbf{Q}_{\mathcal{S}}$. To cast this in the context of Definition 6.1, take $\boldsymbol{\psi} = (\boldsymbol{\alpha}, \boldsymbol{\Sigma})$, $\boldsymbol{\phi} = \boldsymbol{\beta}$, and $\widetilde{\boldsymbol{\phi}}$ to be the ordinary least squares estimator of $\boldsymbol{\beta}$ (2.2). Let $\sigma_X^2 = \mathrm{var}(X)$. The asymptotic covariance matrix of $\widetilde{\boldsymbol{\phi}}$ is $\sigma_X^{-2}\boldsymbol{\Sigma}$, which does not depend on $\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$. Direct application of Definition 6.1 then leads to the $\sigma_X^{-2}\boldsymbol{\Sigma}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$. The equivalence of the envelopes $\mathcal{E}_{\boldsymbol{\sigma}_X^{-2}\boldsymbol{\Sigma}}(\boldsymbol{\beta})$ and $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta})$ follows from the construct leading to Corollary 5.2.

Partial envelopes. In Chapter 3 we considered partial envelopes for $\boldsymbol{\beta}_1$ in the partitioned multivariate linear regression model

$$\mathbf{Y}_i = \boldsymbol{\mu} + \boldsymbol{\beta}\mathbf{X}_i + \boldsymbol{\varepsilon}_i = \boldsymbol{\mu} + \boldsymbol{\beta}_1 X_{1i} + \boldsymbol{\beta}_2\mathbf{X}_{2i} + \boldsymbol{\varepsilon}_i,\ i = 1, \ldots, n,$$

where $\mathbf{Y} \in \mathbb{R}^r$, $\boldsymbol{\beta} \in \mathbb{R}^{r\times p}$, the predictor vector $\mathbf{X} \in \mathbb{R}^p$ is non-stochastic and centered in the sample, the error vectors $\boldsymbol{\varepsilon}_i$ are independent copies of $\boldsymbol{\varepsilon} \sim N(0, \boldsymbol{\Sigma})$. To apply Definition 6.1, the asymptotic covariance matrix of the least squares estimator of $\boldsymbol{\beta}_1$ is $\mathbf{V}_{\boldsymbol{\beta}_1} = (\boldsymbol{\Sigma}_{\mathbf{X}}^{-1})_{11}\boldsymbol{\Sigma}$, where $(\boldsymbol{\Sigma}_{\mathbf{X}}^{-1})_{11}$ is the $(1,1)$ element of the inverse of $\boldsymbol{\Sigma}_{\mathbf{X}} = \lim_{n\to\infty} n^{-1}\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i^T$. The $\mathbf{V}_{\boldsymbol{\beta}_1}$-envelope of $\mathrm{span}(\boldsymbol{\beta}_1)$ is then dictated by Definition 6.1. If $\boldsymbol{\varepsilon}$ is not normal, then the asymptotic variance of the ordinary least squares estimator is the same as that of the maximum likelihood estimator under normality, and the envelope can be viewed as a precursor to improving upon ordinary least squares.

Weighted least squares. Consider a heteroscedastic linear model with data consisting of n independent copies of $(Y, \mathbf{X}, W)$, where $Y \in \mathbb{R}^1$, $\mathbf{X} \in \mathbb{R}^p$, and $W > 0$ is a weight with $\mathrm{E}(W) = 1$:

$$Y = \mu + \boldsymbol{\beta}^T \mathbf{X} + \varepsilon/\sqrt{W}, \tag{6.1}$$

where $\varepsilon \perp\!\!\!\perp (\mathbf{X}, W)$ and $\mathrm{Var}(\varepsilon) = \sigma^2$. The constraint $\mathrm{E}(W) = 1$ is without loss of generality and serves to normalize the weights so they have mean 1 and to make subsequent expressions a bit simpler. Fitting under this model is typically done by using weighted least squares (WLS):

$$(a, \mathbf{b}) = \arg\min_{\mu, \boldsymbol{\beta}} n^{-1} \sum_{i=1}^{n} W_i (Y_i - \mu - \boldsymbol{\beta}^T \mathbf{X}_i)^2, \tag{6.2}$$

where we normalize the sample weights so that $\bar{W} = 1$. Let

$$\begin{aligned} \boldsymbol{\Sigma}_{\mathbf{X}(W)} &= \mathrm{E}\{W(\mathbf{X} - \mathrm{E}(W\mathbf{X}))(\mathbf{X} - \mathrm{E}(W\mathbf{X}))^T\} \\ \boldsymbol{\Sigma}_{\mathbf{X}Y(W)} &= \mathrm{E}[W\{\mathbf{X} - \mathrm{E}(W\mathbf{X})\}\{Y - \mathrm{E}(WY)\}] \end{aligned}$$

denote the weighted covariance matrix of $\mathbf{X}$ and the weighted covariance between $\mathbf{X}$ and Y, and let $\mathbf{S}_{\mathbf{X}(W)}$ and $\mathbf{S}_{\mathbf{X}Y(W)}$ denote their corresponding sample versions. Then $\boldsymbol{\beta} = \boldsymbol{\Sigma}_{\mathbf{X}(W)}^{-1} \boldsymbol{\Sigma}_{\mathbf{X}Y(W)}$, the pre-specified is $\widetilde{\boldsymbol{\beta}} = \mathbf{S}_{\mathbf{X}(W)}^{-1} \mathbf{S}_{\mathbf{X}Y(W)}$ and $\sqrt{n}(\widetilde{\boldsymbol{\beta}} - \boldsymbol{\beta})$ converges to a normal random vector with mean 0 and variance $\mathbf{V}_{\boldsymbol{\beta}} = \sigma^2 \boldsymbol{\Sigma}_{\mathbf{X}(W)}^{-1}$. According to Definition 6.1, we should now strive to estimate the $\sigma^2 \boldsymbol{\Sigma}_{\mathbf{X}(W)}^{-1}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$, which is equal to the $\boldsymbol{\Sigma}_{\mathbf{X}(W)}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$.

Non-linear least squares. Consider the non-linear univariate regression model

$$Y = f(\mathbf{X}, \boldsymbol{\beta}) + \epsilon,$$

where f is a known function of the predictor vector $\mathbf{X} \in \mathbb{R}^p$ and parameter vector $\boldsymbol{\beta} \in \mathbb{R}^q$, and errors ϵ are independent of $\mathbf{X}$ and have mean 0 and variance σ^2. Given a sample $(Y_i, \mathbf{X}_i)$, $i = 1, \ldots, n$, we take the pre-specified estimator to be the the usual least squares estimator of $\boldsymbol{\beta}$:

$$\widetilde{\boldsymbol{\beta}} = \arg\min \sum_{i=1}^{n} (Y_i - f(\mathbf{X}_i, \boldsymbol{\beta}))^2.$$

Let $\mathbf{W} \in \mathbb{R}^{n \times q}$ denote the matrix with rows $\mathbf{w}_i^T$ equal to the partial derivative vectors $\mathbf{w}_i^T = \partial f(\mathbf{X}_i, \boldsymbol{\beta})/\partial \boldsymbol{\beta}^T$, $i = 1, \ldots, n$, evaluated at the true value of $\boldsymbol{\beta}$ and let $\mathbf{V}_{\boldsymbol{\beta}} = \lim_{n \to \infty} \mathbf{W}^T \mathbf{W}/n$. Then under the usual regularity conditions, $\sqrt{n}(\widetilde{\boldsymbol{\beta}} - \boldsymbol{\beta})$ is asymptotically normal with mean 0 and variance $\sigma^2 \mathbf{V}_{\boldsymbol{\beta}}^{-1}$, which leads to the $\mathbf{V}_{\boldsymbol{\beta}}$-envelope of $\mathrm{span}(\boldsymbol{\beta})$.

6.2 Envelope formulation for matrix-valued parameters

Definition 6.1 is sufficiently general to cover a matrix-valued parameter $\boldsymbol{\phi} \in \mathbb{R}^{r \times c}$ by considering the $\mathrm{avar}(\sqrt{n}\mathrm{vec}(\widetilde{\boldsymbol{\phi}}))$-envelope of $\mathrm{span}(\mathrm{vec}(\boldsymbol{\phi}))$. However, matrix-valued parameters come with additional structure that is often desirable to maintain during estimation. For instance, in the multivariate linear model our envelope constructions were constrained to reflect separate row and column reduction of the matrix parameter $\boldsymbol{\beta}$, leading to interpretations in terms of material variation in $\mathbf{X}$ and $\mathbf{Y}$. In this section we indicate how to adapt for a matrix-valued parameter in the spirit of Definition 6.1. To avoid proliferation of notation, we use parameters in envelope descriptions rather than their spans; eg. $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta}) := \mathcal{E}_{\boldsymbol{\Sigma}}(\mathcal{B})$.

Suppose that $\sqrt{n}(\widetilde{\boldsymbol{\phi}} - \boldsymbol{\phi})$ converges to a matrix normal distribution with mean 0, column variance $\boldsymbol{\Delta}_L \in \mathbb{S}^{r \times r}$ and row variance $\boldsymbol{\Delta}_R \in \mathbb{S}^{c \times c}$. (See Dawid (1981) for background on the matrix normal distribution.) Then

$$\sqrt{n}(\mathrm{vec}(\widetilde{\boldsymbol{\phi}}) - \mathrm{vec}(\boldsymbol{\phi})) \to N(0, \boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L), \tag{6.3}$$

and direct application of Definition 6.1 yields the envelope $\mathcal{E}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\mathrm{vec}(\boldsymbol{\phi}))$. The least squares estimator of the coefficient matrix $\boldsymbol{\beta}$ in the multivariate linear model satisfies this condition with $\boldsymbol{\Delta}_R = \boldsymbol{\Sigma}_{\mathbf{X}}^{-1}$ and $\boldsymbol{\Delta}_L = \boldsymbol{\Sigma}$ (Section 2.1). However, this envelope may not preserve the intrinsic row-column structure of $\boldsymbol{\phi}$. In the following definition we introduce a restricted class of envelopes that maintain the matrix structure of $\boldsymbol{\phi}$. In preparation, the Kronecker product of two subspaces $\mathcal{A}$ and $\mathcal{B}$ is defined as $\mathcal{A} \otimes \mathcal{B} = \{\mathbf{a} \otimes \mathbf{b} \mid \mathbf{a} \in \mathcal{A}, \mathbf{b} \in \mathcal{B}\}$. If $\mathbf{A}$ and $\mathbf{B}$ are basis matrices for $\mathcal{A}$ and $\mathcal{B}$ then $\mathrm{span}(\mathbf{A} \otimes \mathbf{B}) = \mathcal{A} \otimes \mathcal{B}$.

Definition 6.2 *Assume that $\widetilde{\boldsymbol{\phi}}$ is asymptotically matrix normal as give in (6.3). Then the tensor envelope for $\boldsymbol{\phi}$, denoted by $\mathcal{K}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\boldsymbol{\phi})$, is defined as the intersection of all reducing subspaces $\mathcal{E}$ of $\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L$ that contain* $\mathrm{span}(\mathrm{vec}(\boldsymbol{\phi}))$ *and can be written as $\mathcal{E} = \mathcal{E}_R \otimes \mathcal{E}_L$ with $\mathcal{E}_R \subseteq \mathbb{R}^c$ and $\mathcal{E}_L \subseteq \mathbb{R}^r$.*

We see from this definition that $\mathcal{K}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\boldsymbol{\phi})$ always exist and is the smallest subspace with the required properties. Let $\boldsymbol{\Gamma}_L \in \mathbb{R}^{r \times d_c}$, $d_c < r$, and $\boldsymbol{\Gamma}_R \in \mathbb{R}^{c \times d_r}$, $d_r < c$ be semi-orthogonal matrices such that $\mathcal{K}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\boldsymbol{\phi}) = \mathrm{span}(\boldsymbol{\Gamma}_R \otimes \boldsymbol{\Gamma}_L)$. By definition, $\mathrm{span}(\boldsymbol{\phi}) \subseteq \mathrm{span}(\boldsymbol{\Gamma}_L)$ and $\mathrm{span}(\boldsymbol{\phi}^T) \subseteq \mathrm{span}(\boldsymbol{\Gamma}_R)$. Hence we have $\boldsymbol{\phi} = \boldsymbol{\Gamma}_L \boldsymbol{\eta} \boldsymbol{\Gamma}_R^T$ and $\mathrm{vec}(\boldsymbol{\phi}) = (\boldsymbol{\Gamma}_R \otimes \boldsymbol{\Gamma}_L)\mathrm{vec}(\boldsymbol{\eta})$ for some $\eta \in \mathbb{R}^{d_c \times d_r}$.

The next proposition shows how to factor $\mathcal{K}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\boldsymbol{\phi}) \in \mathbb{R}^{rc}$ into the tensor product of envelopes $\mathcal{E}_{\boldsymbol{\Delta}_R}(\boldsymbol{\phi}^T) \in \mathbb{R}^r$ and $\mathcal{E}_{\boldsymbol{\Delta}_L}(\boldsymbol{\phi}) \in \mathbb{R}^c$ for the row and column spaces of $\boldsymbol{\phi}$.

These tensor factors are envelopes in smaller spaces that preserve the row and column structure and can facilitate analysis and interpretation.

Proposition 6.1 $\mathcal{K}_{\boldsymbol{\Delta}_R \otimes \boldsymbol{\Delta}_L}(\boldsymbol{\phi}) = \mathcal{E}_{\boldsymbol{\Delta}_R}(\boldsymbol{\phi}^T) \otimes \mathcal{E}_{\boldsymbol{\Delta}_L}(\boldsymbol{\phi})$.

PROOF.

To come $\square$

For example, in reference to the multivariate linear model (2.1), the distribution of $\mathbf{B} = \mathbf{S}_{\mathbf{XY}}^T \mathbf{S}_{\mathbf{X}}^{-1}$ satisfies (6.3) with $\boldsymbol{\Delta}_R = \boldsymbol{\Sigma}_{\mathbf{X}}^{-1}$ and $\boldsymbol{\Delta}_L = \boldsymbol{\Sigma}$. The tensor envelope is then

$$\mathcal{K}_{\boldsymbol{\Sigma}_{\mathbf{X}}^{-1} \otimes \boldsymbol{\Sigma}}(\boldsymbol{\beta}) = \mathcal{E}_{\boldsymbol{\Sigma}_{\mathbf{X}}^{-1}}(\boldsymbol{\beta}^T) \otimes \mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta}).$$

If we are interested in reducing only the column space of $\boldsymbol{\beta}$, which corresponds to response reduction, we would use $\mathbb{R}^p \otimes \mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta})$ for constructing an envelope estimator of $\boldsymbol{\beta}$, and then $\boldsymbol{\beta} = \boldsymbol{\Gamma}_L \boldsymbol{\eta} \mathbf{I}_p = \boldsymbol{\Gamma}_L \boldsymbol{\eta}$ where $\boldsymbol{\Gamma}_L$ is a semi-orthogonal basis for $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta})$, which reproduces the envelope construction of Chapter 2. Similarly, if we are interested only in predictor reduction, we would take $\mathcal{E}_{\boldsymbol{\Sigma}_{\mathbf{X}}}(\boldsymbol{\beta}^T) \otimes \mathbb{R}^r$, which reproduces the envelope construction in Chapter 4. More generally, the definition of the tensor envelope and Proposition 6.1 straightforwardly connects and combines the envelope models in the predictor space and in the response space, allowing for new methodology to be developed.

6.3 Likelihood-based envelope construction

In this section we describe a likelihood-based method of construction that requires $\mathbf{M} > 0$ and is based on searching over all u-dimensional subspaces of $\mathbb{R}^r$, where $u = \dim(\mathcal{E}_{\mathbf{M}}(\mathcal{S}))$. The set of all subspaces of dimension u in $\mathbb{R}^r$ is called a Grassmann manifold and is denoted by $\mathcal{G}^{r \times u}$. A brief introduction to Grassmann manifolds is given in the appendix of this chapter *this location will be changed to the chapter in which the manifolds are first used, likely SDR chapter 1*.

Given the dimension of the envelope, the envelope estimators we have considered so far are all maximum likelihood estimators based on normality assumptions. As a consequence, the partial maximized log likelihood functions $L(\mathbf{G}) = -(n/2)J(\mathbf{G})$ for estimation of a basis $\boldsymbol{\Gamma}$ of $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta})$, $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta}_1)$ or $\mathcal{E}_{\boldsymbol{\Sigma}_{\mathbf{X}}}(\boldsymbol{\beta}^T)$ all have the same form with

$$J(\mathbf{G}) = \log |\mathbf{G}^T \widehat{\mathbf{M}} \mathbf{G}| + \log |\mathbf{G}^T (\widehat{\mathbf{M}} + \widehat{\mathbf{U}})^{-1} \mathbf{G}|, \qquad (6.4)$$

where the positive definite matrix $\widehat{\mathbf{M}}$ and the positive semi-definite matrix $\widehat{\mathbf{U}}$ depend on context. An estimated basis is then $\widehat{\boldsymbol{\Gamma}} = \arg\min J(\mathbf{G})$, where the minimization is carried out over a set of semi-orthogonal matrices whose dimensions depend on the envelope being estimated. Estimates of the remaining parameters are then simple functions of $\widehat{\boldsymbol{\Gamma}}$. To determine the estimator of $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta})$, we have $\widehat{\mathbf{M}} = \mathbf{S}_{\mathbf{Y}|\mathbf{X}}$, $\widehat{\mathbf{M}} + \widehat{\mathbf{U}} = \mathbf{S}_{\mathbf{Y}}$, $\widehat{\boldsymbol{\beta}} = \mathbf{P}_{\widehat{\boldsymbol{\Gamma}}}\widehat{\boldsymbol{\beta}}$ and $\widehat{\boldsymbol{\Sigma}} = \mathbf{P}_{\widehat{\boldsymbol{\Gamma}}}\mathbf{S}_{\mathbf{Y}|\mathbf{X}}\mathbf{P}_{\widehat{\boldsymbol{\Gamma}}} + \mathbf{Q}_{\widehat{\boldsymbol{\Gamma}}}\mathbf{S}_{\mathbf{Y}|\mathbf{X}}\mathbf{Q}_{\widehat{\boldsymbol{\Gamma}}}$. The same forms are used for partial envelopes $\mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta}_1)$, except $\mathbf{Y}$ and $\mathbf{X}_1$ are replaced with the residuals from their linear fits on $\mathbf{X}_2$. For predictor reduction in model (2.1), the envelope $\mathcal{E}_{\boldsymbol{\Sigma}_{\mathbf{X}}}(\boldsymbol{\beta}^T)$ is estimated with $\widehat{\mathbf{M}} = \mathbf{S}_{\mathbf{X}|\mathbf{Y}}$, $\widehat{\mathbf{M}} + \widehat{\mathbf{U}} = \mathbf{S}_{\mathbf{X}}$, $\widehat{\boldsymbol{\beta}} = \mathbf{B}\mathbf{P}^T_{\widehat{\boldsymbol{\Gamma}}(\mathbf{S}_{\mathbf{X}})}$ and $\widehat{\boldsymbol{\Sigma}}_{\mathbf{X}} = \mathbf{P}_{\widehat{\boldsymbol{\Gamma}}}\mathbf{S}_{\mathbf{X}}\mathbf{P}_{\widehat{\boldsymbol{\Gamma}}} + \mathbf{Q}_{\widehat{\boldsymbol{\Gamma}}}\mathbf{S}_{\mathbf{X}}\mathbf{Q}_{\widehat{\boldsymbol{\Gamma}}}$.

Here we use $J(\mathbf{G})$ as a generic objective function for estimating an envelope given estimators of $\mathbf{M}$ and $\mathbf{U}$. Although objective function is inspired by the normal likelihood for the multivariate linear model, neither the linear model nor normality is required in this usage. The next proposition shows that minimizing $J(\mathbf{G})$ returns $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ in the population.

Proposition 6.2 *Let $\mathbf{M} > 0$ and $\mathbf{U} \geq 0$ be symmetric matrices of the same size, let $\boldsymbol{\Gamma}$ denote a semi-orthogonal basis matrix for the $\mathbf{M}$-envelope of $\mathcal{U} = \mathrm{span}(\mathbf{U})$ and let $u = \dim(\mathcal{E}_{\mathbf{M}}(\mathcal{U}))$. Then the envelope can be construced as*

$$\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \arg\min_{\mathcal{T}\in\mathcal{G}^{r\times u}}\{\log|\mathbf{P}_{\mathcal{T}}\mathbf{M}\mathbf{P}_{\mathcal{T}}|_0 + \log|\mathbf{Q}_{\mathcal{T}}(\mathbf{M}+\mathbf{U})\mathbf{Q}_{\mathcal{T}}|_0\}.$$

A semi-orthognal basis matrix $\boldsymbol{\Gamma} \in \mathbb{R}^{r\times u}$ for $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ can be obtained as

$$\begin{aligned}\boldsymbol{\Gamma} &= \arg\min_{\mathbf{G}}\{\log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}_0^T(\mathbf{M}+\mathbf{U})\mathbf{G}_0|\} \\ &= \arg\min_{\mathbf{G}}\{\log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{G}|\},\end{aligned}$$

where $\min_{\mathbf{G}}$ is taken over all semi-orthognal matrices $\mathbf{G} \in \mathbb{R}^{r\times u}$.

The proof of this proposition makes use of the following two lemmas, which may be useful in other contexts. Lemma 6.1 justifies replacing $\log|\mathbf{G}_0^T(\mathbf{M}+\mathbf{U})\mathbf{G}_0|$ with $\log|\mathbf{G}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{G}|$ during the minimization to obtain $\boldsymbol{\Gamma}$.

Lemma 6.1 *Suppose that $\mathbf{A} \in \mathbb{R}^{t\times t}$ is non-singular and that the column-partitioned matrix $(\boldsymbol{\alpha}, \boldsymbol{\alpha}_0) \in \mathbb{R}^{t\times t}$ is orthogonal. Then $|\boldsymbol{\alpha}_0^T\mathbf{A}\boldsymbol{\alpha}_0| = |\mathbf{A}| \times |\boldsymbol{\alpha}^T\mathbf{A}^{-1}\boldsymbol{\alpha}|$.*

PROOF. Define the $t \times t$ matrix

$$\mathbf{K} = \begin{pmatrix} \mathbf{I}_d, \boldsymbol{\alpha}^T\mathbf{A}\boldsymbol{\alpha}_0 \\ 0, \boldsymbol{\alpha}_0^T\mathbf{A}\boldsymbol{\alpha}_0 \end{pmatrix}.$$

Since $(\boldsymbol{\alpha}, \boldsymbol{\alpha}_0)$ is an orthogonal matrix,

$$\begin{aligned} |\boldsymbol{\alpha}_0^T \mathbf{A} \boldsymbol{\alpha}_0| &= |(\boldsymbol{\alpha}, \boldsymbol{\alpha}_0)\mathbf{K}(\boldsymbol{\alpha}, \boldsymbol{\alpha}_0)^T| = |\boldsymbol{\alpha}\boldsymbol{\alpha}^T + \boldsymbol{\alpha}\boldsymbol{\alpha}^T \mathbf{A} \boldsymbol{\alpha}_0 \boldsymbol{\alpha}_0^T + \boldsymbol{\alpha}_0 \boldsymbol{\alpha}_0^T \mathbf{A} \boldsymbol{\alpha}_0 \boldsymbol{\alpha}_0^T| \\ &= |\mathbf{A} - (\mathbf{A} - \mathbf{I}_p)\boldsymbol{\alpha}\boldsymbol{\alpha}^T| = |\mathbf{A}||\mathbf{I}_d - \boldsymbol{\alpha}^T(\mathbf{I}_p - \mathbf{A}^{-1})\boldsymbol{\alpha}| \\ &= |\mathbf{A}||\boldsymbol{\alpha}^T \mathbf{A}^{-1} \boldsymbol{\alpha}|. \end{aligned}$$

□

Lemma 6.2 *Let $\mathbf{O} = (\mathbf{O}_1, \mathbf{O}_2) \in \mathbb{R}^{r \times r}$ be a column partitioned orthogonal matrix and let $\mathbf{A} \in \mathbb{S}^{r \times r}$ be positive definite. Then $|\mathbf{A}| \le |\mathbf{O}_1^T \mathbf{A} \mathbf{O}_1| \times |\mathbf{O}_2^T \mathbf{A} \mathbf{O}_2|$ with equality if and only if $\operatorname{span}(\mathbf{O}_1)$ reduces $\mathbf{A}$.*

PROOF.

$$\begin{aligned} |\mathbf{A}| &= |\mathbf{O}^T \mathbf{A} \mathbf{O}| = \begin{vmatrix} \mathbf{O}_1^T \mathbf{A} \mathbf{O}_1 & \mathbf{O}_1^T \mathbf{A} \mathbf{O}_2 \\ \mathbf{O}_2^T \mathbf{A} \mathbf{O}_1 & \mathbf{O}_2^T \mathbf{A} \mathbf{O}_2 \end{vmatrix} \\ &= |\mathbf{O}_1^T \mathbf{A} \mathbf{O}_1| \times |\mathbf{O}_2^T \mathbf{A} \mathbf{O}_2 - \mathbf{O}_2^T \mathbf{A} \mathbf{O}_1 (\mathbf{O}_1^T \mathbf{A} \mathbf{O}_1)^{-1} \mathbf{O}_1^T \mathbf{A} \mathbf{O}_2| \\ &\le |\mathbf{O}_1^T \mathbf{A} \mathbf{O}_1| \times |\mathbf{O}_2^T \mathbf{A} \mathbf{O}_2|. \end{aligned}$$

□

PROOF OF PROPOSITION 6.2. To demonstrate Proposition 6.2, let $\mathbf{G}$ be a semi-orthogonal basis matrix for $\mathcal{T}$ and let $(\mathbf{G}, \mathbf{G}_0)$ be orthogonal. Then

$$|\mathbf{P}_{\mathcal{T}} \mathbf{M} \mathbf{P}_{\mathcal{T}}|_0 = \left| (\mathbf{G}, \mathbf{G}_0) \begin{pmatrix} \mathbf{G}^T \mathbf{M} \mathbf{G} & 0 \\ 0 & 0 \end{pmatrix} (\mathbf{G}, \mathbf{G}_0)^T \right|_0 = |\mathbf{G}^T \mathbf{M} \mathbf{G}|.$$

Consequently, we can work in terms of bases without loss of generality. Now,

$$\begin{aligned} \log |\mathbf{G}^T \mathbf{M} \mathbf{G}| + \log |\mathbf{G}_0^T (\mathbf{M} + \mathbf{U}) \mathbf{G}_0| &= \log |\mathbf{G}^T \mathbf{M} \mathbf{G}| + \log |\mathbf{G}_0^T \mathbf{M} \mathbf{G}_0 + \mathbf{G}_0^T \mathbf{U} \mathbf{G}_0| \\ &\ge \log |\mathbf{G}^T \mathbf{M} \mathbf{G}| + \log |\mathbf{G}_0^T \mathbf{M} \mathbf{G}_0| \\ &\ge |\mathbf{M}|, \end{aligned}$$

where the second inequality follows from Lemma 6.2. To achieve the lower bound, the second inequality requires that $\operatorname{span}(\mathbf{G})$ reduce $\mathbf{M}$, while the first inequality requires that

$\mathcal{U} \subseteq \mathrm{span}(\mathbf{G})$. The first representation for $\mathbf{\Gamma}$ follows since u is the dimension of the smallest subspace that satisfies these two properties. The second representation for $\mathbf{\Gamma}$ follows immediately from Lemma 6.1. □

The usual requirement that $\mathcal{U} \subseteq \mathrm{span}(\mathbf{M})$ holds automatically in Proposition 6.2 because $\mathbf{M} > 0$. If $\mathbf{M} \geq 0$ and $\mathcal{U} \subseteq \mathrm{span}(\mathbf{M})$, this proposition can be still used as a basis for the construction of $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ by using Proposition 5.6 to first reduce the coordinates.

Being based on a normal likelihood, some interpretations of the objective functions given in Proposition 6.2 parallel those for the objective functions of Chapters 2-4. To see this first factor $\mathbf{U} = \mathbf{u}\mathbf{u}^T$, where $\mathbf{u}$ has full column rank, let $\mathbf{A} = \mathbf{I} + \mathbf{u}^T\mathbf{M}\mathbf{u}$ and use the Woodbury identity to write

$$\begin{aligned}
|\mathbf{G}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{G}| &= |\mathbf{G}^T(\mathbf{M}+\mathbf{u}\mathbf{u}^T)^{-1}\mathbf{G}| \\
&= |\mathbf{G}^T\{\mathbf{M} - \mathbf{M}\mathbf{u}\mathbf{A}^{-1}\mathbf{u}^T\mathbf{M}^{-1}\}\mathbf{G}| \\
&= |\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G} - \mathbf{G}^T\mathbf{M}^{-1}\mathbf{u}\mathbf{A}^{-1}\mathbf{u}^T\mathbf{M}^{-1}\mathbf{G}| \\
&= |\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}| \\
&\quad \times |\mathbf{I} - \mathbf{A}^{-1/2}\mathbf{u}^T\mathbf{M}^{-1}\mathbf{G}(\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G})^{-1}\mathbf{G}^T\mathbf{M}^{-1}\mathbf{u}\mathbf{A}^{-1/2}| \\
&= |\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}| \times |\mathbf{I} - \mathbf{A}^{-1/2}\mathbf{u}^T\mathbf{M}^{-1/2}\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}\mathbf{M}^{-1/2}\mathbf{u}\mathbf{A}^{-1/2}| \\
&= |\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}| \times |\mathbf{I} - \mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}\mathbf{M}^{-1/2}\mathbf{u}\mathbf{A}^{-1}\mathbf{u}^T\mathbf{M}^{-1/2}\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}|
\end{aligned}$$

Let $\mathbf{\Gamma}$ be a semi-orthogonal basis matrix for $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$. Since $\mathrm{span}(\mathbf{u}) \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, we can write $\mathbf{u} = \mathbf{\Gamma}\boldsymbol{\eta}$ for some $\boldsymbol{\eta}$ with full column rank. Further, since $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ reduces $\mathbf{M}$ we have $\mathbf{M}^{-1/2}\mathbf{u} = \mathbf{\Gamma}\mathbf{v}$ for some $\mathbf{v}$ with full column rank. Then substituting into the last expression above we have

$$|\mathbf{G}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{G}| \quad = \quad |\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}| \times |\mathbf{I} - \mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}\mathbf{\Gamma}\mathbf{v}\mathbf{A}^{-1}\mathbf{v}^T\mathbf{\Gamma}^T\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}|.$$

With this expansion the objective function of Proposition 6.2 can be written as

$$\begin{aligned}
k(\mathbf{G}) := &\ \log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{G}| \\
= &\ \log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}| + \log|\mathbf{I} - \mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}\mathbf{\Gamma}\mathbf{v}\mathbf{A}^{-1}\mathbf{v}^T\mathbf{\Gamma}^T\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}|.
\end{aligned} \tag{6.5}$$

The terms in this expansion play different roles in determining a solution. The following lemma deals with the first two terms.

Lemma 6.3 *The function* $f(\mathbf{G}) := \log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}^T\mathbf{M}^{-1}\mathbf{G}|$ *is minimized over semi-orthogonal matrices* $\mathbf{G}$ *by choosing* $\mathbf{G}$ *to span any reducing subspace of* $\mathbf{M}$.

PROOF. Let $(\mathbf{G}, \mathbf{G}_0)$ be an orthogonal matrix, where $\mathrm{span}(\mathbf{G})$ reduces $\mathbf{M}$. Using Lemma 6.1, we have

$$f(\mathbf{G}) = \log|\mathbf{G}^T\mathbf{M}\mathbf{G}| + \log|\mathbf{G}_0^T\mathbf{M}\mathbf{G}_0| - \log|\mathbf{M}|.$$

It follows from conclusion 3 of Corollary 5.1 that $f(\mathbf{G})$ is constant for all $\mathbf{G}$ that reduce $\mathbf{M}$; that is, $f(\mathbf{G}) = 0$ for all $\mathbf{G}$ that reduce $\mathbf{M}$. It follows from Lemma 6.2 that this is the minimum value for $f(\mathbf{G})$, and thus the conclusion follows. □

Lemma 6.3 says in effect that the role of the first two terms on the right hand side of (6.5) is to pull solutions toward reducing subspaces of $\mathbf{M}$, without distinguishing between the subspaces themselves. It must then be that the final term on the right hand side of (6.5) represents the signal and serves to distinguish between the reducing subspaces of $\mathbf{M}$. Reasoning heuristically, the role of the projection $\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}}$ is to "shrink" the factor $\mathbf{\Gamma}\mathbf{v}\mathbf{A}^{-1}\mathbf{v}^T\mathbf{\Gamma}^T$ and thus make the determinant larger. If we choose $\mathbf{G} = \mathbf{\Gamma}$ then, $\mathbf{P}_{\mathbf{M}^{-1/2}\mathbf{G}} = \mathbf{P}_{\mathbf{\Gamma}}$ and there is no shrinkage, which tends to minimize the final term on the right side of (6.5).

In practice it will be necessary to replace $\mathbf{M}$ and $\mathbf{U}$ with estimators, say $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$. If these are $\sqrt{n}$-consistent estimators of $\mathbf{M}$ and $\mathbf{U}$, then the corresponding solution $\widehat{\mathbf{\Gamma}}$ provides a $\sqrt{n}$-consistent estimator $\mathbf{P}_{\widehat{\mathbf{\Gamma}}}$ of $\mathbf{P}_{\mathbf{\Gamma}}$. However, in the present use of $J(\mathbf{G})$ it may not be clear how to choose $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$, particularly since there may be many choices that lead to consistent estimators of $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ as implied by the relationships described in Section 5.3. This is where Definition 6.1 plays a crucial role.

Definition 6.1 reproduces the partial envelopes for $\boldsymbol{\beta}_1$ and the envelopes for $\boldsymbol{\beta}$ when it is a vector; that is, when $r = 1$ and $p > 1$ or when $r > 1$ and $p = 1$. It also reproduces the the partially maximized log likelihood function (6.4) by setting $\mathbf{M} = \mathbf{V}_{\boldsymbol{\phi}}(\boldsymbol{\theta})$ and $\mathbf{U} = \boldsymbol{\phi}\boldsymbol{\phi}^T$. For instance, to apply Definition 6.1 for the partial envelope of $\boldsymbol{\beta}_1$, the asymptotic covariance matrix of the maximum likelihood estimator of $\boldsymbol{\beta}_1$ is $\mathbf{V}_{\boldsymbol{\beta}_1} = (\mathbf{\Sigma}_{\mathbf{X}}^{-1})_{11}\mathbf{\Sigma}$, where $(\mathbf{\Sigma}_{\mathbf{X}}^{-1})_{11}$ is the $(1,1)$ element of the inverse of $\mathbf{\Sigma}_{\mathbf{X}} = \lim_{n\to\infty} n^{-1}\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i^T$. Consequently, $\mathcal{E}_{\mathbf{V}_{\boldsymbol{\beta}_1}}(\boldsymbol{\beta}_1) = \mathcal{E}_{\mathbf{\Sigma}}(\boldsymbol{\beta}_1)$, and thus Definition 6.1 recovers the partial envelopes of Chapter 3. To construct the partially maximized log likelihood (6.4) we set $\mathbf{M} = \mathbf{V}_{\boldsymbol{\beta}_1}$ and $\mathbf{U} = \boldsymbol{\beta}_1\boldsymbol{\beta}_1^T$. Then using sample versions and letting $\mathbf{b}_1$ denote the first column of the ordinary least squares estimator $\mathbf{B}$ gives

$$\begin{aligned} J(\boldsymbol{\Gamma}) &= \log|(\mathbf{S}_{\mathbf{X}}^{-1})_{11}\boldsymbol{\Gamma}\mathbf{S}_{\mathbf{Y}|\mathbf{X}}\boldsymbol{\Gamma}^T| + \log|\boldsymbol{\Gamma}\{(\mathbf{S}_{\mathbf{X}}^{-1})_{11}\mathbf{S}_{\mathbf{Y}|\mathbf{X}} + \mathbf{b}_1\mathbf{b}_1^T\}^{-1}\boldsymbol{\Gamma}^T| \\ &= \log|\boldsymbol{\Gamma}\mathbf{S}_{\mathbf{Y}|\mathbf{X}}\boldsymbol{\Gamma}^T| + \log|\boldsymbol{\Gamma}\mathbf{S}_{\mathbf{Y}|\mathbf{X}_2}^{-1}\boldsymbol{\Gamma}^T|, \end{aligned}$$

which is the partially maximized log-likelihood of Chapter 3. It is important to note that, although $\mathcal{E}_{\mathbf{V}_{\boldsymbol{\beta}_1}}(\boldsymbol{\beta}_1) = \mathcal{E}_{\boldsymbol{\Sigma}}(\boldsymbol{\beta}_1)$, Definition 6.1 requires that we use $\mathbf{V}_{\boldsymbol{\beta}_1} = (\boldsymbol{\Sigma}_{\mathbf{X}}^{-1})_{11}\boldsymbol{\Sigma}$ and not $\boldsymbol{\Sigma}$ alone.

6.4 Sequential likelhood-based envelope construction

The method that stems from Proposition 6.2 works well in practice when the dimension involved in the Grassmann optimization not too big. It takes $u(r-u)$ real numbers to uniquely specify a u-dimensional subspace of $\mathbb{R}^r$. Grassmann optimization of a sample version of the objective function in Proposition 6.2 seems quite feasible when $u(r-u)$ is at most, say, 100. Grassmann optimization can be annoyingly slow when $u(r-u)$ is large, and the solution $\widehat{\boldsymbol{\Gamma}}$ returned may correspond to a local rather than global minimum of the objective function, particularly when the signal, represented by the "size" of $\widehat{\mathbf{U}}$ relative to the size of $\widehat{\mathbf{M}}$, is small. For instance, if $r = 40$ and $u = 1$ then $u(r-u) = 39$, which does not represent a burden. On the other hand if $r = 200$ and $u = 50$ then $u(r-u) = 7500$, which could lead to computational challenges. In this section we describe a sequential version of the construction in Proposition 6.2 that requires optimization in $r-1$ dimensions in the first step, and reduces the optimization dimension by 1 in each subsequent step. This sequential likelihood-based algorithm reduces the computational burden dramatically with little loss of effectiveness.

Sequential likelihood-based algorithm. This algorithm requires $\mathbf{M} > 0$. Let $\mathbf{g}_k \in \mathbb{R}^r$, $k = 1, \ldots, u$, be the stepwise directions obtained. Let $\mathbf{G}_k = (\mathbf{g}_1, \ldots, \mathbf{g}_k)$, let $(\mathbf{G}_k, \mathbf{G}_{0k})$ be an orthogonal basis for $\mathbb{R}^r$ and set initial value $\mathbf{g}_0 = \mathbf{G}_0 = 0$, then for $k = 0, \ldots, u-1$, get

$$\begin{aligned} \mathbf{w}_{k+1} &= \arg\min_{\mathbf{w}\in\mathbb{R}^{p-k}} \phi_k(\mathbf{w}), \text{ subject to } \mathbf{w}^T\mathbf{w} = 1, \\ \mathbf{g}_{k+1} &= \mathbf{G}_{0k}\mathbf{w}_{k+1}, \end{aligned}$$

where $\phi_k(\mathbf{w}) = \log(\mathbf{w}^T\mathbf{G}_{0k}^T\mathbf{M}\mathbf{G}_{0k}\mathbf{w}) + \log(\mathbf{w}^T\left\{\mathbf{G}_{0k}^T(\mathbf{M}+\mathbf{U})\mathbf{G}_{0k}\right\}^{-1}\mathbf{w})$ for $\mathbf{w} \in \mathbb{R}^{r-k}$.

On the first pass through the algorithm, $k = 0$ and we take $\mathbf{G}_{00} = \mathbf{I}_r$. With $\mathbf{M} = \boldsymbol{\Sigma}$ and $\mathbf{U} = \boldsymbol{\beta}\boldsymbol{\Sigma}_{\mathbf{X}}\boldsymbol{\beta}^T$, the result is the same as that of Chapter 2 with $u = 1$. The first iteration gives $\mathbf{g}_1 = \mathbf{w}_1 \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, even if $u > 1$, as shown in Proposition 6.3. For the second iteration we construct $\mathbf{G}_{01}$ orthogonal to $\mathbf{w}_1$ and then use Proposition 5.7 to reduce the coordinates, $\mathbf{M} \mapsto \mathbf{G}_{01}^T\mathbf{M}\mathbf{G}_{01}$ and $\mathbf{U} \mapsto \mathbf{G}_{01}^T\mathbf{U}\mathbf{G}_{01}$, and obtain $\mathbf{w}_2 \in \mathcal{E}_{\mathbf{G}_{01}^T\mathbf{M}\mathbf{G}_{01}}(\mathbf{G}_{01}^T\mathbf{U})$. It then follows from Proposition 5.7 that $\mathbf{g}_2 = \mathbf{G}_{01}\mathbf{w}_2 \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$. The conclusion for subsequent directions is obtained similarly.

Proposition 6.3 *The sequential likelihood-based algorithm returns $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ in the population; that is,* $\operatorname{span}(\mathbf{G}_u) = \mathcal{E}_{\mathbf{M}}(\mathcal{U})$.

PROOF.

Let $\boldsymbol{\Gamma} \in \mathbb{R}^{r\times u}$ be a semi-orthogonal basis matrix for $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$. Then we can write $\mathbf{M} = \boldsymbol{\Gamma}\boldsymbol{\Omega}\boldsymbol{\Gamma}^T + \boldsymbol{\Gamma}_0\boldsymbol{\Omega}_0\boldsymbol{\Gamma}_0^T$ by Proposition 5.1, where $\boldsymbol{\Omega} > 0$, $\boldsymbol{\Omega}_0 > 0$ and $(\boldsymbol{\Gamma}, \boldsymbol{\Gamma}_0) \in \mathbb{R}^r$ is orthogonal basis for $\mathbb{R}^r$. Since $\mathcal{U} \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$ we also have the decomposition $\mathbf{M} + \mathbf{U} = \boldsymbol{\Gamma}\boldsymbol{\Phi}\boldsymbol{\Gamma}^T + \boldsymbol{\Gamma}\boldsymbol{\Omega}_0\boldsymbol{\Gamma}_0^T$, where $\boldsymbol{\Phi} > 0$. We first need to solve the optimization for the first direction $\mathbf{g}_1 = \arg\min_{\mathbf{g}\in\mathbb{R}^r} \phi_0(\mathbf{g})$, where $\phi_0(\mathbf{g}) = \log(\mathbf{g}^T\mathbf{M}\mathbf{g}) + \log(\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g})$ and the minimization is subject to constraint $\mathbf{g}^T\mathbf{g} = 1$. Let $\mathbf{g} = \boldsymbol{\Gamma}\mathbf{h} + \boldsymbol{\Gamma}_0\mathbf{h}_0$ for some $\mathbf{h} \in \mathbb{R}^u$ and $\mathbf{h}_0 \in \mathbb{R}^{(r-u)}$. Consider the equivalent unconstrained optimization,

$$\mathbf{g}_1 = \arg\min_{\mathbf{g}\in\mathbb{R}^r} \left\{\log(\mathbf{g}^T\mathbf{M}\mathbf{g}) + \log(\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g}) - 2\log(\mathbf{g}^T\mathbf{g})\right\}.$$

Then we will have the same solution as the original problem up to an arbitrary scaling constant. Next, we plug-in these expressions for $\mathbf{g}$, $\mathbf{M}+\mathbf{U}$ and $\mathbf{M}$,

$$\begin{aligned} f(\mathbf{h},\mathbf{h}_0) &:= \log(\mathbf{g}^T\mathbf{M}\mathbf{g}) + \log(\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g}) - 2\log(\mathbf{g}^T\mathbf{g}) \\ &= \log\{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0\mathbf{h}_0\} + \log\{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0^{-1}\mathbf{h}_0\} \\ &\quad -2\log\{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0\}. \end{aligned}$$

The desired conclusion will follow by showing that $\arg\min_{\mathbf{h}_0} f(\mathbf{h},\mathbf{h}_0) = 0$ for any fixed $\mathbf{h} \neq 0$.

Taking partial derivative with respect to $\mathbf{h}_0$, we have

$$\frac{\partial}{\partial\mathbf{h}_0} f(\mathbf{h},\mathbf{h}_0) = \frac{2\boldsymbol{\Omega}_0\mathbf{h}_0}{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0\mathbf{h}_0} + \frac{2\boldsymbol{\Omega}_0^{-1}\mathbf{h}_0}{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0^{-1}\mathbf{h}_0} - \frac{4\mathbf{h}_0}{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0}.$$

To get a stationary point, we set this derivative to zero, obtaining

$$\left\{\frac{2\boldsymbol{\Omega}_0}{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0\mathbf{h}_0} + \frac{2\boldsymbol{\Omega}_0^{-1}}{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0^{-1}\mathbf{h}_0}\right\}\mathbf{h}_0 = \left\{\frac{4}{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0}\right\}\mathbf{h}_0.$$

Define the positive definite matrix $\mathbf{A}_0$ as

$$\mathbf{A}_0 = \left\{ \frac{2\boldsymbol{\Omega}_0}{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0\mathbf{h}_0} + \frac{2\boldsymbol{\Omega}_0^{-1}}{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h} + \mathbf{h}_0^T\boldsymbol{\Omega}_0^{-1}\mathbf{h}_0} \right\} \Big/ \left\{ \frac{4}{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0} \right\}.$$

Then $\mathbf{A}_0\mathbf{h}_0 = \mathbf{h}_0$ has a solution only as an eigenvector of $\mathbf{A}_0$. The eigenvectors of $\mathbf{A}_0$ are exactly the same as those of $\boldsymbol{\Omega}_0$. Hence, we have $\mathbf{h}_0$ equals 0 or any eigenvector $\ell_k(\boldsymbol{\Omega}_0)$ of $\boldsymbol{\Omega}_0$. Therefore, the minimum value of $f(\mathbf{h}, \mathbf{h}_0)$ has to be obtained by 0 or $\ell_k(\boldsymbol{\Omega}_0)$ (since $\mathbf{h}_0 = \infty$ can be easily eliminated). Restricting $\boldsymbol{\Omega}_0\mathbf{h}_0 = \lambda\mathbf{h}_0$, we have

$$\begin{aligned} f(\mathbf{h}, \mathbf{h}_0) &= \log\left\{ \frac{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h} + \lambda\mathbf{h}_0^T\mathbf{h}_0}{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0} \right\} + \log\left\{ \frac{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h} + \lambda^{-1}\mathbf{h}_0^T\mathbf{h}_0}{\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0} \right\} \\ &= \log\left\{ \frac{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} W_h + \lambda(1 - W_h) \right\} + \log\left\{ \frac{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} W_h + \lambda^{-1}(1 - W_h) \right\} \end{aligned}$$

where $W_h = \mathbf{h}^T\mathbf{h}/(\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0)$ is a weight in the interval $[0, 1]$. Because $\log()$ is concave, we have $\log(aW_h + b(1 - W_h)) \geq W_h \log(a) + (1 - W_h)\log(b)$, with strict inequality when $W_h \in (0, 1)$ and $a \neq b$. Hence,

$$\begin{aligned} f(\mathbf{h}, \mathbf{h}_0) &\geq W_h \left\{ \log\frac{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} + \log\frac{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} \right\} + (1 - W_h)\left\{ \log(\lambda) + \log(\lambda^{-1}) \right\} \\ &= W_h f(\mathbf{h}, 0). \end{aligned}$$

Let $\mathbf{h}_{\min} = \arg\min_{\mathbf{h}\in\mathbb{R}^u} f(\mathbf{h}, 0)$. Then, repeating the last result for clarity,

$$f(\mathbf{h}, \mathbf{h}_0) \geq W_h f(\mathbf{h}, 0) \geq W_h f(\mathbf{h}_{\min}, 0) \geq f(\mathbf{h}_{\min}, 0),$$

where last inequality holds because

$$\min_{\mathbf{h}\in\mathbb{R}^u} f(\mathbf{h}, 0) < 0. \tag{6.6}$$

We defer the proof of (6.6) to the end of this proof. This lower bound on $f(\mathbf{h}, \mathbf{h}_0)$, which is negative, is attained when $\mathbf{h}_0 = 0$ so $W_h = 1$ and $\mathbf{h} = \mathbf{h}_{\min}$. So we have the minimum found at $W_h = \mathbf{h}^T\mathbf{h}/(\mathbf{h}^T\mathbf{h} + \mathbf{h}_0^T\mathbf{h}_0) = 1$, or equivalently, $\mathbf{g} = \boldsymbol{\Gamma}\mathbf{h} \in \operatorname{span}(\boldsymbol{\Gamma})$. This setting is unique since the $\log$ is a strictly concave function.

For the $(k+1)$-th direction, $\mathbf{g}_{k+1} = \mathbf{G}_{0k}\mathbf{w}_{k+1}$ where $\mathbf{w}_{k+1} = \arg\min_{\mathbf{w}\in\mathbb{R}^{r-k}} \phi_k(\mathbf{w})$, $\text{subject to } \mathbf{w}^T\mathbf{w} = 1$. Because

$$\phi_k(\mathbf{w}) = \log(\mathbf{w}^T\mathbf{G}_{0k}^T\mathbf{M}\mathbf{G}_{0k}\mathbf{w}) + \log(\mathbf{w}^T \left\{ \mathbf{G}_{0k}^T(\mathbf{M} + \mathbf{U})\mathbf{G}_{0k} \right\}^{-1} \mathbf{w})$$

has the same form as $\phi_0(\mathbf{g})$, we have

$$\mathbf{w}_{k+1} \in \mathcal{E}_{\mathbf{G}_{0k}^T\mathbf{M}\mathbf{G}_{0k}}(\mathbf{G}_{0k}^T\mathcal{U}).$$

Therefore $\mathbf{g}_{k+1} = \mathbf{G}_{0k}\mathbf{w}_{k+1} \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$ by Proposition 5.7.

We conclude the proof by demonstrating (6.6). We first show that $\min_{\mathbf{h}\in\mathbb{R}^u} f(\mathbf{h}, 0) \leq 0$ and then we assume the equality to conclude the proof by contradiction. Define the following two functions,

$$\begin{aligned} F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) &:= \log \frac{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} + \log \frac{\mathbf{h}^T\boldsymbol{\Phi}^{-1}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} = f(\mathbf{h}, 0), \\ F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1}) &:= \log \frac{\mathbf{h}^T\boldsymbol{\Omega}\mathbf{h}}{\mathbf{h}^T\mathbf{h}} + \log \frac{\mathbf{h}^T\boldsymbol{\Omega}^{-1}\mathbf{h}}{\mathbf{h}^T\mathbf{h}}, \end{aligned}$$

where $F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1})$ is a re-expression of $f(\mathbf{h}, 0)$ to display $\boldsymbol{\Omega}$ and $\boldsymbol{\Phi}^{-1}$ as arguments. Recall that $\boldsymbol{\Phi} - \boldsymbol{\Omega} \geq 0$, and hence $F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) \leq F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1})$ for any $\mathbf{h}$. Consider the minimum of both $F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1})$ and $F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1})$, we have

$$\min_{\mathbf{h}} f(\mathbf{h}, 0) = \min_{\mathbf{h}} F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) \leq \min_{\mathbf{h}} F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1}) = 0,$$

where the minimum of the right hand side is zero by taking $\mathbf{h}$ equals to any eigenvector of $\boldsymbol{\Omega}$ (cf. Lemma 6.3). So we know that $f(\mathbf{h}, 0) \leq 0$.

Now we assume that $\min_{\mathbf{h}} F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) = 0$. Then for an arbitrary $\mathbf{h}$,

$$0 \leq F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) \leq F(\mathbf{h}, \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1}).$$

Let $\mathbf{h}_i = \boldsymbol{\ell}_i(\boldsymbol{\Omega})$, $i = 1, \ldots, u$, be the i-th unit eigenvector of $\boldsymbol{\Omega}$ and plug $\mathbf{h}_i$ into the above inequalities, we have

$$0 \leq F(\mathbf{h}_i; \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) \leq F(\mathbf{h}_i; \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1}) = 0,\ i = 1, \ldots, u,$$

which implies

$$0 = F(\mathbf{h}_i; \boldsymbol{\Omega}, \boldsymbol{\Phi}^{-1}) = F(\mathbf{h}_i; \boldsymbol{\Omega}, \boldsymbol{\Omega}^{-1}) = 0,\ i = 1, \ldots, u,$$

and more explicitly,

$$\mathbf{h}_i^T\boldsymbol{\Phi}^{-1}\mathbf{h}_i = \mathbf{h}_i^T\boldsymbol{\Omega}^{-1}\mathbf{h}_i,\ i = 1, \ldots, u,$$

which implies $\boldsymbol{\Phi} = \boldsymbol{\Omega}$ because that $\boldsymbol{\Phi},\ \boldsymbol{\Omega} \in \mathbb{R}^{u\times u}$ and $\mathbf{h}_i$, $i = 1, \ldots, u$, are u linear independent vectors. Then by definition $\mathbf{U} = \boldsymbol{\Gamma}(\boldsymbol{\Phi} - \boldsymbol{\Omega})\boldsymbol{\Gamma}^T = 0$ leads to contradiction since $\mathrm{span}(\mathbf{U})$ is not contained in the envelope spanned by $\boldsymbol{\Gamma}$. $\square$

The previous proposition shows that the sequential likelihood-based methods gives the desired answer in the population and it is an essential ingredient in showing $\sqrt{n}$-consistency:

Proposition 6.4 *Let $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$ be $\sqrt{n}$-consistent estimators of $\mathbf{M}$ and $\mathbf{U}$, and let $\widehat{\mathbf{G}}_u$ denote the estimated basis for $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ from the sequential likelihood-based algorithm using $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$. Then $\mathbf{P}_{\widehat{\mathbf{G}}_u}$ is a $\sqrt{n}$-consistent estimator of $\mathbf{P}_{\mathcal{E}}$, the projection onto $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$.*

PROOF. This proof that the sample algorithm is $\sqrt{n}$-consistent makes use of classical results in the theory of extremum estimators (see, for example, Theorems 4.1.1 and 4.1.3 in Amemiya, T. (1985). *Advanced Econometrics*, Harvard University Press.) We review these results briefly and then sketch how they can be used to prove the $\sqrt{n}$-consistency for the algorithm.

Let $Q_n(\mathbf{Y}, \boldsymbol{\theta})$ be a real-valued function of the random variables $\mathbf{Y} = (Y_1, \ldots, Y_n)^T$ and the parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_K)^T$. We shall sometimes write $Q_n(\mathbf{Y}, \boldsymbol{\theta})$ more compactly as $Q_n(\boldsymbol{\theta})$. Let the parameter space be $\boldsymbol{\Theta}$ and let the true value of $\boldsymbol{\theta}$ be $\boldsymbol{\theta}_t \in \boldsymbol{\Theta}$. The following assumptions (A)-(F) are used to establish asymptotic properties of the extremum estimator, $\widehat{\boldsymbol{\theta}}_n = \arg\max_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} Q_n(\mathbf{Y}, \boldsymbol{\theta})$:

(A) The parameter space $\boldsymbol{\Theta}$ is a compact subset of $\mathbb{R}^K$.

(B) $Q_n(\mathbf{Y}, \boldsymbol{\theta})$ is continuous in $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ for all $\mathbf{Y}$ and is a measurable function of $\mathbf{Y}$ for all $\boldsymbol{\theta} \in \boldsymbol{\Theta}$.

(C) $n^{-1}Q_n(\boldsymbol{\theta})$ converges to a nonstochastic function $Q(\boldsymbol{\theta})$ in probability uniformly in $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ as n goes to infinity, and $Q(\boldsymbol{\theta})$ attains a unique global maximum at $\boldsymbol{\theta}_t$.

(D) $\partial^2 Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T$ exists and is continuous in an open, convex neighborhood of $\boldsymbol{\theta}_t$.

(E) $n^{-1}\left\{\partial^2 Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T\right\}_{\boldsymbol{\theta}=\boldsymbol{\theta}_n^*}$ converges to a finite nonsingular matrix

$$\mathbf{A}(\boldsymbol{\theta}) = \lim_{n\to\infty} \mathrm{E}_{\boldsymbol{\theta}_t}\left\{n^{-1}\left(\partial^2 Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T\right)\right\},$$

for any random sequences $\boldsymbol{\theta}_n^*$ such that $\operatorname{plim}(\boldsymbol{\theta}_n^*) = \boldsymbol{\theta}_t$.

(F) $n^{-1/2}\left\{\partial Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}\right\}_{\boldsymbol{\theta}=\boldsymbol{\theta}_t} \to N(0, \mathbf{B}(\boldsymbol{\theta}_t))$, where

$$\mathbf{B}(\boldsymbol{\theta}) = \lim_{n\to\infty} \mathrm{E}_{\boldsymbol{\theta}_t}\left\{n^{-1}\left(\partial Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}\right\}\left\{\partial Q_n(\boldsymbol{\theta})/\partial\boldsymbol{\theta}^T\right)\right\}.$$

Under assumptions (A)-(D), $\widehat{\boldsymbol{\theta}}_n$ converges to $\boldsymbol{\theta}_t$ in probability. Under assumptions (A)-(F), then $\sqrt{n}(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_t) \to N(0, \mathbf{A}^{-1}(\boldsymbol{\theta}_t)\mathbf{B}(\boldsymbol{\theta}_t)\mathbf{A}^{-1}(\boldsymbol{\theta}_t))$ (Amemiya, 1985).

To adapt these results for the first step of the algorithm, let $\boldsymbol{\theta} = \mathbf{g}$ whose true value is denoted by $\mathbf{g}_t$. The parameter space is the 1D manifold $\boldsymbol{\Theta} = \mathcal{G}_{(p,1)}$ which is a compact set of $\mathbb{R}^{p\times 1}$, so condition (A) is satisfied. The objective function depends on the random variables $\mathbf{Y}$ only through $(\widehat{\mathbf{M}}, \widehat{\mathbf{U}})$. The specific function to be maximized is

$$Q_n(\mathbf{g}) = -n/2\log(\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g}) - n/2\log(\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}) + n\log(\mathbf{g}^T\mathbf{g}). \tag{6.7}$$

Condition (B) then holds. Although $\arg\max Q_n(\mathbf{g})$ is not unique, $\mathrm{span}(\arg\max Q_n(\mathbf{g}))$ is unique and we can choose one unique value for the maximizing argument by, say, setting the norm equal to 1 (see Jennrich, R. I. (1969). Asymptotic Properties of Non-linear Least Squares Estimators. *Annals of Mathematical Statistics* **40**, 633–43.)

We next verify condition (C) that $n^{-1}Q_n(\mathbf{g})$ converges uniformly to

$$Q(\mathbf{g}) = -1/2\log(\mathbf{g}^T\mathbf{M}\mathbf{g}) - 1/2\log(\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g}) + \log(\mathbf{g}^T\mathbf{g}). \tag{6.8}$$

We have shown in Proposition 6.3 that the population objective function $Q(\mathbf{g})$ attains the unique global maximum at $\mathbf{g}_t$. For simplicity, we assume $\mathbf{M}$ and $\mathbf{M}+\mathbf{U}$ have distinct eigenvalues so that $\mathbf{g}_t$ is the unique maximum of $Q(\mathbf{g})$ in the 1D manifold $\boldsymbol{\Theta}$. For the case where there are multiple local maxima of $Q(\mathbf{g})$, we can obtain similar results by applying Theorem 4.1.2 in Amemiya (1985). Since $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$ are $\sqrt{n}$-consistent for $\mathbf{M}$ and $\mathbf{U}$, the eigenvectors and eigenvalues of $\widehat{\mathbf{M}}$, $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{M}}+\widehat{\mathbf{U}}$ are $\sqrt{n}$-consistent for the eigenvectors and eigenvalues of their population counterparts. Then $n^{-1}Q_n(\mathbf{g})$ converge in probability to $Q(\mathbf{g})$ uniformly in $\mathbf{g}$, as can be seen from the following argument.

$$\begin{aligned} n^{-1}Q_n(\mathbf{g}) - Q(\mathbf{g}) &= -1/2\left(\log(\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g}) - \log(\mathbf{g}^T\mathbf{M}\mathbf{g})\right) \\ &\quad -1/2\left(\log(\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}) - \log(\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g})\right) \\ &= -1/2\log\left[\frac{\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g}}{\mathbf{g}^T\mathbf{M}\mathbf{g}}\right] - 1/2\log\left[\frac{\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}}{\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g}}\right]. \end{aligned}$$

Hence, $\sup_{\mathbf{g}\in\boldsymbol{\Theta}}\log(\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g}/\mathbf{g}^T\mathbf{M}\mathbf{g}) = \sup_{\mathbf{g}\in\boldsymbol{\Theta}}\log(\mathbf{g}^T\mathbf{M}^{-1/2}\widehat{\mathbf{M}}\mathbf{M}^{-1/2}\mathbf{g}/\mathbf{g}^T\mathbf{g})$, which equals to the logarithm of the largest eigenvalue of $\mathbf{M}^{-1/2}\widehat{\mathbf{M}}\mathbf{M}^{-1/2}$ and converges to 0 in probability. Similarly, $\sup_{\mathbf{g}\in\boldsymbol{\Theta}}\log[\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}/\mathbf{g}^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{g}]$ converges to zero in probability. Therefore, $n^{-1}Q_n(\mathbf{g})$ converges to $Q(\mathbf{g})$ in probability uniformly in $\mathbf{g}\in\boldsymbol{\Theta}$.

From conditions (A)-(C) we can conclude that $\mathbf{P}_{\widehat{\mathbf{G}}_1}$ converges in probability to $\mathbf{P}_{\mathcal{E}}$. We need conditions (D)-(F) to get convergence at the $\sqrt{n}$ rate.

By straightforward calculation, condition (D) follows from the second derivative matrix

$$
\begin{aligned}
n^{-1}\frac{\partial^2 Q_n(\mathbf{g})}{\partial\mathbf{g}\partial\mathbf{g}^T} = {} & 2(\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g})^{-2}(\widehat{\mathbf{M}}\mathbf{g}\mathbf{g}^T\widehat{\mathbf{M}}) - (\mathbf{g}^T\widehat{\mathbf{M}}\mathbf{g})^{-1}\widehat{\mathbf{M}} \\
& + 2\left[\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}\right]^{-2}\left[(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\right] \\
& - \left[\mathbf{g}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}\right]^{-1}(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1} - 2(\mathbf{g}^T\mathbf{g})^{-2}\mathbf{P}_{\mathbf{g}} + (\mathbf{g}^T\mathbf{g})^{-1}\mathbf{I}_p.
\end{aligned}
$$

Condition (E) holds because the above quantity is a smooth function of $\mathbf{g}$, $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{M}}+\widehat{\mathbf{U}}$.

Last, we need to verify condition (F). To demonstrate $\sqrt{n}$-consistency of the first step, we need to show only that

$$
n^{-1}\left\{\partial Q_n(\mathbf{g})/\partial\mathbf{g}\right\}_{\mathbf{g}=\mathbf{g}_t} = -(\mathbf{g}_t^T\widehat{\mathbf{M}}\mathbf{g}_t)^{-1}\widehat{\mathbf{M}}\mathbf{g}_t - (\mathbf{g}_t^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}_t)^{-1}(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\mathbf{g}_t + 2\mathbf{g}_t. \tag{6.9}
$$

has order $O_p(1/\sqrt{n})$. From the proof of Proposition 6.3, we know that $\left\{\partial Q(\mathbf{g})/\partial\mathbf{g}\right\}_{\mathbf{g}=\mathbf{g}_t} = 0$. Then the result follows from the fact that $n^{-1}\partial Q_n(\mathbf{g})/\partial\mathbf{g}$ is a smooth function of $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{M}}+\widehat{\mathbf{U}}$ which are $\sqrt{n}$-consistent estimators.

So far, we have verified the conditions $(A)-(F)$ so that the sample estimator $\mathrm{span}(\widehat{\mathbf{g}}_1)$ will be $\sqrt{n}$-consistent for the population estimator. For the $(k+1)$-th direction, $k < u$, let $\widehat{\mathbf{G}}_k$ denote a $\sqrt{n}$-consistent estimator of the first k directions and let $(\widehat{\mathbf{G}}_k, \widehat{\mathbf{G}}_{0k})$ be an orthogonal matrix. The $(k+1)$-th direction is defined by $\mathbf{g}_{k+1} = \widehat{\mathbf{G}}_{0k}\mathbf{w}_{k+1}$ where the parameters are $\mathbf{w}_{k+1} \in \mathbf{\Theta}_{k+1} \subset \mathbb{R}^{p-k}$ and the parameter space is $\mathbf{\Theta}_{k+1} = \mathcal{G}_{p-k,1}$. We show that we can obtain a $\sqrt{n}$-consistent estimator $\widehat{\mathbf{w}}_{k+1}$, so the $\sqrt{n}$-consistency of $\widehat{\mathbf{g}}_{k+1} = \widehat{\mathbf{G}}_{0k}\widehat{\mathbf{w}}_{k+1}$ then follows. We define our objective function $Q_n(\mathbf{w})$ and $Q(\mathbf{w})$ as

$$
\begin{aligned}
Q_n(\mathbf{w}) &= -n/2\log(\mathbf{w}^T(\widehat{\mathbf{G}}_{0k}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})\widehat{\mathbf{G}}_{0k})^{-1}\mathbf{w}) - n/2\log(\mathbf{w}^T\widehat{\mathbf{G}}_{0k}^T\widehat{\mathbf{M}}\widehat{\mathbf{G}}_{0k}\mathbf{w}) \\
&\quad + n\log(\mathbf{w}^T\mathbf{w}) \\
Q(\mathbf{w}) &= -1/2\log(\mathbf{w}^T(\mathbf{G}_{0k}^T(\mathbf{M}+\mathbf{U})\mathbf{G}_{0k})^{-1}\mathbf{w}) - 1/2\log(\mathbf{w}^T\mathbf{G}_{0k}^T\mathbf{M}\mathbf{G}_{0k}\mathbf{w}) \\
&\quad + \log(\mathbf{w}^T\mathbf{w})
\end{aligned}
$$

Following the same logic as verifying the conditions for the first direction, we can see that $\widehat{\mathbf{w}} = \arg\max Q_n(\mathbf{w})$ will be $\sqrt{n}$-consistent for $\mathbf{v}_t = \arg\max Q(\mathbf{w})$ by noticing that $(\widehat{\mathbf{G}}_{0k}^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})\widehat{\mathbf{G}}_{0k})^{-1}$ and $\widehat{\mathbf{G}}_{0k}^T\widehat{\mathbf{M}}\widehat{\mathbf{G}}_{0k}$ are $\sqrt{n}$-consistent estimators for $(\mathbf{G}_{0k}^T(\mathbf{M}+\mathbf{U})\mathbf{G}_{0k})^{-1}$ and $\mathbf{G}_{0k}^T\mathbf{M}\mathbf{G}_{0k}$. Since all the u directions will be $\sqrt{n}$-consistent, the projection onto $\widehat{\mathbf{G}}_u = (\widehat{\mathbf{g}}_1, \ldots, \widehat{\mathbf{g}}_u)$ will be a $\sqrt{n}$-consistent estimator for the projection onto the envelope $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$. $\square$

6.5 Sequential moment-based envelope construction

6.5.1 Basic algorithm

Let $\mathbf{u} \in \mathbb{R}^{r\times p}$ with $\mathrm{rank}(\mathbf{u}) \le p$, let $\mathcal{U} = \mathrm{span}(\mathbf{u}) \subseteq \mathrm{span}(\mathbf{M})$, where $\mathbf{M} \in \mathbb{S}^{r\times r}$ is a positive semi-definite matrix. In this section we describe a sequential method for finding $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$, the $\mathbf{M}$-envelope of $\mathcal{S}$, based only on knowledge of $\mathbf{u}$ and $\mathbf{M}$. Let $u = \dim(\mathcal{E}_{\mathbf{M}}(\mathcal{U}))$. Essentially an abstraction of the SIMPLS method for PLS discussed in Chapter 4, the algorithm proceeds by finding a sequence of r-dimensional vectors $\mathbf{w}_0$, $\mathbf{w}_1, \dots, \mathbf{w}_u$, with $\mathbf{w}_0 = 0$, whose cumulative spans are strictly increasing and converge to $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ after u steps. Let $\mathbf{W}_k = (\mathbf{w}_0, \mathbf{w}_1, \dots, \mathbf{w}_k) \in \mathbb{R}^{r\times k}$ and let $\mathcal{W}_k = \mathrm{span}(\mathbf{W}_k)$. Then the $\mathbf{w}_k$'s are constructed so that

$$\mathcal{W}_0 \subset \mathcal{W}_1 \subset \dots \subset \mathcal{W}_{u-1} \subset \mathcal{W}_u = \mathcal{E}_{\mathbf{M}}(\mathcal{U}). \tag{6.10}$$

Let $\mathbf{U} = \mathbf{u}\mathbf{u}^T$, so $\mathrm{span}(\mathbf{U}) = \mathrm{span}(\mathbf{u})$. The algorithm is based on the following sequence of constrained optimizations. Starting with $\mathbf{w}_1$ since $\mathbf{w}_0 = 0$ is a known starting vector. For $k = 0, 1, ..., u-1$ find

$$\begin{aligned}
\mathbf{w}_{k+1} &= \arg\max_{\mathbf{w}} \mathbf{w}^T\mathbf{U}\mathbf{w}, \text{ subject to} && (6.11)\\
& \mathbf{w}^T\mathbf{M}\mathbf{W}_k = 0 && (6.12)\\
& \mathbf{w}^T\mathbf{w} = 1. && (6.13)
\end{aligned}$$

As shown in Section 6.5.2 the algorithm can also be stated without explicit reference to the constraints: Set $\mathbf{w}_0 = 0$ and $\mathbf{W}_0 = \mathbf{w}_0$. For $k = 0, 1, \dots, u-1$, set

$$\begin{aligned}
\mathcal{E}_k &= \mathrm{span}(\mathbf{M}\mathbf{W}_k)\\
\mathbf{w}_{k+1} &= \boldsymbol{\ell}_1(\mathbf{Q}_{\mathcal{E}_k}\mathbf{U}\mathbf{Q}_{\mathcal{E}_k})\\
\mathbf{W}_{k+1} &= (\mathbf{w}_0, \dots, \mathbf{w}_k, \mathbf{w}_{k+1}).
\end{aligned}$$

The algorithm continues until $\mathbf{Q}_{\mathcal{E}_k}\mathbf{U} = 0$, at which point $k = u$ and $\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \mathcal{W}_u = \mathrm{span}(\mathbf{W}_u)$.

Viewing $\mathbf{U}$ and $\mathbf{M}$ as population parameters from a statistical perspective, this algorithm is Fisher consistent for the envelope $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$. Substituting $\sqrt{n}$ consistent estimators for $\mathbf{U}$ and $\mathbf{M}$, the algorithm provides also a $\sqrt{n}$ consistent estimator for $\mathbf{P}_{\mathcal{E}}$. Even so, application of the algorithm could still seem elusive in practice because there are several ways in which to choose $\mathbf{U}$ and $\mathbf{M}$ that yield the same envelope in the population. For instance, choosing $\mathbf{U} = \mathbf{u}\mathbf{A}\mathbf{u}^T$ for any non-singular $\mathbf{A} \in \mathbb{S}^{p\times p}$ also yields $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ in the population because $\mathcal{S} = \mathrm{span}(\mathbf{u}) = \mathrm{span}(\mathbf{u}\mathbf{A}\mathbf{u}^T)$. Similarly, from (5.7) in Corollary 5.2, replacing $\mathbf{M}$ with $\mathbf{M}^k$ also yields $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ in the population. Although the population changes indicated here have no impact on the end result of the algorithm, they will produce different results in application when $\mathbf{u}$ and $\mathbf{M}$ are replaced by $\sqrt{n}$ consistent estimators.

Consider for example the problem of estimating the envelope $\mathcal{E}_{\mathbf{\Sigma}}(\mathcal{B})$ for response reduction in the multivariate regression of a response vector $\mathbf{Y}$ on a predictor vector $\mathbf{X}$, as discussed in Chapter 2. A seemingly natural choice in practical application might be $\widehat{\mathbf{u}} = \mathbf{B} = \mathbb{Y}^T\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}$ (cf. (2.2)), leading to

$$\widehat{\mathbf{U}} = \mathbf{B}\mathbf{B}^T = \mathbb{Y}^T\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-2}\mathbb{X}^T\mathbb{Y}.$$

However, $\widehat{\mathbf{U}}$ is not invariant under non-singular linear transformations $\mathbf{X} \mapsto \mathbf{A}\mathbf{X}$, and consequently the results of the sample algorithm will depend on the scaling of the predictors. Appealing to invariance then leads to a different choice:

$$\widehat{\mathbf{U}} = \mathbf{B}(\mathbb{X}^T\mathbb{X})\mathbf{B}^T = \mathbb{Y}^T\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y} = \mathbb{Y}^T\mathbf{P}_{\mathbb{X}}\mathbb{Y},$$

which is invariant under transformations $\mathbf{X} \mapsto \mathbf{A}\mathbf{X}$. Choosing this form for $\widehat{\mathbf{U}}$ and $\widehat{\mathbf{M}} = \mathbf{S}_{\mathbf{Y}|\mathbf{X}}$ may then lead to a useful envelope algorithm.

A potential advantage of this algorithm, which we will continue to use in later chapters, is that it does not require that $\mathbf{M}$ be non-singular, although it still requires $\mathcal{S} \subseteq \mathrm{span}(\mathbf{M})$. This suggests that it may form a starting point for methodology to deal with settings in which the estimator of $\mathbf{M}$ is singular.

6.5.2 Justification of the algorithm

The next lemma will facilitate a demonstration that the sequence so constructed has property (6.10).

Lemma 6.4 *Let $\mathbf{U} \in \mathbb{S}^{r\times r}$ and $\mathbf{V} \in \mathbb{S}^{r\times r}$ be positive semi-definite matrices, let $\mathcal{S}$ be a u-dimensional subspace of $\mathbb{R}^r$ with semi-orthogonal basis matrix $\mathbf{\Gamma} \in \mathbb{R}^{r\times u}$, let $\mathcal{T}$ be a u_1-dimensional subspace of $\mathbb{R}^r$ that is orthogonal to $\mathcal{S}$, $u_1 = \dim(\mathcal{T})$, and let $u_2 = \dim\{(\mathcal{S}+\mathcal{T})^{\perp}\}$. Assume that $\mathbf{\Gamma}^T\mathbf{V}\mathbf{\Gamma} > 0$. Then*

$$\begin{aligned}
\mathbf{w}_{\max} &= \arg\max_{D_1} \mathbf{w}^T\mathbf{P}_{\mathcal{S}}\mathbf{U}\mathbf{P}_{\mathcal{S}}\mathbf{w} \\
&= \arg\max_{D_2} \mathbf{w}^T\mathbf{P}_{\mathcal{S}}\mathbf{U}\mathbf{P}_{\mathcal{S}}\mathbf{w} \\
&= \mathbf{\Gamma}(\mathbf{\Gamma}^T\mathbf{V}\mathbf{\Gamma})^{-1/2}\boldsymbol{\ell}_1\{(\mathbf{\Gamma}^T\mathbf{V}\mathbf{\Gamma})^{-1/2}\mathbf{\Gamma}^T\mathbf{U}\mathbf{\Gamma}(\mathbf{\Gamma}^T\mathbf{V}\mathbf{\Gamma})^{-1/2}\},
\end{aligned}$$

where

$$
\begin{aligned}
D_1 &= \{\mathbf{w} | \mathbf{w}^T \mathbf{P}_{\mathcal{S}} \mathbf{V} \mathbf{P}_{\mathcal{S}} \mathbf{w} + \mathbf{w}^T \mathbf{P}_{\mathcal{T}} \mathbf{V} \mathbf{P}_{\mathcal{T}} \mathbf{w} = 1\}, \\
D_2 &= \{\mathbf{w} | \mathbf{w}^T \mathbf{P}_{\mathcal{S}} \mathbf{V} \mathbf{P}_{\mathcal{S}} \mathbf{w} = 1\},
\end{aligned}
$$

and $\ell_1(\mathbf{A})$ is any eigenvector in the first eigenspace of $\mathbf{A}$. Clearly, $\mathbf{w}_{\max} \in \mathcal{S}$, although it is not necessarily unique.

PROOF. Let $\mathbf{\Gamma}_1$ be a semi-orthogonal basis matrix for $\mathcal{T}$ and let $\mathbf{\Gamma}_2$ be a semi-orthogonal basis matrix for $(\mathcal{S} + \mathcal{T})^\perp$ so that $(\mathbf{\Gamma}, \mathbf{\Gamma}_1, \mathbf{\Gamma}_2) \in \mathbb{R}^{r \times r}$ is an orthogonal matrix. Let $\mathbf{s} = \mathbf{\Gamma}^T \mathbf{w}$, $\mathbf{t} = \mathbf{\Gamma}_1^T \mathbf{w}$ and $\mathbf{v} = \mathbf{\Gamma}_2^T \mathbf{w}$. Then expressing $\mathbf{w}$ in the coordinates of $(\mathbf{\Gamma}, \mathbf{\Gamma}_1, \mathbf{\Gamma}_2)$, we have $\mathbf{w} = \mathbf{\Gamma}\mathbf{s} + \mathbf{\Gamma}_1 \mathbf{t} + \mathbf{\Gamma}_2 \mathbf{v}$ and $\mathbf{w}_{\max} = \mathbf{\Gamma}\mathbf{s}_{\max} + \mathbf{\Gamma}_1 \mathbf{t}_{\max} + \mathbf{\Gamma}_2 \mathbf{v}_{\max}$, where $\mathbf{s}_{\max} = \arg\max \mathbf{s}^T \mathbf{\Gamma}^T \mathbf{U} \mathbf{\Gamma} \mathbf{s}$ is now over all vectors $\mathbf{s} \in \mathbb{R}^u$, $\mathbf{t} \in \mathbb{R}^{u_1}$ and $\mathbf{v} \in \mathbb{R}^{u_2}$ such that $\mathbf{s}^T \mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma} \mathbf{s} + \mathbf{t}^T \mathbf{\Gamma}_1^T \mathbf{V} \mathbf{\Gamma}_1 \mathbf{t} = 1$, and $(\mathbf{s}_{\max}, \mathbf{t}_{\max}, \mathbf{v}_{\max})$ is the triplet of values at which the maximum occurs. Since $\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma} > 0$ we can make a change of variable in $\mathbf{s}$ without affecting $\mathbf{t}$ or $\mathbf{v}$. Let $\mathbf{d} = (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{1/2} \mathbf{s}$. Then $\mathbf{s}_{\max} = (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2} \mathbf{d}_{\max}$, where

$$
\mathbf{d}_{\max} = \arg\max \mathbf{d}^T (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2} \mathbf{\Gamma}^T \mathbf{U} \mathbf{\Gamma} (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2} \mathbf{d}
$$

and the maximum is computed over all vectors $(\mathbf{d}, \mathbf{t}, \mathbf{v})$ such that $\mathbf{d}^T \mathbf{d} + \mathbf{t}^T \mathbf{\Gamma}_1^T \mathbf{V} \mathbf{\Gamma}_1 \mathbf{t} = 1$. We know that the inverse $(\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1}$ exists because of the condition $\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma} > 0$. Clearly, the maximum is achieved when $\mathbf{t} = 0$ and $\mathbf{v} = 0$ and then $\mathbf{d}_{\max}$ is the first eigenvector of $(\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2} \mathbf{\Gamma}^T \mathbf{U} \mathbf{\Gamma} (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2}$ and $\mathbf{w}_{\max} = \mathbf{\Gamma} \mathbf{s}_{\max} = \mathbf{\Gamma} (\mathbf{\Gamma}^T \mathbf{V} \mathbf{\Gamma})^{-1/2} \mathbf{d}_{\max}$. □

The first step in demonstrating that the sequence constructed by (6.11) - (6.13) has property (6.10) is to incorporate $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ into the algorithm. For notational convenience we shorten $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ to $\mathcal{E}$ when used as a subscript. Since $\mathcal{U}$ is contained in $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$, $\mathcal{U} = \mathrm{span}(\mathbf{U}) \subseteq \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, we can substitute into (6.11) $\mathbf{w}^T \mathbf{U} \mathbf{w} = \mathbf{w}^T \mathbf{P}_{\mathcal{E}} \mathbf{U} \mathbf{P}_{\mathcal{E}} \mathbf{w}$. We know from Proposition 5.1 that $\mathbf{M} = \mathbf{P}_{\mathcal{E}} \mathbf{M} \mathbf{P}_{\mathcal{E}} + \mathbf{Q}_{\mathcal{E}} \mathbf{M} \mathbf{Q}_{\mathcal{E}}$. Substituting this into (6.12) we have $\mathbf{w}^T \mathbf{M} \mathbf{W}_k = 0$ if and only if $\mathbf{w}^T \mathbf{P}_{\mathcal{E}} \mathbf{M} \mathbf{P}_{\mathcal{E}} \mathbf{W}_k + \mathbf{w}^T \mathbf{Q}_{\mathcal{E}} \mathbf{M} \mathbf{Q}_{\mathcal{E}} \mathbf{W}_k = 0$. These considerations lead to the following equivalent statement of the algorithm. For $k = 0, 1, ..., u-1$ find

$$
\begin{aligned}
\mathbf{w}_{k+1} &= \arg\max_{\mathbf{w}} \mathbf{w}^T \mathbf{P}_{\mathcal{E}} \mathbf{U} \mathbf{P}_{\mathcal{E}} \mathbf{w}, \text{ subject to} && (6.14) \\
& \mathbf{w}^T \mathbf{P}_{\mathcal{E}} \mathbf{M} \mathbf{P}_{\mathcal{E}} \mathbf{W}_k + \mathbf{w}^T \mathbf{Q}_{\mathcal{E}} \mathbf{M} \mathbf{Q}_{\mathcal{E}} \mathbf{W}_k = 0 && (6.15) \\
& \mathbf{w}^T \mathbf{P}_{\mathcal{E}} \mathbf{w} + \mathbf{w}^T \mathbf{Q}_{\mathcal{E}} \mathbf{w} = 1. && (6.16)
\end{aligned}
$$

We next establish (6.10) by induction, starting with an analysis of (6.14) - (6.16) for $k = 0$.

First direction vector $\mathbf{w}_1$. For the first vector $\mathbf{w}_1$, only the length constraint (6.16) is operational since $\mathbf{w}_0 = 0$. It follows from Lemma 6.4 with $\mathbf{V} = \mathbf{I}_r$ and $\mathcal{T} = \mathcal{S}^\perp$ that

$$\mathbf{w}_1 = \boldsymbol{\Gamma}\boldsymbol{\ell}_1(\boldsymbol{\Gamma}^T\mathbf{U}\boldsymbol{\Gamma}) = \boldsymbol{\ell}_1(\mathbf{P}_\mathcal{E}\mathbf{U}\mathbf{P}_\mathcal{E}) = \boldsymbol{\ell}_1(\mathbf{U}) \in \operatorname{span}(\mathbf{M}),$$

where $\boldsymbol{\Gamma}$ is a semi-orthogonal basis matrix for $\mathcal{E}_\mathbf{M}(\mathcal{U})$. Clearly, $\mathbf{w}_1 \in \mathcal{S} \subseteq \mathcal{E}_\mathbf{M}(\mathcal{U})$, so trivially $\mathcal{W}_0 \subset \mathcal{W}_1 \subseteq \mathcal{E}_\mathbf{M}(\mathcal{U})$ with equality if and only if $u = 1$.

Second direction vector $\mathbf{w}_2$. Next, assume that $u \geq 2$ and consider the second vector $\mathbf{w}_2$. In that case $\mathcal{W}_1 \subset \mathcal{E}_\mathbf{M}(\mathcal{U})$ and so the second addend on the left of (6.15) is 0. Consequently,

$$\begin{aligned} \mathbf{w}_2 &= \arg\max_{\mathbf{w}} \mathbf{w}^T\mathbf{P}_\mathcal{E}\mathbf{U}\mathbf{P}_\mathcal{E}\mathbf{w}, \text{ subject to} && (6.17)\\ & \quad\ \mathbf{w}^T\mathbf{P}_\mathcal{E}\mathbf{M}\mathbf{P}_\mathcal{E}\mathbf{w}_1 = 0 && (6.18)\\ & \quad\ \mathbf{w}^T\mathbf{P}_\mathcal{E}\mathbf{w} + \mathbf{w}^T\mathbf{Q}_\mathcal{E}\mathbf{w} = 1. && (6.19) \end{aligned}$$

Condition (6.18) holds if and only if $\mathbf{w}$ is orthogonal to $\mathbf{P}_\mathcal{E}\mathbf{M}\mathbf{P}_\mathcal{E}\mathbf{w}_1$. Letting $\mathcal{E}_1 = \operatorname{span}(\mathbf{P}_\mathcal{E}\mathbf{M}\mathbf{P}_\mathcal{E}\mathbf{w}_1)$ for notational convenience, $\mathbf{w}$ is then constrained to be of the form $\mathbf{w} = \mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}}$ for $\widetilde{\mathbf{w}} \in \mathbb{R}^r$. This form for $\mathbf{w}$ satisfies (6.18) by construction, leaving only the length constraint.

We need to deal with $\mathbf{P}_\mathcal{E}\mathbf{w} = \mathbf{P}_\mathcal{E}\mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}}$ and $\mathbf{Q}_\mathcal{E}\mathbf{w} = \mathbf{Q}_\mathcal{E}\mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}}$ to write the algorithm in terms of $\widetilde{\mathbf{w}}$: $\mathbf{Q}_\mathcal{E}\mathbf{Q}_{\mathcal{E}_1} = \mathbf{Q}_\mathcal{E}$, $\mathcal{E}_1 = \operatorname{span}(\mathbf{P}_\mathcal{E}\mathbf{M}\mathbf{P}_\mathcal{E}\mathbf{w}_1) \subset \mathcal{E}_\mathbf{M}(\mathcal{U})$, (the strict containment holds because $u \geq 2$) and thus $\mathbf{Q}_{\mathcal{E}_1}\mathbf{P}_\mathcal{E} = \mathbf{P}_\mathcal{E} - \mathbf{P}_{\mathcal{E}_1}$ is the projection onto $\mathcal{E}_\mathbf{M}(\mathcal{U}) \setminus \mathcal{E}_1$, the part of $\mathcal{E}_\mathbf{M}(\mathcal{U})$ that is orthogonal to $\mathcal{E}_1$. Let $\mathcal{D}_1 = \mathcal{E}_\mathbf{M}(\mathcal{U}) \setminus \mathcal{E}_1$ and $\mathbf{P}_{\mathcal{D}_1} = \mathbf{P}_\mathcal{E} - \mathbf{P}_{\mathcal{E}_1}$. It follows that the length condition (6.19) can be written as

$$\begin{aligned} \mathbf{w}^T\mathbf{P}_\mathcal{E}\mathbf{w} + \mathbf{w}^T\mathbf{Q}_\mathcal{E}\mathbf{w} &= \widetilde{\mathbf{w}}^T\mathbf{Q}_{\mathcal{E}_1}\mathbf{P}_\mathcal{E}\mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}} + \widetilde{\mathbf{w}}^T\mathbf{Q}_{\mathcal{E}_1}\mathbf{Q}_\mathcal{E}\mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}}\\ &= \widetilde{\mathbf{w}}^T\mathbf{P}_{\mathcal{D}_1}\widetilde{\mathbf{w}} + \widetilde{\mathbf{w}}^T\mathbf{Q}_\mathcal{E}\widetilde{\mathbf{w}} = 1. \end{aligned}$$

Then the algorithm for $\widetilde{\mathbf{w}}_2$ becomes

$$\begin{aligned} \widetilde{\mathbf{w}}_2 &= \arg\max_{\mathbf{w}} \mathbf{w}^T\mathbf{P}_{\mathcal{D}_1}\mathbf{U}\mathbf{P}_{\mathcal{D}_1}\mathbf{w}, \text{ subject to} && (6.20)\\ & \quad\ \mathbf{w}^T\mathbf{P}_{\mathcal{D}_1}\mathbf{w} + \mathbf{w}^T\mathbf{Q}_\mathcal{E}\mathbf{w} = 1. && (6.21) \end{aligned}$$

Let $\boldsymbol{\Gamma}_1$ be a semi-orthogonal basis matrix for $\mathcal{D}_1$. It follows from Lemma 6.4 with $\mathbf{V} = \mathbf{I}_r$, $\mathcal{U} = \mathcal{D}_1$ and $\mathcal{T} = \mathcal{E}_\mathbf{M}^\perp(\mathcal{U})$ that

$$\widetilde{\mathbf{w}}_2 = \boldsymbol{\Gamma}_1\boldsymbol{\ell}_1(\boldsymbol{\Gamma}_1^T\mathbf{U}\boldsymbol{\Gamma}_1) = \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_1}\mathbf{U}\mathbf{P}_{\mathcal{D}_1}) = \boldsymbol{\ell}_1(\mathbf{Q}_{\mathcal{E}_1}\mathbf{U}\mathbf{Q}_{\mathcal{E}_1}) \in \operatorname{span}(\mathbf{M})$$

and thus that $\mathbf{w}_2 = \mathbf{Q}_{\mathcal{E}_1}\widetilde{\mathbf{w}}_2 = \widetilde{\mathbf{w}}_2$.

Termination. If $\mathbf{P}_{\mathcal{D}_1}\mathbf{U} = 0$ the algorithm will terminate and then $\mathrm{span}(\mathbf{w}_1) = \mathcal{E}_{\mathbf{M}}(\mathcal{U})$. To see why this conclusion holds, we have $\mathbf{P}_{\mathcal{D}_1}\mathbf{U} = 0$ is equivalent to $\mathbf{P}_{\mathcal{E}_1}\mathbf{U} = \mathbf{U}$, so $\mathcal{U} = \mathrm{span}(\mathbf{U}) \subseteq \mathcal{E}_1$. The conclusion will follow if, when $\mathbf{P}_{\mathcal{E}_1}\mathbf{U} = \mathbf{U}$, we can show that $\mathcal{E}_1 = \mathrm{span}(\mathbf{w}_1)$ and that $\mathcal{E}_1$ reduces $\mathbf{M}$, because then $\mathcal{E}_1$ will be a reducing subspace of $\mathbf{M}$ that contains $\mathcal{U}$. Now, we know that

$$\mathcal{E}_1 = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{w}_1) = \mathrm{span}(\mathbf{M}\mathbf{w}_1) = \mathbf{M}\mathrm{span}(\boldsymbol{\ell}_1(\mathbf{U})).$$

Assuming that $\mathbf{P}_{\mathcal{E}_1}\mathbf{U} = \mathbf{U}$ gives

$$\mathcal{E}_1 = \mathbf{M}\mathrm{span}(\boldsymbol{\ell}_1(\mathbf{U})) = \mathbf{M}\mathrm{span}(\boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{E}_1}\mathbf{U}\mathbf{P}_{\mathcal{E}_1})).$$

The subspace $\mathcal{E}_1$ has dimension 1 and thus $\mathcal{U}$, which is assumed to be nontrivial, must have dimension 1. It follows that $\mathrm{span}(\mathbf{w}_1) = \mathrm{span}(\boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{E}_1}\mathbf{U}\mathbf{P}_{\mathcal{E}_1})) = \mathcal{E}_1$ and thus $\mathcal{E}_1 = \mathbf{M}\mathcal{E}_1$, so $\mathcal{E}_1$ reduces $\mathbf{M}$.

In sum, $\mathbf{w}_1 \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, $\mathbf{w}_2 \in \mathcal{D}_1 = \mathcal{E}_{\mathbf{M}}(\mathcal{U}) \setminus \mathcal{E}_1 \subset \mathcal{E}_{\mathbf{M}}(\mathcal{U})$. If $\mathbf{w}_1$ and $\mathbf{w}_2$ are linearly independent. then $\mathcal{W}_0 \subset \mathcal{W}_1 \subset \mathcal{W}_2 \subseteq \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, with equality if and only if $u = 2$.

$(q+1)$**-st direction vector** $\mathbf{w}_{q+1}$**,** $q < u$**.** The reasoning here parallels that for $\mathbf{w}_2$. Consider weight matrices $\mathbf{W}_k = (\mathbf{w}_0, \ldots, \mathbf{w}_k)$, with $\mathbf{w}_k \in \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, $k = 0, 1, \ldots, q$. Assuming that the columns of $\mathbf{W}_k$ are linearly independent, the weight matrices must satisfy

$$\mathcal{W}_0 \subset \mathcal{W}_1 \subset \ldots \subset \mathcal{W}_{q-1} \subset \mathcal{W}_q \subset \mathcal{E}_{\mathbf{M}}(\mathcal{U})$$

by construction. For $k = 0, 1, \ldots, q-1$, let $\mathcal{E}_k = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_k)$ and $\mathcal{D}_k = \mathcal{E}_{\mathbf{M}}(\mathcal{U}) \setminus \mathcal{E}_k$ so that $\mathbf{P}_{\mathcal{D}_k} = \mathbf{P}_{\mathcal{E}} - \mathbf{P}_{\mathcal{E}_k}$. As a consequence of the structure assumed for the $\mathbf{W}_k$'s, the $\mathcal{D}_k$'s are properly nested subspaces

$$\mathcal{D}_{q-1} \subset \ldots \mathcal{D}_1 \subset \mathcal{D}_0 = \mathcal{E}_{\mathbf{M}}(\mathcal{U}).$$

To use induction, we now must show that $\mathcal{W}_q \subset \mathcal{W}_{q+1} \subseteq \mathcal{E}_{\mathbf{M}}(\mathcal{U})$, with equality in the last containment if and only if $q + 1 = u$, starting from representations (6.14) - (6.16). Since $\mathcal{W}_q \subset \mathcal{E}_{\mathbf{M}}(\mathcal{U})$ the second addend on the left of (6.15) is again 0 and the $q+1$-st step of the algorithm becomes

$$\mathbf{w}_{q+1} = \arg\max_{\mathbf{w}} \mathbf{w}^T\mathbf{P}_{\mathcal{E}}\mathbf{U}\mathbf{P}_{\mathcal{E}}\mathbf{w}, \text{ subject to} \tag{6.22}$$

$$\mathbf{w}^T\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_q = 0 \tag{6.23}$$

$$\mathbf{w}^T\mathbf{P}_{\mathcal{E}}\mathbf{w} + \mathbf{w}^T\mathbf{Q}_{\mathcal{E}}\mathbf{w} = 1. \tag{6.24}$$

Condition (6.23) holds if and only if $\mathbf{w}$ is orthogonal to $\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_q$, so $\mathbf{w}$ is then constrained to be of the form $\mathbf{w} = \mathbf{Q}_{\mathcal{E}_q}\widetilde{\mathbf{w}}$ for $\widetilde{\mathbf{w}} \in \mathbb{R}^r$, where $\mathcal{E}_q = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_q)$. This form for $\mathbf{w}$ satisfies (6.23) by construction, leaving only the length constraint. Straightforwardly,

$$\mathcal{E}_{q-1} = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_{q-1}) \subset \mathcal{E}_q = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_q) \subset \mathcal{E}_{\mathbf{M}}(\mathcal{U}),$$

and $\mathbf{Q}_{\mathcal{E}_q}\mathbf{P}_{\mathcal{E}} = \mathbf{P}_{\mathcal{E}} - \mathbf{P}_{\mathcal{E}_q}$ is a projection onto the part of $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ that is orthogonal to $\mathcal{E}_q$. Let $\mathcal{D}_q = \mathcal{E}_{\mathbf{M}}(\mathcal{U}) \setminus \mathcal{E}_q \subset \mathcal{D}_{q-1}$. Then we can use $\widetilde{\mathbf{w}}$ to rewrite the algorithm in terms of only the criterion and the length constraint leading to

$$\widetilde{\mathbf{w}}_{q+1} = \arg\max_{\mathbf{w}} \mathbf{w}^T\mathbf{P}_{\mathcal{D}_q}\mathbf{U}\mathbf{P}_{\mathcal{D}_q}\mathbf{w}, \text{ subject to} \tag{6.25}$$

$$\mathbf{w}^T\mathbf{P}_{\mathcal{D}_q}\mathbf{w} + \mathbf{w}^T\mathbf{Q}_{\mathcal{E}}\mathbf{w} = 1. \tag{6.26}$$

Let $\mathbf{\Gamma}_q$ be a semi-orthogonal basis matrix for $\mathcal{D}_q$. It follows from Lemma 6.4 with $\mathbf{V} = \mathbf{I}_r$, $\mathcal{U} = \mathcal{D}_q$ and $\mathcal{T} = \mathcal{E}_{\mathbf{M}}^{\perp}(\mathcal{U})$ that

$$\widetilde{\mathbf{w}}_{q+1} = \mathbf{\Gamma}_q\boldsymbol{\ell}_1(\mathbf{\Gamma}_q^T\mathbf{U}\mathbf{\Gamma}_q) = \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_q}\mathbf{U}\mathbf{P}_{\mathcal{D}_q}) = \boldsymbol{\ell}_1(\mathbf{Q}_{\mathcal{E}_q}\mathbf{U}\mathbf{Q}_{\mathcal{E}_q}) \in \mathrm{span}(\mathbf{M})$$

and thus that $\mathbf{w}_{q+1} = \mathbf{Q}_{\mathcal{E}_q}\widetilde{\mathbf{w}}_{q+1} = \widetilde{\mathbf{w}}_{q+1}$. With $\mathbf{W}_{q+1} = (\mathbf{W}_q, \mathbf{w}_{q+1})$, it follows that $\mathcal{W}_q \subset \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_{q+1}) = \mathcal{W}_{q+1} \subseteq \mathcal{E}_{\mathbf{M}}(\mathcal{U})$.

Termination. The algorithm will terminate the first time $\mathbf{P}_{\mathcal{D}_q}\mathbf{U} = 0$ or, equivalently, $\mathbf{P}_{\mathcal{E}_q}\mathbf{U} = \mathbf{U}$ so $\mathcal{S} \subseteq \mathcal{E}_q$. We need to show that $\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \mathrm{span}(\mathbf{W}_q) = \mathcal{E}_q$ to insure that the algorithm produces the envelope at termination. It is sufficient to show that $\mathrm{span}(\mathbf{W}_q) = \mathcal{E}_q$ and that $\mathcal{E}_q$ reduces $\mathbf{M}$. Now,

$$\begin{aligned}\mathcal{E}_q &= \mathrm{span}(\mathbf{M}\mathbf{W}_q) = \mathrm{span}(\mathbf{P}_{\mathcal{E}}\mathbf{M}\mathbf{P}_{\mathcal{E}}\mathbf{W}_q) \\ &= \mathbf{M}\mathrm{span}\{\boldsymbol{\ell}_1(\mathbf{U}), \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_1}\mathbf{U}\mathbf{P}_{\mathcal{D}_1}), \ldots \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_{q-1}}\mathbf{U}\mathbf{P}_{\mathcal{D}_{q-1}})\}\end{aligned}$$

Substituting the condition $\mathbf{P}_{\mathcal{E}_q}\mathbf{U} = \mathbf{U}$, we have

$$\begin{aligned}\mathcal{E}_q &= \mathbf{M}\mathrm{span}\{\boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{E}_q}\mathbf{U}\mathbf{P}_{\mathcal{E}_q}), \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_1}\mathbf{P}_{\mathcal{E}_q}\mathbf{U}\mathbf{P}_{\mathcal{E}_q}\mathbf{P}_{\mathcal{D}_1}), \ldots \boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{D}_{q-1}}\mathbf{P}_{\mathcal{E}_q}\mathbf{U}\mathbf{P}_{\mathcal{E}_q}\mathbf{P}_{\mathcal{D}_{q-1}})\} \\ &= \mathbf{M}\mathrm{span}\{\boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{E}_q}\mathbf{U}\mathbf{P}_{\mathcal{E}_q}), \boldsymbol{\ell}_1[(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_1})\mathbf{U}(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_1})], \\ &\quad \ldots, \boldsymbol{\ell}_1[(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_{q-1}})\mathbf{U}(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_{q-1}})]\}.\end{aligned}$$

The argument to the span in the right hand side of the last expression contains q linearly independent terms, each of which is in $\mathcal{E}_q$, and thus these terms must span $\mathcal{E}_q$. Thus

$$\begin{aligned}\mathcal{E}_q &= \mathrm{span}\{\boldsymbol{\ell}_1(\mathbf{P}_{\mathcal{E}_q}\mathbf{U}\mathbf{P}_{\mathcal{E}_q}), \boldsymbol{\ell}_1[(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_1})\mathbf{U}(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_1})], \\ &\quad \ldots, \boldsymbol{\ell}_1[(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_{q-1}})\mathbf{U}(\mathbf{P}_{\mathcal{E}_q} - \mathbf{P}_{\mathcal{E}_{q-1}})]\},\end{aligned}$$

and

$$\mathcal{E}_q = \mathbf{M}\mathrm{span}(\mathbf{W}_q) = \mathbf{M}\mathcal{E}_q.$$

It follows that $\mathcal{E}_q = \mathrm{span}(\mathbf{W}_q)$, that $\mathcal{E}_q$ reduces $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ and thus that $q = u$. We have therefore verified that the sequence generated by the algorithm satisfies (6.10).

6.5.3 Krylov matrices and $\dim(\mathcal{U}) = 1$

The algorithm simplifies considerably when $\dim(\mathcal{U}) = 1$, so $\mathbf{U} = \mathbf{u}\mathbf{u}^T$ with $\mathbf{u} \in \mathbb{R}^r$. In that case, we have that $\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \mathrm{span}(\mathbf{u}, \mathbf{M}^1\mathbf{u}, \ldots, \mathbf{M}^{u-1}\mathbf{u})$. The sequence $\mathbf{M}\mathbf{u}, \mathbf{M}^2\mathbf{u}, \ldots, \mathbf{M}^{u-1}\mathbf{u}$ is called a Krylov sequence in numerical analysis. We proceed sequentially to see how this conclusion arises. The first direction vector is simply $\mathbf{w}_1 = \boldsymbol{\ell}_1(\mathbf{U}) \propto \mathbf{u}$. The second direction vector is

$$\mathbf{w}_2 = \boldsymbol{\ell}_1(\mathbf{Q}_{\mathcal{E}_1}\mathbf{U}\mathbf{Q}_{\mathcal{E}_1}) \propto \mathbf{Q}_{\mathcal{E}_1}\mathbf{u} = \mathbf{u} - \mathbf{P}_{\mathcal{E}_1}\mathbf{u}.$$

Thus,

$$\begin{aligned}
\mathrm{span}(\mathbf{W}_2) &= \mathrm{span}(\mathbf{u}, \mathbf{u} - \mathbf{P}_{\mathcal{E}_1}\mathbf{u}) = \mathrm{span}(\mathbf{u}, \mathbf{P}_{\mathcal{E}_1}\mathbf{u}) \\
&= \mathrm{span}(\mathbf{u}, \mathbf{P}_{\mathbf{M}\mathbf{u}}\mathbf{u}) = \mathrm{span}(\mathbf{u}, \mathbf{M}^1\mathbf{u}).
\end{aligned}$$

Proceeding by induction, assume that $\mathrm{span}(\mathbf{W}_k) = \mathrm{span}(\mathbf{u}, \mathbf{M}^1\mathbf{u}, \ldots, \mathbf{M}^{k-1}\mathbf{u})$ for $k = 1, \ldots, q$. Then next direction vector is given by

$$\mathbf{w}_{q+1} = \boldsymbol{\ell}(\mathbf{Q}_{\mathcal{E}_q}\mathbf{U}\mathbf{Q}_{\mathcal{E}_q}) \propto \mathbf{Q}_{\mathcal{E}_q}\mathbf{u} = \mathbf{u} - \mathbf{P}_{\mathcal{E}_q}\mathbf{u},$$

and therefore

$$\mathrm{span}(\mathbf{W}_{q+1}) = \mathrm{span}(\mathbf{u}, \mathbf{M}^1\mathbf{u}, \ldots, \mathbf{M}^{q-1}\mathbf{u}, \mathbf{P}_{\mathcal{E}_q}\mathbf{u}).$$

Since $\mathbf{P}_{\mathcal{E}_q}\mathbf{u} = \mathbf{P}_{\mathbf{M}\mathbf{W}_q}\mathbf{u}$, we can write $\mathbf{P}_{\mathcal{E}_q}\mathbf{u}$ as a linear combination of the q spanning vectors $\mathbf{M}^1\mathbf{u}, \mathbf{M}^2\mathbf{u}, \ldots, \mathbf{M}^q\mathbf{u}$. It follows that

$$\mathrm{span}(\mathbf{W}_{q+1}) = \mathrm{span}(\mathbf{u}, \mathbf{M}^1\mathbf{u}, \mathbf{M}^2\mathbf{u}, \ldots, \mathbf{M}^q\mathbf{u}).$$

6.5.4 Variations on the basic algorithm

It follows from Corollary 5.2 that there are many variations on the choice of $\mathbf{U}$ and $\mathbf{M}$ that lead to the same envelope. For example, replacing $\mathbf{U}$ with $f^*(\mathbf{M})\mathbf{U}f^*(\mathbf{M})$ produces the same envelope after u steps, as does replacing $\mathbf{M}$ by $f^*(\mathbf{M})$ for a strictly monotonic f.

Such modifications may alter the individual direction vectors $\mathbf{w}_k$ but they will not change $\mathcal{W}_u = \mathcal{E}_{\mathbf{M}}(\mathcal{U})$ in the end.

Variations on the length constraint (6.13) are more involved. Consider replacing the length constraint $\mathbf{w}^T\mathbf{w} = 1$ with $\mathbf{w}^T\mathbf{V}\mathbf{w}$, where $\mathbf{V} \in \mathbb{S}^{r\times r}$ is positive definite, without altering the rest of the algorithm in (6.11) and (6.12). This variation can be studied straightforwardly by changing coordinates to represent it in the form of the original algorithm. Let $\mathbf{h} = \mathbf{V}^{1/2}\mathbf{w}$ and $\mathbf{H}_k = \mathbf{V}^{1/2}\mathbf{W}_k$. Then the algorithm in the $\mathbf{h}$ coordinates is

$$\mathbf{h}_{k+1} = \arg\max_{\mathbf{h}} \mathbf{h}^T\mathbf{V}^{-1/2}\mathbf{U}\mathbf{V}^{-1/2}\mathbf{h}, \text{ subject to} \tag{6.27}$$

$$\mathbf{h}^T\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}\mathbf{H}_k = 0 \tag{6.28}$$

$$\mathbf{h}^T\mathbf{h} = 1, \tag{6.29}$$

which produces $\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathbf{V}^{-1/2}\mathcal{U})$ after u steps. After transforming back to the $\mathbf{w}$ coordinate we have the resulting subspace $\mathbf{V}^{-1/2}\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathbf{V}^{-1/2}\mathcal{U})$. The question now at hand is when this subspace results in $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$; that is, when is it true that

$$\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \mathbf{V}^{-1/2}\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathbf{V}^{-1/2}\mathcal{U})? \tag{6.30}$$

Before considering general conditions on $\mathbf{V}$ that guarantee (6.30), we examine the special case in which $\mathbf{M} > 0$ and $\mathbf{V} = \mathbf{M}$. In that case,

$$\mathbf{V}^{-1/2}\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathbf{V}^{-1/2}\mathcal{U}) = \mathbf{M}^{-1/2}\mathcal{E}_{\mathbf{I}_r}(\mathbf{M}^{-1/2}\mathcal{U}) = \mathbf{M}\mathcal{U},$$

where the second equality follows from Propostion 5.3. Let the columns of the symmetric matrix $\mathbf{U}$ be a basis for $\mathcal{U}$ and let $d = \dim(\mathcal{U})$. The subspace $\mathbf{M}\mathcal{U}$ is the span of the eigenvectors of $\mathbf{U}$ relative to $\mathbf{M}$; that is, the span of the solutions $\boldsymbol{\ell}_j$, $j = 1,\ldots,d$, of $\mathbf{U}\boldsymbol{\ell}_j = \lambda\mathbf{M}\boldsymbol{\ell}_j$ subject to the constraints that $\boldsymbol{\ell}_j^T\mathbf{M}\boldsymbol{\ell}_j = 1$ and $\boldsymbol{\ell}_j^T\mathbf{M}\boldsymbol{\ell}_k = 0$ for $k = 1,\ldots,j-1$. We summarize the results of this discussion in the following lemma for later reference.

Lemma 6.5 *If the length constraint (6.13) in the envelope algorithm (6.11)–(6.13) is replaced with* $\mathbf{w}^T\mathbf{M}\mathbf{w} = 1$, *then the revised algorithm ends with* $\mathbf{M}\mathcal{U}$ *after* $\dim(\mathcal{U})$ *steps.*

Turning to a discussion of conditions on $\mathbf{V}$ that ensure (6.30), we know from Proposition 5.4 that if $\mathbf{V}$ commutes with $\mathbf{M}$ and $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ reduces $\mathbf{V}$ then

$$\mathbf{V}^{-1/2}\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathbf{V}^{-1/2}\mathcal{U}) = \mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathcal{U}).$$

From Proposition 5.3 we will have $\mathcal{E}_{\mathbf{M}}(\mathcal{U}) = \mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathcal{U})$ if the eigenspaces of $\mathbf{M}$ that are not orthogonal to $\mathcal{U}$ are the same as the eigenspaces of $\mathcal{E}_{\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2}}(\mathcal{U})$ that are not orthogonal to $\mathcal{U}$. In reference to Corollary 5.2, these sufficient conditions are satisfies when $\mathbf{V} = f^*(\mathbf{M})$ and $f(\cdot)$ is strictly monotonic. In particular, we can use $\mathbf{V} = \mathbf{M}^a$ for $a \in \mathbb{R}^1$ and $a \neq 1$ without altering the end result of the algorithm. The case where $\mathbf{V} = \mathbf{M}$ is non-singular fails because then $f(\cdot)$ is the identity ($a = 1$), $\mathbf{V}^{-1/2}\mathbf{M}\mathbf{V}^{-1/2} = \mathbf{I}_r$, and consequently its eigenspaces are not the same as those of $\mathbf{M}$.

The envelope algorithm is also invariant under choices of a positive semi-definite $\mathbf{V} \geq 0$ when $\mathbf{V}$ satisfies the previous conditions for the positive definite case: $\mathbf{V}$ commutes with $\mathbf{M}$, $\mathrm{span}(\mathbf{V}) \subseteq \mathrm{span}(\mathbf{M})$ and $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ reduces $\mathbf{V}$. This can be demonstrated by adapting the justification presented in Section 6.5.1 reasoning as follows. Since $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ reduces $\mathbf{V}$, we have $\mathbf{V} = \boldsymbol{\Gamma}(\boldsymbol{\Gamma}^T\mathbf{V}\boldsymbol{\Gamma})\boldsymbol{\Gamma}^T + \boldsymbol{\Gamma}_0(\boldsymbol{\Gamma}_0^T\mathbf{V}\boldsymbol{\Gamma}_0)\boldsymbol{\Gamma}_0^T$ and $\boldsymbol{\Gamma}^T\mathbf{V}\boldsymbol{\Gamma} > 0$. Consequently, the rank deficiency in $\mathbf{V}$ is manifested only in $\boldsymbol{\Gamma}_0^T\mathbf{V}\boldsymbol{\Gamma}_0$. The part of $\mathbf{V}$ that is orthogonal to $\mathcal{E}_{\mathbf{M}}(\mathcal{U})$ plays no role in the algorithm and consequently we can modify $\boldsymbol{\Gamma}_0^T\mathbf{V}\boldsymbol{\Gamma}_0$ to make it non-singular without affecting the outcome, leading back to the full rank case.

Problems

Problem 6.1 *Propose a solution to the estimation problem given in Problem 1.6, providing justification. Is your solution the same as the MLE?*

Problem 6.2 *Prove Proposition 6.1.*

Problem 6.3 *Consider the OLS estimator $\mathbf{B} \in \mathbb{R}^p$ of the coefficient vector $\boldsymbol{\beta}$ in the multivariate linear model with $r = 1$ and $p > 1$, so there is a single response. Show that objective function (6.4) yields objective function (4.8) when the sample versions $\mathbf{V}_{\boldsymbol{\beta}}$ and $\mathbf{U} = \boldsymbol{\beta}\boldsymbol{\beta}^T$ are used for $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{U}}$.*