Robust Causal Estimation in the Large-Sample Limit without Strict Faithfulness

Ioan Gabriel Bucur **Tom Claassen** **Tom Heskes**
Radboud University Nijmegen

Appendix A Recovering B and V from $\hat{\mathbf{\Sigma}}$

$$\mathbf{\Sigma} = \mathbf{V}^{\frac{1}{2}}(\mathbf{I} - \tilde{\mathbf{B}})^{-1}(\mathbf{I} + \tilde{\mathbf{C}}\tilde{\mathbf{C}}^T)(\mathbf{I} - \tilde{\mathbf{B}})^{-T}\mathbf{V}^{\frac{1}{2}} \, . \tag{1}$$

We propose a procedure to recover the parameters over the observed variables $(\mathbf{B}, \mathbf{V})$ from Equation 1 when given the covariance matrix $\hat{\mathbf{\Sigma}}$ and the structural coefficients $\mathbf{C}$.

The procedure is as follows:

1. $\mathbf{Q} = \text{chol}(\hat{\mathbf{\Sigma}})$
2. $\mathbf{L} = \text{chol}(\mathbf{I} + \tilde{\mathbf{C}}\tilde{\mathbf{C}}^T)$
3. After plugging in the Cholesky decompositions into Equation 1, we obtain:
$$\mathbf{Q} = \mathbf{V}^{\frac{1}{2}}(\mathbf{I} - \tilde{\mathbf{B}})^{-1}\mathbf{L} \implies \mathbf{V}^{\frac{1}{2}}(\mathbf{I} - \tilde{\mathbf{B}})^{-1} = \mathbf{Q}\mathbf{L}^{-1}$$
4. Since $(\mathbf{I} - \tilde{\mathbf{B}})^{-1}$ is a term with ones on the diagonal, it follows that $\mathbf{V}^{\frac{1}{2}} = \text{diag}(\mathbf{Q}\mathbf{L}^{-1})$.
5. Finally, we recover $\tilde{\mathbf{B}} = \mathbf{I} - \mathbf{L}\mathbf{Q}^{-1}\mathbf{V}^{\frac{1}{2}}$ and $\mathbf{B} = \mathbf{V}^{\frac{1}{2}}\tilde{\mathbf{B}}\mathbf{V}^{-\frac{1}{2}} = \mathbf{I} - \mathbf{V}^{\frac{1}{2}}\mathbf{L}\mathbf{Q}^{-1}$.

Appendix B Hessian

Here we compute the Hessian matrix of the log-likelihood per data point w.r.t. $\mathbf{\Theta} = (\mathbf{B}, \mathbf{V})$ evaluated at the maximum likelihood solution. With covariance matrix $\mathbf{\Sigma}$ and $\mathbf{K} = \mathbf{\Sigma}^{-1}$, we have:

$$\frac{1}{N}\partial^2_{\alpha,\beta} \log \mathcal{L} = \mathbf{H}_{\alpha,\beta} = -\frac{1}{2}\sum_{i,j,k,l} \mathbf{\Sigma}_{ik}\mathbf{\Sigma}_{jl}\partial_\alpha \mathbf{K}_{ij}\partial_\beta \mathbf{K}_{kl} \, .$$

With $\mathbf{\Delta} \equiv \mathbf{I} - \tilde{\mathbf{B}}$ and $\mathbf{\Omega} \equiv \mathbf{I} + \tilde{\mathbf{C}}\tilde{\mathbf{C}}^T$, we can write

$$\mathbf{\Sigma}_{ij} = \sqrt{v_i v_j}(\mathbf{\Delta}^{-1}\mathbf{\Omega}\mathbf{\Delta}^{-T})_{ij} \equiv \sqrt{v_i v_j}\tilde{\mathbf{\Sigma}}_{ij}$$

and

$$\mathbf{K}_{ij} = \frac{1}{\sqrt{v_i v_j}}(\mathbf{\Delta}^T\mathbf{\Omega}^{-1}\mathbf{\Delta})_{ij} \equiv \frac{1}{\sqrt{v_i v_j}}\tilde{\mathbf{K}}_{ij} \, ,$$

so that

$$\frac{\partial \mathbf{K}_{ij}}{\partial b_{pq}} = -\frac{1}{\sqrt{v_i v_j}}\left[\mathbf{Z}_{pi}\delta_{qj} + \mathbf{Z}_{pj}\delta_{qi}\right] \, ,$$

with $\mathbf{Z} \equiv \mathbf{\Omega}^{-1}\mathbf{\Delta} = \mathbf{\Delta}^{-T}\tilde{\mathbf{K}}$, and

$$\frac{\partial \mathbf{K}_{ij}}{\partial v_r} = -\frac{\mathbf{K}_{ij}}{2v_r}\left[\delta_{ri} + \delta_{rj}\right] \, .$$

Some bookkeeping yields

$$-\frac{\partial^2 \log \mathcal{L}}{\partial b_{pq}\partial b_{rs}} = \tilde{\mathbf{\Sigma}}_{qs}(\mathbf{\Omega}^{-1})_{pr} + (\mathbf{\Delta}^{-1})_{sp}(\mathbf{\Delta}^{-1})_{qr} \, ,$$

and

$$-\frac{\partial^2 \log \mathcal{L}}{\partial v_r \partial v_s} = \frac{1}{4 v_r v_s}\left[\delta_{rs} + \tilde{\mathbf{\Sigma}}_{rs}\tilde{\mathbf{K}}_{rs}\right] \, ,$$

and

$$-\frac{\partial^2 \log \mathcal{L}}{\partial b_{pq}\partial v_r} = \frac{1}{2v_r}\left[\tilde{\mathbf{\Sigma}}_{rq}(\tilde{\mathbf{K}}\mathbf{\Delta}^{-1})_{rp} + \delta_{rq}(\mathbf{\Delta}^{-1})_{rp}\right] \, .$$

Or, in terms of $\mathbf{Q} = \text{chol}(\hat{\mathbf{\Sigma}})$ and $\mathbf{L} = \text{chol}(\mathbf{I} + \tilde{\mathbf{C}}\tilde{\mathbf{C}}^T)$,

$$\begin{aligned}-\frac{\partial^2 \log \mathcal{L}}{\partial b_{pq}\partial b_{rs}} =& \frac{1}{\sqrt{v_q v_s}}\big[(\mathbf{Q}\mathbf{Q}^T)_{qs}(\mathbf{L}^{-T}\mathbf{L}^{-1})_{pr} \\ &+ (\mathbf{Q}\mathbf{L}^{-1})_{sp}(\mathbf{Q}\mathbf{L}^{-1})_{qr}\big] \, ,\end{aligned}$$

and

$$-\frac{\partial^2 \log \mathcal{L}}{\partial v_r \partial v_s} = \frac{1}{4 v_r v_s}\left[\delta_{rs} + (\mathbf{Q}\mathbf{Q}^T)_{rs}(\mathbf{Q}^{-T}\mathbf{Q}^{-1})_{rs}\right] \, ,$$

and

$$-\frac{\partial^2 \log \mathcal{L}}{\partial b_{pq}\partial v_r} = \frac{1}{2v_r\sqrt{v_q}}\left[(\mathbf{Q}\mathbf{Q}^T)_{rq}(\mathbf{Q}^{-T}\mathbf{L}^{-1})_{rp} + \delta_{rq}(\mathbf{Q}\mathbf{L}^{-1})_{rp}\right] .$$