Targeted Principal Components Regression

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1 Preliminaries

Recall the functions

$$g(\theta) = g(\theta; y, x) = -\log |\Omega| + (y - \beta^{\mathsf{T}} x)^{\mathsf{T}} \Omega(y - \beta^{\mathsf{T}} x) + \log |\tau I_p + \Psi| + x^{\mathsf{T}} (\tau I_p + \Psi)^{-1} x,$$

$$G(\theta) = G(\theta; \theta_*) = -\log |\Omega| + \operatorname{tr} \{ (\beta - \beta_*)^{\mathsf{T}} (\tau_* I_p + \Psi_*) (\beta - \beta_*) \Omega \} + \operatorname{tr} (\Omega \Omega_*^{-1}) + \log |\tau I_p + \Psi| + \operatorname{tr} \{ (\tau I_p + \Psi)^{-1} (\tau_* I_p + \Psi_*) \},$$
and $G_n(\theta) = G_n(\theta; Y_1, X_1, \dots, Y_n, X_n) = n^{-1} \sum_{i=1}^n g(\theta; Y_i, X_i).$ Let $\Sigma_X = \tau I_p + \Psi$; then
$$G_n(\theta) = -\log |\Omega| + n^{-1} \operatorname{tr} \{ (Y - X\beta)^{\mathsf{T}} (Y - X\beta) \Omega \} + \log |\Sigma_X| + n^{-1} \operatorname{tr} (X^{\mathsf{T}} X \Sigma_X^{-1}).$$

The gradient $\nabla g = \nabla_{\theta} g$ is characterized by

$$\nabla_{\beta}g(\theta) = -2x(y - \beta^{\mathsf{T}}x)^{\mathsf{T}}\Omega;$$

$$\nabla_{\Omega}g(\theta) = -\Omega^{-1} + (y - \beta^{\mathsf{T}}x)(y - \beta^{\mathsf{T}}x)^{\mathsf{T}};$$

$$\nabla_{\tau}g(\theta) = \operatorname{tr}(\Sigma_X^{-1} - \Sigma_X^{-1}xx^{\mathsf{T}}\Sigma_X^{-1});$$

$$\nabla_{\Psi}g(\theta) = \Sigma_X^{-1} - \Sigma_X^{-1}xx^{\mathsf{T}}\Sigma_X^{-1}.$$

By differentiating these expressions, one gets that the non-zero blocks of the Hessian $\nabla^2 g$

are given by

$$\nabla_{\beta}^{2}g(\theta) = 2\Omega \otimes xx^{\mathsf{T}};$$

$$\nabla_{\beta\Omega}^{2}g(\theta) = -2I_{r} \otimes x(y - \beta^{\mathsf{T}}x)^{\mathsf{T}};$$

$$\nabla_{\Omega}^{2}g(\theta) = \Omega^{-1} \otimes \Omega^{-1};$$

$$\nabla_{\tau}^{2}g(\theta) = \operatorname{tr}\{-\Sigma_{X}^{-2} + \Sigma_{X}^{-2}xx^{\mathsf{T}}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}xx^{\mathsf{T}}\Sigma_{X}^{-2}\};$$

$$\nabla_{\tau\Psi}^{2}g(\theta) = -\Sigma_{X}^{-2} + \Sigma_{X}^{-2}xx^{\mathsf{T}}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}xx^{\mathsf{T}}\Sigma_{X}^{-2};$$

$$\nabla_{\Psi}^{2}g(\theta) = -\Sigma_{X}^{-2} \otimes \Sigma_{X}^{-1} + \Sigma_{X}^{-1} \otimes \Sigma_{X}^{-1}xx^{\mathsf{T}}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}xx^{\mathsf{T}}\Sigma_{X}^{-1} \otimes \Sigma_{X}^{-1}.$$

The gradient ∇G is characterized by

$$\nabla_{\beta}G(\theta) = 2\Sigma_{X*}(\beta - \beta_{*})\Omega;$$

$$\nabla_{\Omega}G(\theta) = -\Omega^{-1} + (\beta - \beta_{*})^{\mathsf{T}}\Sigma_{X*}(\beta - \beta_{*}) + \Omega_{*}^{-1};$$

$$\nabla_{\tau}G(\theta) = \operatorname{tr}\{\Sigma_{X}^{-1} - \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-1}\};$$

$$\nabla_{\Psi}G(\theta) = \Sigma_{X}^{-1} - \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-1}.$$

The non-zero blocks of the Hessian $\nabla^2 G$ are given by

$$\nabla_{\beta}^{2}G(\theta) = 2\Omega \otimes \Sigma_{X*};$$

$$\nabla_{\beta\Omega}^{2}G(\theta) = 2I_{r} \otimes \Sigma_{X*}(\beta - \beta_{*});$$

$$\nabla_{\Omega}^{2}G(\theta) = \Omega^{-1} \otimes \Omega^{-1};$$

$$\nabla_{\tau}^{2}G(\theta) = \operatorname{tr}\{-\Sigma_{X}^{-2} + \Sigma_{X}^{-2}\Sigma_{X*}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-2}\};$$

$$\nabla_{\tau\Psi}^{2}G(\theta) = -\Sigma_{X}^{-2} + \Sigma_{X}^{-2}\Sigma_{X*}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-2};$$

$$\nabla_{\Psi}^{2}G(\theta) = -\Sigma_{X}^{-1} \otimes \Sigma_{X}^{-1} + \Sigma_{X}^{-1} \otimes \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-1} + \Sigma_{X}^{-1}\Sigma_{X*}\Sigma_{X}^{-1} \otimes \Sigma_{X}^{-1}.$$

2 Proofs

2.1 Proof of Proposition 2.1

Consider an enlarged parameter set Θ_1 where Ψ is of rank at most k and has a spectral decomposition UDU^T , $D \in \mathbb{R}^{k \times k}$, such that $\beta = U\gamma$ for some $\gamma \in \mathbb{R}^{k \times r}$; that is, β is in the column space of U, but not necessarily in that of Ψ if some diagonal elements of D are equal to zero. Clearly, G_n can be defined the same way on Θ_1 as on Θ . The enlarged parameter set is useful because it is closed. To see this, pick a convergent sequence $\{\theta_m\} \in \Theta_1$; we need to show the limit point $\theta \in \Theta_1$. It straightforward to show Ω , τ , and Ψ must be symmetric and positive semi-definite, so we omit the details. To see the rank of Ψ is at most k, suppose for contradiction it has k+1 strictly positive eigenvalues. Then by Weyl's perturbation theorem (Bhatia, 2012, Corollary III.2.6), so does Ψ_m for all large enough m, which is a contradiction to $\Psi_m \in \mathcal{S}$. Because $\Psi \in \mathcal{S}$, we can write $\Psi = UDU^\mathsf{T}$ and it remains to show $P_U\beta = \beta$. To that end, write $\Psi_m = U_m D_m U_m^\mathsf{T}$ and $\beta_m = U_m \gamma_m$ for every m. Since $\|\beta_m\| = \|\gamma_m\|$ and

 β_m converges, $\{\gamma_m\}$ is bounded. Similarly, $\{D_m\}$ is bounded and $\{U_m\}$ is a sequence in the compact set of $p \times k$ semi-orthogonal matrices. Thus, we can pick out a subsequence along which γ_m , D_m , and U_m converge to some limits γ , D, and U. The diagonal elements of D are non-negative since those of D_m are and U is a semi-orthogonal matrix by closedness. Thus, along this subsequence we get by taking limits on both sides of the identities $\beta_m = U_m \gamma_m$ and $\Psi_m = U_m D_m U_m^\mathsf{T}$ that $\beta = U \gamma$ and $\Psi = U D U^\mathsf{T}$, which proves Θ_1 is closed.

Next, we show there exists a compact $A \subseteq \Theta_1$ such that $G_n(\theta) > G_n(\theta_0)$ for all $\theta \in \Theta_1 \setminus A$ and some arbitrary but fixed $\theta_0 \in \Theta$. Unconstrained partial minimization in β and Σ_X shows $G_n(\theta) \ge -\log |\Omega| + \operatorname{tr}(Y^\mathsf{T}Q_XY\Omega) + \log |X^\mathsf{T}X/n| + \operatorname{tr}(I_p)$, which tends to ∞ if $\lambda_{\max}(\Omega) \to \infty$ or $\lambda_{\min}(\Omega) \to 0$; this is so because $Y^\mathsf{T}Q_XY$ is positive definite when [Y,X] has full column rank. Similarly, unconstrained partial minimization in β and Ω shows $G_n(\theta) \ge \log |Y^\mathsf{T}Q_XY/n| + \operatorname{tr}(I_r) + \log |\tau I_p + \Psi| + n^{-1}\operatorname{tr}\{X^\mathsf{T}X(\tau I_p + \Psi)^{-1}\}$, which since $X^\mathsf{T}X$ is positive definite when [Y,X] and hence X has full column rank, tends to ∞ if $\tau \to \infty$, $\tau \to 0$, or $\lambda_{\max}(\Psi) \to \infty$. Unconstrained partial minimization in Ω and Σ_X gives $G_n(\theta) \ge \log |(Y - X\beta)^\mathsf{T}(Y - X\beta)/n| + \operatorname{tr}(I_r) + \log |X^\mathsf{T}X/n| + \operatorname{tr}(I_p)$, which tends to ∞ if $\|\beta\| \to \infty$ since $X^\mathsf{T}X$ is positive definite. Thus, we can take $A = \{\theta \in \Theta_1 : \|\beta\| \le c, c^{-1} \le \lambda_{\min}(\Omega) \le \lambda_{\max}(\Omega) \le c, c^{-1} \le \tau \le c, \lambda_{\max}(\Psi) \le c\}$ for some large enough $c < \infty$. Using that Θ_1 is closed and A is bounded by construction, it is routine to show A is a closed and bounded subset of \mathbb{R}^d and hence compact.

Now, G_n is continuous at points where $\tau > 0$ and $\lambda_{\min}(\Omega) > 0$ and hence attains its minimum over A, which must be a minimum over Θ_1 by the above. To show G_n attains its minimum over Θ it thus suffices to show that for any minimizer $\hat{\theta}$ over Θ_1 , it must hold that $\hat{\Psi}$ has rank k so that $\hat{\theta} \in \Theta$. Consider a point θ such that Ψ has rank s < k. Then for any $v \neq 0$ such that $\Psi v = 0$, $\Psi + vv^{\mathsf{T}}$ has rank $s + 1 \leq k$ and $\Psi + vv^{\mathsf{T}} \in \mathcal{S}$. Moreover, β is in the column space of [U, v] since it is in that of U. Thus, if we can show setting $v \neq 0$ decreases the objective function, no point with the rank of Ψ equal to s < k can be a minimizer, and hence we are done. Consider the function of v defined for a fixed θ by $\log |\Sigma_X + vv^{\mathsf{T}}| + n^{-1} \operatorname{tr}\{(\Sigma_X + vv^{\mathsf{T}})^{-1}X^{\mathsf{T}}X\} = \log |\Sigma_X| + \log(1 + v^{\mathsf{T}}\Sigma_X^{-1}v) + n^{-1} \operatorname{tr}(X^{\mathsf{T}}X\Sigma_X^{-1}) - n^{-1}v^{\mathsf{T}}\Sigma_X^{-1}X^{\mathsf{T}}X\Sigma_X^{-1}v(1 + v^{\mathsf{T}}\Sigma_X^{-1}v)^{-1}$, where we used the matrix determinant lemma and the Sherman-Morrison formula. Now observe that if v is orthogonal to the s leading eigenvectors of Σ_X , then $v^{\mathsf{T}}\Sigma_X v = \tau ||v||^2$ and $v^{\mathsf{T}}\Sigma_X^{-1}v = \tau^{-1}||v||^2$. Let $c = ||v||^2$. Then, with the spectral decomposition $\Sigma_X^{-1} = \sum_{j=1}^p \lambda_j^{-1}(\Sigma_X)u_ju_j^{\mathsf{T}}$, the terms of the objective that depend on v are

$$\log(1 + \tau^{-1}c) - \frac{c\tau^{-1}\left(\sum_{j=s+1}^{p} v^{\mathsf{T}} u_{j} u_{j}^{\mathsf{T}}\right) \left(S_{X}/\tau\right) \left(\sum_{j=s+1}^{p} u_{j} u_{j}^{\mathsf{T}} v\right)}{1 + \tau^{-1}c}$$

Consider a $v \propto u_j$ for some $j \in \{s+1,\ldots,p\}$. The last display then becomes $\log(1+\tau^{-1}c)-(1+\tau^{-1}c)^{-1}c\tau^{-1}u_j^{\mathsf{T}}(S_X/\tau)u_j$. By making the change of variables $t=c\tau^{-1}$ and letting $a=u_j^{\mathsf{T}}S_Xu_j/\tau$ one gets $\log(1+t)-(1+t)^{-1}ta$ which is minimized by t=a-1, which is feasible and non-zero if a>1. To see $\hat{\tau}>\lambda_{\min}(S_X)$ and hence a>1, let VHV^{T} be a spectral decomposition of Σ_X , where the diagonal elements of H are the eigenvalues $h_j=\lambda_j(\Sigma_X)$. It follows that $h_{k+1}=\cdots=h_p=\tau$ and the first k columns of V are those of U. The part of G_n depending on H is $\log |\Sigma_X|+\operatorname{tr}(S_X\Sigma_X^{-1})=\sum_{j=1}^p \{\log h_j+h_j^{-1}a_j\}$, where $a_j=V_j^{\mathsf{T}}X^{\mathsf{T}}XV_j/n$.

The derivative of this with respect to h_j is $h_j^{-1} - h_j^{-2} a_j$ if $j \geq k$ and $(p-k)h_j^{-1} - h_j^{-2} \sum_{j=k+1}^p a_j$ if j = k+1. Suppose that $h_p < \lambda_{\min}(S_X)$; then since $\sum_{j=k+1}^p a_j \geq (p-k)\lambda_{\min}(S_X)$, the derivative for h_p is negative. That is, moving $h_p = \tau$ towards h_k does not affect the ordering of the eigenvalues but decreases the objective function. The same holds for every h_j , so for a minimizer it must be that $\hat{h}_1 \geq \cdots \geq \hat{h}_p = \hat{\tau} \geq \lambda_{\min}(S_X)$. A similar argument shows $\hat{h}_1 \leq \lambda_{\max}(S_X)$. It remains to show $\hat{\tau} \neq \lambda_{\min}(S_X)$. Suppose $\hat{h}_1 = \lambda_{\min}(S_X)$, then in fact $h_j = \lambda_{\min}(S_X)$ for all j giving $\lambda_{\min}(S_X)$ multiplicity p, contradicting $\lambda_{k+1}(S_X) > \lambda_p(S_X)$. But then, by the same argument as when showing $\hat{\tau} \geq \lambda_{\min}(S_X)$, it must be that $\hat{h}_2 > \lambda_{\min}(S_X)$ since otherwise the objective could be decreased by moving \hat{h}_2 towards \hat{h}_1 . Continuing this process shows $\hat{h}_{k+1} > \lambda_{\min}(S_X)$ as desired.

2.2 Proof of Theorem 2.2

We start with a lemma.

Lemma A. Condition (i) of Theorem 2.2 implies, for a generic $0 < c < \infty$ that may change between claims but does not depend on r or p: (a) $c^{-1} \le \lambda_{\min}(\Omega_*) \le \lambda_{\max}(\Omega_*) \le c$, (b) $c^{-1} \le \lambda_{\min}(\Omega_*^{-1} + \beta_*^\mathsf{T} \Sigma_{X*} \beta) \le \lambda_{\min}(\Sigma_{X*}) \le \lambda_{\min}(\Sigma_{X*}) \le \lambda_{\min}(\Sigma_{X*}) \le c$, and (d) $\|\beta_*\| \le c$.

Proof. Claim (a) follows from observing that $\Omega_*^{-1} = \Sigma_*/\Sigma_{X*}$ is the Schur-complement of Σ_{X*} in Σ_* (Smith, 1992, Theorem 5), while (b) and (c) are by the Cauchy interlacing theorem. Now (d) follows since $c \geq v^{\mathsf{T}}(\Omega_*^{-1} + \beta_*^{\mathsf{T}}\Sigma_{X*}\beta_*)v \geq \lambda_{\min}(\Omega_*) + \|\beta_*\|\lambda_{\min}(\Sigma_{X*}) \geq c^{-1} + c^{-1}\|\beta_*\|$ so that $\|\beta_*\| \leq c^2 - 1$.

We next show G_n concentrates around G on suitably chosen subsets of Θ . For any c > 1 define the set A = A(c) by

$$A = \{ \theta \in \Theta : \|\beta\| \le c, c^{-1} \le \lambda_{\min}(\Omega), \le \lambda_{\max}(\Omega) \le c, c^{-1} \le \tau \le c, \lambda_{\max}(\Psi) \le c \}.$$
 (1)

Lemma B. Under the conditions of Theorem 2.2, for all $c < \infty$ large enough and any $\epsilon > 0$,

$$\operatorname{pr}\left(\sup_{\theta\in A(c)}|G_n(\theta)-G(\theta)|\geq\epsilon\right)\to 0.$$

Proof. We have

$$G_n(\theta) - G(\theta) = n^{-1} \operatorname{tr}\{(Y - X\beta)^{\mathsf{T}}(Y - X\beta)\Omega\} - \operatorname{tr}\{(\beta - \beta_*)^{\mathsf{T}}\Sigma_{X*}(\beta - \beta_*)\Omega\} - \operatorname{tr}(\Omega\Omega_*^{-1}) + n^{-1} \operatorname{tr}(X^{\mathsf{T}}X\Sigma_X^{-1}) - \operatorname{tr}(\Sigma_{X*}\Sigma_X^{-1}).$$

We show that the suprema of lines one and two over A are both $o_p(1)$ and start with the first. Let $\varepsilon = Y - X\beta_*$, $\tilde{\beta} = \beta_* - \beta$, and $S_Y = Y^\mathsf{T} Y/n$. Then the first line is

$$n^{-1}\operatorname{tr}\{(\varepsilon^{\mathsf{T}}\varepsilon+2\varepsilon^{\mathsf{T}}X\tilde{\beta}+\tilde{\beta}^{\mathsf{T}}X^{\mathsf{T}}X\tilde{\beta})\Omega\}-\operatorname{tr}(\tilde{\beta}^{\mathsf{T}}\Sigma_{X*}\tilde{\beta}\Omega)-\operatorname{tr}(\Omega\Omega_{*}^{-1})$$

or

$$\operatorname{tr}\{(S_{\varepsilon} - \Omega_{*}^{-1})\Omega\} + 2\operatorname{tr}\{(S_{\varepsilon X}\tilde{\beta})\Omega\} + \operatorname{tr}\{\tilde{\beta}(S_{X} - \Sigma_{X*})\tilde{\beta}\Omega\}$$

Thus, repeatedly using that $\operatorname{tr}(A) \leq r \|A\|$ for any $A \in \mathbb{R}^{r \times r}$ and that operator norms are sub-multiplicative, the absolute value of the first line is upper bounded on A by

$$rc\|S_{\varepsilon} - \Omega_{*}^{-1}\| + 4rc\|S_{\varepsilon X}\| + 4rc^{3}\|S_{X} - \Sigma_{X*}\|,$$

where we implicitly assumed that the c in the definition of A and condition (i) of Theorem 2.2 are the same, which can always be arranged by picking the larger of the two, so that $\|\beta - \beta_*\| \le 2c$ on A. But the last display is $o_p(1)$ by condition (ii) of Theorem 2.2.

Now, the second line whose supremum we need to show is $o_p(1)$ is, by the Woodbury identity $\Sigma_X = \tau^{-1}I_p - \tau^{-2}U(D^{-1} + \tau^{-1}I_k)^{-1}U^{\mathsf{T}}$ with spectral decomposition $\Psi = UDU^{\mathsf{T}}$,

$$\operatorname{tr}\{(S_X - \Sigma_{X*})\Sigma_X^{-1}\} = \tau^{-1}\operatorname{tr}(S_X - \Sigma_{X*}) - \tau^{-2}\operatorname{tr}\{U^{\mathsf{T}}(S_X - \Sigma_{X*})U(D^{-1} + \tau^{-1}I_k)^{-1}\}.$$

The absolute value of first term is, on A, less than $c \operatorname{tr}(S_X - \Sigma_{X*})$ which is $o_p(1)$ by condition (iii) of Theorem 2.2. Also on A, the absolute value of the second term is, since $U \in \mathbb{R}^{p \times k}$, less than $c^2 k \|(S_X - \Sigma_{X*})(D^{-1} + \tau^{-1}I_k)^{-1}\| \leq c^3 k \|S_X - \Sigma_{X*}\|$, which is $o_p(1)$ by condition (ii) of Theorem 2.2.

Lemma C. Under the conditions of Theorem 2.2, there exists a $0 < c < \infty$ such that

$$\operatorname{pr}\left(\arg\min_{\theta\in\Theta}G_n(\theta)\subseteq A(c)\right)\to 1.$$

Proof. Because $\tau_* \geq c^{-1} > 0$, condition (ii) of Theorem 2.2 implies $S_X = X^{\mathsf{T}} X / n$ is invertible with probability tending to one, so it suffices to consider outcomes with invertible S_X . Pick $\hat{\theta} \in \arg\min_{\theta \in \Theta} G_n(\theta)$; if none exists we are done trivially.

Let $\hat{\Psi} = \hat{U}\hat{D}\hat{U}^{\mathsf{T}}$ by spectral decomposition and pick a $\hat{\gamma}$ such that $\hat{\beta} = \hat{U}\hat{\gamma}$. Since $\hat{\theta}$ is a minimizer $\hat{\gamma}$ minimizes $\gamma \mapsto \operatorname{tr}\{(Y - X\hat{U}\gamma)^{\mathsf{T}}(Y - X\hat{U}\gamma)\hat{\Omega}\}$; that is, $\hat{\gamma} = (\hat{U}^{\mathsf{T}}S_X\hat{U})^{-1}\hat{U}^{\mathsf{T}}S_{XY}$. Thus, using that the spectral norm is submultiplicative,

$$\|\hat{\beta}\| = \|\hat{\gamma}\| \le \|(\hat{U}^{\mathsf{T}} S_X \hat{U})^{-1}\| \|\hat{U}^{\mathsf{T}} S_{XY}\| \le \lambda_{\min}(S_X)^{-1} \|S_X\|^{1/2} \|S_Y\|^{1/2}$$

which by condition (ii) of Theorem 2.2 tends in probability to $\tau_*^{-1}\{\tau_* + \lambda_{\max}(\Psi_*)\}^{1/2}\|\Omega_*^{-1} + \beta_* \Sigma_{X*} \beta_*\|^{1/2} \leq 2^{1/2} c^2$, where the inequality is by condition (i). Thus, with probability tending to one, every minimizer satisfies $\|\hat{\beta}\| \leq c$ for some large enough c. Next, since $\hat{\Omega} = (Y^{\mathsf{T}} Q_{X\hat{U}} Y/n)^{-1}$ and the column space of $X\hat{U}$ is a subset of that of X, it follows that

$$\lambda_{\min}(Y^{\mathsf{T}}Q_XY/n) \le \lambda_{\min}(\hat{\Omega}^{-1}) \le \lambda_{\max}(\hat{\Omega}^{-1}) \le \lambda_{\max}(Y^{\mathsf{T}}Y/n).$$

By condition (ii), the left-most and right-most expressions tend to, respectively, $0 < \lambda_{\min}(\Omega_*^{-1})$ and $\lambda_{\max}(\Omega_*^{-1} + \beta_*^\mathsf{T} \Sigma_{X*} \beta_*) < \infty$, from which it follows, by condition (i), that $c^{-1} \leq \lambda_{\min}(\hat{\Omega}) \leq \lambda_{\max}(\hat{\Omega}) \leq c$ with probability tending to one for some large enough c. That $\hat{\tau} \leq c$ and $\lambda_{\max}(\hat{\Psi}) \leq c$ follows similarly from Proposition 2.1 and conditions (i) and (ii).

Lemma D. Under condition (i) of Theorem 2.2, there exists a $\delta > 0$, which can depend on c but not p, such that, for every $\theta \in A(c)$,

$$G(\theta) - G(\theta_*) \ge \delta \|\theta - \theta_*\|_M^2$$

Proof. The inequality is an equality if $\theta = \theta_*$, so pick a $\theta \neq \theta_*$ and let $\epsilon = \|\theta - \theta_*\|_M > 0$. By definition of $\|\cdot\|_M$, it must hold that (a) $\|\beta - \beta_*\| = \epsilon$, (b) $\|\Omega - \Omega_*\| = \epsilon$, (c) $|\tau - \tau_*| = \epsilon$, or (d) $\|\Psi - \Psi_*\| = \epsilon$. Let $G_1(\theta) = -\log |\Omega| + \operatorname{tr}\{(\beta - \beta_*)^\mathsf{T}(\tau_* I_p + \Psi_*)(\beta - \beta_*)\Omega\} + \operatorname{tr}(\Omega\Omega_*^{-1})$ and $G_2(\theta) = \log |\Sigma_X| + \operatorname{tr}(\Sigma_X^{-1}\Sigma_{X*})$. Since both G_1 and G_2 are minimized by θ_* , we have

$$G(\theta) - G(\theta_*) \ge \max\{G_1(\theta) - G_1(\theta_*), G_2(\theta) - G_2(\theta_*)\}.$$

Thus, it suffices to show that if either of (a) – (d) holds, then at least one of the terms in the maximum on the right-hand side are greater than $\epsilon^2 \delta$ for some $\delta > 0$ not depending on p.

Consider first G_2 and let $\Omega_X = \Sigma_X^{-1} = (\tau I_p + \Psi)^{-1}$. The map $\operatorname{vec}(\Omega_X) \mapsto G_2(\theta)$ is convex with gradient vanishing at $\operatorname{vec}(\Omega_{X*})$ and Hessian $\Sigma_X \otimes \Sigma_X$. Thus, $G_2(\theta) - G(\theta_*) \geq 2^{-1}\lambda_{\min}(\Sigma_X \otimes \Sigma_X) \| \operatorname{vec}(\Omega_X) - \operatorname{vec}(\Omega_X) \|^2 \geq 2^{-1}\tau^2 \|\Omega_X - \Omega_{X*}\|^2$. Now $\|\Sigma_X - \Sigma_{X*}\| = \|\Sigma_X(\Omega_X - \Omega_{X*})\Sigma_{X*}\| \leq \|\Sigma_X\| \|\Sigma_{X*}\| \|\Omega_X - \Omega_{X*}\|$, so $G_2(\theta) - G_2(\theta_*) \geq 2^{-1}\tau^2 \|\Sigma_X - \Sigma_{X*}\|^2 / (\|\Sigma_X\| + \|\Sigma_{X*}\|)^2 \geq 2^{-3}c^{-4} \|\Sigma_X - \Sigma_{X*}\|$. Now suppose (c) holds, then $\|\Sigma_X - \Sigma_{X*}\| \geq \epsilon$ by Weyl's inequalities, so we can take $\delta = 2^{-3}c^{-4}$. Next suppose (d) holds. If $|\tau - \tau_*| \geq \epsilon/2$, then we can take $\delta = 2^{-4}c^{-4}$ by the same argument as before, so suppose $|\tau - \tau_*| < \epsilon/2$. Write $\Sigma_X - \Sigma_{X*} = \Psi - \Psi_* + (\tau - \tau_*)I_p$. Then for any unit-length v, $v^{\mathsf{T}}(\Sigma_X - \Sigma_{X*})v = v^{\mathsf{T}}(\Psi - \Psi_*)v + (\tau - \tau_*)$. It follows, since the spectral norm of a symmetric matrix is its largest absolute eigenvalue, that $\|\Sigma_X - \Sigma_{X*}\| \geq \epsilon/2$, and hence we can take $\delta = 2^{-4}c^{-4}$.

Consider now G_1 and suppose (a) holds. Minimize partially in Ω , which amounts to setting $\Omega^{-1} = (\beta - \beta_*)^\mathsf{T} \Sigma_{X*} (\beta - \beta_*) + \Omega_*^{-1}$. One obtains that $G_1(\theta) - G_1(\theta_*)$ is lower bounded by $\log |(\beta - \beta_*)^\mathsf{T} \Sigma_{X*} (\beta - \beta_*) + \Omega_*^{-1}| - \log |\Omega_*^{-1}|$. By the mean value theorem and using that the gradient of $\Omega^{-1} \mapsto \log |\Omega^{-1}|$ is $\operatorname{tr}(\Omega)$, the last display is equal to $\operatorname{tr}\{\tilde{\Omega}(\beta - \beta_*)^\mathsf{T} \Sigma_{X*} (\beta - \beta_*)\}$, where $\tilde{\Omega}^{-1} = \Omega_*^{-1} + s(\beta - \beta_*)^\mathsf{T} \Sigma_{X*} (\beta - \beta_*)$ for some $s \in [0, 1]$. But the last trace is a quadratic in $\operatorname{vec}(\beta)$ with Hessian $\tilde{\Omega} \otimes \Sigma_X$. The eigenvalues of $\tilde{\Omega}^{-1}$ are less than $c + c^3$, so the eigenvalues of the Hessian, which are the products of the eigenvalues of the terms, are greater than $c^{-1}(c+c^3)^{-1}$. Thus, we can take $\delta = 2^{-1}(c^{-2} + c^{-4})$.

Finally, suppose (b) holds and minimize partially in β ; that is, set $\beta = \beta_*$. One gets $G_1(\theta) - G(\theta_*) \ge -\log |\Omega| + \operatorname{tr}(\Omega\Omega_*^{-1}) + \log |\Omega_*| - \operatorname{tr}(I_r)$. We already know this is a convex function of $\operatorname{vec}(\Omega)$ which is minimized at $\operatorname{vec}(\Omega_*)$ and with Hessian $\Omega^{-1} \otimes \Omega^{-1}$. Thus, $G_1(\theta) - G_1(\theta_*) \ge \|\Omega - \Omega_*\|_F^2 2^{-1} c^{-2} \ge \|\Omega - \Omega_*\|^2 2^{-1} c^{-2}$, so we can take $\delta = 2^{-1} c^{-2}$. To conclude, we have shown the claim holds with $\delta = \min\{2^{-4} c^{-4}, 2^{-1} (c^{-2} + c^{-4}), 2^{-1} c^{-2}\}$

Proof of Theorem 2.2. The existence part follows from Proposition 2.1 and conditions (i) and (ii). Pick an $\epsilon > 0$ and a c large enough that Lemma B and C hold on A = A(c). By increasing c and decreasing ϵ if necessary, we may assume $B = \{\theta : \|\theta - \theta_*\|_M < \epsilon\} \subset A(c)$. On $A \setminus B$, $G(\theta) \geq G(\theta_*) + \delta \epsilon^2$ by Lemma D. Thus, by Lemma B, $G_n(\theta) > G(\theta_*) + \delta \epsilon^2/2$ with probability tending to one. Also with probability tending to one, $G_n(\theta_*) < G(\theta_*) + \delta \epsilon^2$. Thus, with probability tending to one, using Lemma C for the first equality, $\arg \min_{\theta \in \Theta} G_n(\theta) = \arg \min_{\theta \in A} G_n(\theta) = \arg \min_{\theta \in B} G_n(\theta)$, which completes the proof.

2.3 Proof of Theorem 2.4

Lemma E. Under the conditions of Theorem 2.4, $\sqrt{n}\nabla G_n(\theta_*)$ tends in distribution to a multivariate normal vector with mean zero and positive definite covariance matrix with finite entries.

Proof. The gradient of $g(\cdot;z)$ at θ_* , with $\varepsilon = y - \beta_*^\mathsf{T} x$, has subvectors given by the vectorizations of $\nabla_\beta g(\theta_*;z) = -2x\varepsilon^\mathsf{T}\Omega_*$, $\nabla_\Omega g(\theta_*;z) = -\Omega_*^{-1} + \varepsilon\varepsilon^\mathsf{T}$, $\nabla_\Psi g(\theta_*;z) = \Sigma_{X*}^{-1} - \Sigma_{X*}^{-1}xx^\mathsf{T}\Sigma_{X*}^{-1}$, and $\nabla_\tau g(\theta_*;z) = \operatorname{tr}\{\nabla_\Psi g(\theta_*;z)\}$. Consider, for example, the subvector $\operatorname{vec}\{\nabla_\beta g(\theta_*;z)\} = -2(\Omega_* \otimes I_p) \operatorname{vec}(x\varepsilon^\mathsf{T})$. Observe $\mathbb{E}(X_i\varepsilon_i^\mathsf{T}) = 0$ and hence $n^{-1/2}\sum_{i=1}^n \operatorname{vec}\{\nabla_\beta g(\theta_*;Z_i)\} = -2(\Omega_* \otimes I_p)n^{-1/2}\sum_{i=1}^n \operatorname{vec}(X_i\varepsilon_i^\mathsf{T})$ tends to a multivariate normal vector by assumption (iii). All the other subvectors, and the full vector, can be treated similarly, using for $\nabla_\tau g(\theta_*;z)$ that $\operatorname{tr}(\Sigma_{X*}^{-1}xx^\mathsf{T}\Sigma_{X*}^{-1}) = \operatorname{tr}(\Sigma_{X*}^{-2}xx^\mathsf{T}) = \operatorname{vec}(\Sigma_{X*}^{-2})^\mathsf{T} \operatorname{vec}(xx^\mathsf{T})$.

Lemma F. Under the conditions of Theorem 2.4, $g(\theta; z) = g(\theta_*; z) + \nabla g(\theta_*; z)^{\mathsf{T}}(\theta - \theta_*) + \|\theta - \theta_*\| r(\theta; z)$ with a $r(\theta; z)$ that is stochastically equicontinuous in the sense that for every $\epsilon > 0$ and $\delta > 0$, there exists a $\rho > 0$ such that

$$\limsup_{n\to\infty} \operatorname{pr}^* \left(\sup_{\|\theta-\theta_*\|<\rho} \left| n^{-1/2} \sum_{i=1}^n [r(\theta; Z_i) - \mathbb{E}\{r(\theta, Z_i)\}] \right| > \delta \right) < \epsilon,$$

where the superscript * denotes outer probability.

Proof. Consider the function $h(s) = g(\theta_* + s(\theta - \theta_*); z)$, so that $g(\theta; z) - g(\theta_*; z) = h(1) - h(0)$. Taylor expansion with integral-form remainder gives $h(s) = h(0) + h'(0)s + \int_0^s h''(t)(s-t)dt$, where $h'(s) = \nabla g(\theta_* + s(\theta - \theta_*); z)^\mathsf{T}(\theta - \theta_*)$ and $h''(s) = (\theta - \theta_*)^\mathsf{T} \nabla^2 g(\theta_* + s(\theta - \theta_*); z)(\theta - \theta_*)$. Thus, $r(\theta_*; z) = 0$ and for $\theta \neq \theta_*$

$$r(\theta; z) = \frac{(\theta - \theta_*)^\mathsf{T}}{\|\theta - \theta_*\|} \int_0^1 \nabla^2 g(\theta_* + s(\theta - \theta_*); z) (1 - s) \mathrm{d}s(\theta - \theta_*).$$

Denote the middle term (matrix) by $K(\theta;z)$ so that $r(\theta;z) = \|\theta-\theta_*\|^{-1}(\theta-\theta_*)^{\mathsf{T}}K(\theta;z)(\theta-\theta_*)$. Blocks of the matrix K correspond to blocks of $\nabla^2 g$. For example, the leading $pr \times pr$ block of K is $K_1(\theta;z) = \int \{\Omega_* + s(\Omega - \Omega_*)\}(1-s)\mathrm{d}s \otimes xx^{\mathsf{T}}$, and hence $n^{-1}\sum_{i=1}^n [K_1(\theta;Z_i) - \mathbb{E}\{K_1(\theta;Z_i)\}] = \int \{\Omega_* + s(\Omega - \Omega_*)\}(1-s)\mathrm{d}s \otimes n^{-1/2}\sum_{i=1}^n \{X_iX_i^{\mathsf{T}} - \Sigma_{X_*}\}$. The elements of the right-hand matrix are $O_p(1)$ since the vectorization satisfies a central limit theorem by condition (iii). The elements of the left-hand matrix are bounded on a neighborhood of θ_* . Thus, the elements of $n^{-1}\sum_{i=1}^n [K_1(\theta;Z_i) - \mathbb{E}\{K_1(\theta;Z_i)\}]$ are $O_p(1)$ uniformly in θ on a neighborhood of θ_* . Similar arguments for the other blocks, using that the inverse covariance matrices in the Hessian have bounded eigenvalues on small enough neighborhoods of θ_* since $\lambda_{\min}(\Omega_*) > 0$ and $\tau_* > 0$, show the elements of $n^{-1/2}\sum_{i=1}^n [K(\theta;Z_i) - \mathbb{E}\{K(\theta;Z_i)\}]$ are $O_p(1)$ uniformly in θ on a neighborhood of θ_* . The result follows since $|n^{-1/2}\sum_{i=1}^n [r(\theta;Z_i) - \mathbb{E}\{r(\theta,Z_i)\}]| = |\|\theta - \theta_*\|^{-1}(\theta - \theta_*)^{\mathsf{T}}n^{-1/2}\sum_{i=1}^n [K(\theta;Z_i) - \mathbb{E}\{K(\theta;Z_i)\}](\theta - \theta_*) \leq \|\theta - \theta_*\|\|n^{-1/2}\sum_{i=1}^n [K(\theta;Z_i) - \mathbb{E}\{K(\theta;Z_i)\}]\|$.

Proof of Theorem 2.4. We verify the conditions of Theorem 4.4 from Geyer (1994). Chernoff-regularity is from Theorem 2.6. Assumption A is verified by noting G is minimized at $\theta_* \in \Theta$, $\nabla G(\theta_*) = 0$, and that G has a local quadratic approximation with $o(\|\theta - \theta_*\|^2)$ remainder around θ_* by Taylor's theorem since the third order derivatives are bounded for θ close to θ_* . The last statement follows from differentiating the expressions for $\nabla^2 G(\theta)$ and observing that powers of Ω and Σ_X are bounded around θ_* since $\lambda_{\min}(\Omega_*) > 0$ and $\tau_* > 0$. Assumptions B and C are verified in Lemmas F and E, respectively. Assumption D holds since $\hat{\theta}$ is a minimizer by assumption.

2.4 Proof of Theorem 2.6

The following lemma is from Li et al. (2019).

Lemma G. Let $\mathcal{R} \subseteq \mathbb{R}^{p \times p}$ be the set of $p \times p$ matrices of rank k and A an arbitrary point in \mathcal{R} with singular value decomposition $A = UDV^{\mathsf{T}}$, $D \in \mathbb{R}^{k \times k}$; then $T_{\mathcal{R}}(A) = \{B \in \mathbb{R}^{p \times p} : Q_U B Q_V = 0\}$.

Proof of Lemma 2.5. Using the definition, if $C_m \to C$, $a_m \downarrow 0$, and $\Psi + a_m C_m \in \mathcal{S}$ for all n, then C_m and hence C must be symmetric. Next, let \mathcal{R} be the set of $p \times p$ matrices of rank k. Since $\Psi \in \mathcal{S} \subseteq \mathcal{R}$, it is immediate from the definition that $\tilde{T}_{\mathcal{S}}(\Psi) \subseteq T_{\mathcal{S}}(\Psi) \subseteq T_{\mathcal{R}}(\Psi)$. But Lemma G says $T_{\mathcal{R}}(\Psi) = \{C \in \mathbb{R}^{p \times p} : Q_U C Q_U\}$, so we have proved $\tilde{T}_{\mathcal{S}}(\Psi) \subseteq T_{\mathcal{S}}(\Psi) \subseteq \{C \in \mathbb{R}^{p \times p} : C = C^{\mathsf{T}}, Q_U C Q_U = 0\}$. To prove the reverse inclusions, pick arbitrary symmetric C such that $Q_U C Q_U = 0$ and $a_m \downarrow 0$. We must find $C_m \to C$ satisfying $\Psi + a_m C_m \in \mathcal{S}$ for all m. To that end, consider $C_m = C$ and $\Psi_m = \Psi + a_m C$. For any v such that $P_U v = 0$, $v^{\mathsf{T}} \Psi_m v = v^{\mathsf{T}} Q_U (\Psi + a_m C) Q_U v = 0$, while for any v such that $P_U v \neq 0$, $v^{\mathsf{T}} \Psi_m v \geq \|P_U v\| \lambda_k(\Psi) - a_m \|C\|$, which is strictly positive for small enough a_m . It follows that the null spaces of Ψ_n and Ψ agree and that $v^{\mathsf{T}} \Psi_m v > 0$ for any v not in that null space. Thus, as desired, Ψ_m is positive semi-definite with rank k. For the at most finitely many m where a_m is not small enough, we may take $C_m = 0$ without affecting the conclusion, and this completes the proof. \square

Proof of Theorem 2.6. The claims that $O = O^{\mathsf{T}}$ and $t \in \mathbb{R}$ are straightforward to verify using the definition so we omit the details. That $C = C^{\mathsf{T}}$ and $Q_{\Psi}CQ_{\Psi} = 0$ is by Lemma 2.5. To see that $P_{\Psi}B = B$, consider arbitrary sequences $a_m \downarrow 0$ and $(B_m, O_m, t_m, C_m) \to (B, O, t, C)$ satisfying Definition 2.1; that is, $\theta_m = \theta + a_m(B_m, O_m, t_m, C_m)$ is in the parameter set for all (large enough) m. Since Ψ has k strictly positive eigenvalues, so does $\Psi_m = \Psi + a_m C_m$ for all large enough m, and hence Ψ_m has rank at least k; thus, it in fact has rank k since θ_m is in the parameter set. Let $\Psi = UDU^{\mathsf{T}}$ and consider $Q_U\beta_m = Q_U(\beta + a_m B_m) = a_m Q_U B_m$. Since θ_m is in the parameter set, we can also write $\beta_m = (\Psi + a_m C_m)\gamma_m$ for some γ_m and get $Q_U\beta_m = a_m Q_U C_m \gamma_m$. Thus, dividing by a_m we get $Q_UB_m = Q_U C_m \gamma_m$. If we can ensure $\{\gamma_m\}$ is bounded so that it has a convergent subsequence, then we are done upon taking limits along that subsequence to get $Q_UB = Q_UC\gamma = 0$ since $Q_UC = 0$. To see that $\{\gamma_m\}$ can be selected to be bounded, note that we may restrict attention to γ_m in the row space of Ψ_m , which is also its column space. Thus, $\gamma_m = U_m\alpha_m = \sum_{j=1}^k \alpha_{mj}u_{mj}$ and $\beta_m = \Psi_m\gamma_m = \sum_{j=1}^k \lambda_j(\Psi_m)\alpha_{mj}u_j$. The norm $\|\beta_m\|$ is bounded since β_m converges and

its square is equal to $\|\sum_{j=1}^k \lambda_j(\Psi_m)\alpha_{mj}u_j\|^2 = \sum_{j=1}^k \lambda_j(\Psi_m)^2\alpha_{mj}^2 \ge \lambda_k(\Psi_m)^2\sum_{j=1}^k \alpha_{mj}^2 = \lambda_k(\Psi_m)^2\|\gamma_m\|$, so $\|\gamma_m\| \le \lambda_k(\Psi_m)^{-1}\|\beta_m\|$, which for all large enough m is bounded by, say, $2\|\beta\|\lambda_k(\Psi)^{-1} < \infty$.

3 Additional details

The objective function in Section 3.1 is

$$-\log |\Omega| + n^{-1} \operatorname{tr} \{ (Y - XL\gamma)^{\mathsf{T}} (Y - XL\gamma)\Omega \} + \log |\tau (I_p + LL^{\mathsf{T}})| + \tau^{-1} \operatorname{tr} \{ S_X (I_p + LL^{\mathsf{T}})^{-1} \}.$$

Differentiating with respect to γ , Ω , and τ and setting those derivatives to zero gives

$$\log |Y^{\mathsf{T}}Q_{XL}Y/n| + \operatorname{tr}(I_r) + \log [\operatorname{tr}\{S_X(I_p + LL^{\mathsf{T}})^{-1}\}] + \log |I_p + LL^{\mathsf{T}}| + 1.$$

We derive the gradient of H_n assuming its argument L is an unconstrained matrix; the gradient under the restriction that $L_{i,j} = 0$ for j > i is obtained by setting the corresponding elements of the unconstrained gradient to zero. The differential of $Q_{XL} = I_n - XL(L^{\mathsf{T}}X^{\mathsf{T}}XL)^{-1}L^{\mathsf{T}}X^{\mathsf{T}}$ is

$$\begin{split} dQ_{XL} &= -X(dL)(L^\mathsf{T} X^\mathsf{T} X L)^{-1} L^\mathsf{T} X^\mathsf{T} \\ &+ X L (L^\mathsf{T} X^\mathsf{T} X L)^{-1} [(dL)^\mathsf{T} X^\mathsf{T} X L + L^\mathsf{T} X^\mathsf{T} X dL] (L^\mathsf{T} X^\mathsf{T} X L)^{-1} L^\mathsf{T} X^\mathsf{T} \\ &- X L (L^\mathsf{T} X^\mathsf{T} X L)^{-1} (dL)^\mathsf{T} X^\mathsf{T}. \end{split}$$

Thus, the differential of $\log |Y^{\mathsf{T}}Q_{XL}Y|$ is, with $S = Y^{\mathsf{T}}Q_{XL}Y$,

$$\begin{split} d\log|Y^\mathsf{T}Q_{XL}Y| &= -\operatorname{tr}\left[S^{-1}Y^\mathsf{T}X(dL)(L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}Y\right] \\ &+ \operatorname{tr}\left[S^{-1}Y^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}[(dL)^\mathsf{T}X^\mathsf{T}XL + L^\mathsf{T}X^\mathsf{T}XdL](L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}Y\right] \\ &- \operatorname{tr}\left[S^{-1}Y^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}(dL)^\mathsf{T}X^\mathsf{T}Y\right] \\ &= -\operatorname{tr}\left[(L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}YS^{-1}Y^\mathsf{T}XdL\right] \\ &+ \operatorname{tr}\left[(dL)^\mathsf{T}X^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}YS^{-1}Y^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}\right] \\ &+ \operatorname{tr}\left[(L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}YS^{-1}Y^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}L^\mathsf{T}X^\mathsf{T}XdL\right] \\ &- \operatorname{tr}\left[(dL)^\mathsf{T}X^\mathsf{T}YS^{-1}Y^\mathsf{T}XL(L^\mathsf{T}X^\mathsf{T}XL)^{-1}\right] \,. \end{split}$$

Thus, $\nabla \log |Y^{\mathsf{T}} Q_{XL} Y|$ is

$$\nabla \log |Y^{\mathsf{T}}Q_{XL}Y| = -2X^{\mathsf{T}}YS^{-1}Y^{\mathsf{T}}XL(L^{\mathsf{T}}X^{\mathsf{T}}XL)^{-1} + 2X^{\mathsf{T}}XL(L^{\mathsf{T}}X^{\mathsf{T}}XL)^{-1}L^{\mathsf{T}}X^{\mathsf{T}}YS^{-1}Y^{\mathsf{T}}XL(L^{\mathsf{T}}X^{\mathsf{T}}XL)^{-1}$$

Finally,

$$\nabla \log |I_p + LL^\mathsf{T}| = 2(I_p + LL^\mathsf{T})^{-1}L,$$

and

$$\nabla \log \operatorname{tr} \left[X^{\mathsf{T}} X (I_p + L L^{\mathsf{T}})^{-1} \right] = -\frac{2}{\operatorname{tr} \left[X^{\mathsf{T}} X (I_p + L L^{\mathsf{T}})^{-1} \right]} (I_p + L L^{\mathsf{T}})^{-1} X^{\mathsf{T}} X (I_p + L L^{\mathsf{T}})^{-1} L.$$

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