Matrix Formulas That Is Usefull In Least Square Analysis

(You could always swap indexes properly to get similar results)

1 Difference of Quadratic Forms, Inverse Matrices and Solution of Linear Systems

For invertable $(n_1 + n_2 + n_3) \times (n_1 + n_2 + n_3)$ matrix R (no need symmetric)

$$R = \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{bmatrix}^{-1} = \begin{bmatrix} Q^{(xx)} & Q^{(xy)} & Q^{(xz)} \\ Q^{(yx)} & Q^{(yy)} & Q^{(yz)} \\ Q^{(zx)} & Q^{(zy)} & Q^{(zz)} \end{bmatrix}$$
(1)

For any $\begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix} (n_4 \times (n_1 + n_2 + n_3) \text{ matrix})$

Define

(replace transpose \cdot^T to conjugate transpose \cdot^H for matrix with complex entries)

$$\begin{aligned} \operatorname{SS}_{R[x,z]} &= \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{array} \right] \left[\begin{array}{ccc} R^{(xx)} & R^{(xz)} \\ R^{(zx)} & R^{(zz)} \end{array} \right]^{-1} \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{array} \right]^{T} \\ \operatorname{SS}_{R[x,y,z]} &= \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} & \vec{r}^{(x|z)} \end{array} \right] \left[\begin{array}{ccc} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{array} \right]^{-1} \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{array} \right]^{T} \\ &\left[\begin{array}{ccc} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{array} \right] \left[\begin{array}{ccc} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{array} \right] = \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{array} \right] \\ &\left[\begin{array}{ccc} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{array} \right] \left[\begin{array}{ccc} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(yz)} & R^{(yz)} & R^{(zz)} \end{array} \right]^{T} = \left[\begin{array}{ccc} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{array} \right] \end{aligned}$$

Then the difference of the quadratic form is

(Assume the inverse matries in the expressions are all valid, pseudo-inverse could also work)

$$SS_{R[x,y,z]} - SS_{R[x,z]} = \vec{a}^{(12)} \left(Q^{(yy)} \right)^{-1} \left(\vec{a}_T^{(12)} \right)^T$$
(2)

The $(Q^{(yy)})^{-1}$ might be expressed as (Swap index x and z will give another expression)

$$\left(Q^{(yy)}\right)^{-1} = R^{(yy)} - R^{(yx)} \left(R^{(xx)}\right)^{-1} R^{(xy)}
- \left(R^{(yz)} - R^{(yx)} \left(R^{(xx)}\right)^{-1} R^{(xz)}\right) \left(R^{(zz)} - R^{(zx)} \left(R^{(xx)}\right)^{-1} R^{(xz)}\right)^{-1} \left(R^{(zy)} - R^{(zx)} \left(R^{(xx)}\right)^{-1} R^{(xy)}\right)
- \left(R^{(yz)} - R^{(yx)} \left(R^{(xx)}\right)^{-1} R^{(xz)}\right) \left(R^{(zz)} - R^{(zx)} \left(R^{(xx)}\right)^{-1} R^{(xz)}\right)^{-1} \left(R^{(zy)} - R^{(zx)} \left(R^{(xx)}\right)^{-1} R^{(xy)}\right)
- \left(R^{(yz)} - R^{(yx)} \left(R^{(xx)}\right)^{-1} R^{(xz)}\right) \left(R^{(xz)} - R^{(xz)} \left(R^{(xx)}\right)^{-1} R^{(xy)}\right)^{-1} R^{(xy)} \right)$$

The inverse matrices have relation

$$\begin{bmatrix} P^{(xx)} & P^{(xy)} \\ P^{(yx)} & P^{(yy)} \end{bmatrix} \triangleq \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1} = \begin{bmatrix} Q^{(xx)} & Q^{(xy)} \\ Q^{(yx)} & Q^{(yy)} \end{bmatrix} - \begin{bmatrix} Q^{(xz)} \\ Q^{(yz)} \end{bmatrix} \begin{pmatrix} Q^{(zz)} \end{pmatrix}^{-1} \begin{bmatrix} Q^{(zx)} & Q^{(zy)} \end{bmatrix}$$
(4)

$$\left(Q^{(zz)}\right)^{-1} = R^{(zz)} - \begin{bmatrix} R^{(zx)} & R^{(zy)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1} \begin{bmatrix} R^{(xz)} \\ R^{(yz)} \end{bmatrix}$$

If we solve

$$\left[\begin{array}{cc} \vec{b}^{(11)} & \vec{b}^{(12)} \end{array} \right] \left[\begin{array}{cc} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{array} \right] = \left[\begin{array}{cc} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} \end{array} \right]$$

Then there is relation

(There are 6 of these relations)

$$b^{(12)} = a^{(12)} - a^{(13)} \left(Q^{(zz)} \right)^{-1} Q^{(zy)} \tag{5}$$

$$a^{(12)} \left(I - \left(Q^{(yy)} \right)^{-1} Q^{(yz)} \left(Q^{(zz)} \right)^{-1} Q^{(zy)} \right) = b^{(12)} + b^{(13)}_{[xz]} \left(Q^{(zz)} \right)^{-1} Q^{(zy)}$$
 (6)

or (due to Eq.(4))

$$a^{(12)} \left(Q^{(yy)} \right)^{-1} P^{(yy)} = b^{(12)} + b^{(13)} \left(Q^{(zz)} \right)^{-1} Q^{(zy)}$$

Also

$$\vec{b}^{(11)} = \vec{a}^{(11)} - a^{(13)} \left(Q^{(zz)} \right)^{-1} Q^{(zx)}$$

In matrix form

$$\left[\vec{b}^{(11)} \quad \vec{b}^{(12)} \right] = \left[\vec{a}^{(11)} \quad \vec{a}^{(12)} \right] - a^{(13)} \left(Q^{(zz)} \right)^{-1} \left[Q^{(zx)} \quad Q^{(zy)} \right]$$

2 Appendix: Formulas Used to Derive Above Results

2.1 Binomial inverse theorem

$$(A + UBV)^{-1} = A^{-1} - A^{-1}UB (B + BVA^{-1}UB)^{-1} BVA^{-1}$$

Specially

$$(A - BD^{-1}C)^{-1} = A^{-1} + A^{-1}B(D - CA^{-1}B)CA^{-1}$$

2.2 Inverse of $(n_1 + n_2) \times (n_1 + n_2)$ matrix

(Assume the inverse matries in the expressions are all valid)

Use row elimination, get

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^{-1} = \begin{bmatrix} (a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1} & -(a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1}a_{12}a_{22}^{-1} \\ -(a_{22} - a_{21}a_{11}^{-1}a_{12})^{-1}a_{21}a_{11}^{-1} & (a_{22} - a_{21}a_{11}^{-1}a_{12})^{-1} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11}^{-1} + a_{11}^{-1}a_{12} (a_{22} - a_{21}a_{11}^{-1}a_{12})^{-1} a_{21}a_{11}^{-1} & -a_{11}^{-1}a_{12} (a_{22} - a_{21}a_{11}^{-1}a_{12})^{-1} \\ -a_{22}^{-1}a_{21} (a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1} & a_{22}^{-1} + a_{21}^{-1}a_{21} (a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1} a_{12}a_{22}^{-1} \end{bmatrix}$$

2.2.1 Known inverse matrix, get inverse of sub matrix

Known

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^{-1} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

Then a_{22}^{-1} can get from

$$a_{22}^{-1} = b_{22} - b_{21} (b_{11})^{-1} b_{12}$$

2.3 Inverse of $(n_1 + n_2 + n_3) \times (n_1 + n_2 + n_3)$ maxtrix

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}^{-1} = UD^{-1}L$$

$$U = \begin{bmatrix} I & -a_{11}^{-1}a_{12} & a_{11}^{-1}a_{12} \left(a_{22} - a_{21}a_{11}^{-1}a_{12}\right)^{-1} \left(a_{23} - a_{21}a_{11}^{-1}a_{13}\right) - a_{11}^{-1}a_{13} \\ O & I & -\left(a_{22} - a_{21}a_{11}^{-1}a_{12}\right)^{-1} \left(a_{23} - a_{21}a_{11}^{-1}a_{13}\right) \\ O & O & I \end{bmatrix}$$

$$L = \begin{bmatrix} I & O & O \\ -a_{21}a_{11}^{-1} & I & O & O \\ \left(a_{32} - a_{31}a_{11}^{-1}a_{12}\right)\left(a_{22} - a_{21}a_{11}^{-1}a_{12}\right)^{-1}a_{21}a_{11}^{-1} - a_{31}a_{11}^{-1} & -\left(a_{32} - a_{31}a_{11}^{-1}a_{12}\right)\left(a_{22} - a_{21}a_{11}^{-1}a_{12}\right)^{-1} & I \end{bmatrix}$$

$$D = \begin{bmatrix} a_{11} & O & O & O \\ O & a_{22} - a_{21}a_{11}^{-1}a_{12} & O & O \\ O & O & a_{33} - a_{31}a_{11}^{-1}a_{13} - \left(a_{32} - a_{31}a_{11}^{-1}a_{12}\right)\left(a_{22} - a_{21}a_{11}^{-1}a_{12}\right)^{-1}\left(a_{23} - a_{21}a_{11}^{-1}a_{13}\right) \end{bmatrix}$$

Note:

$$\begin{bmatrix} 1 & a_{12} & a_{13} \\ 0 & 1 & a_{23} \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} b_1 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & b_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ c_{21} & 1 & 0 \\ c_{31} & c_{32} & 1 \end{bmatrix} = \begin{bmatrix} b_1 + a_{12}b_2c_{21} + a_{13}b_3c_{31} & a_{12}b_2 + a_{13}b_3c_{32} & a_{13}b_3 \\ b_2c_{21} + a_{23}b_3c_{31} & b_2 + a_{23}b_3c_{32} & a_{23}b_3 \\ b_3c_{31} & b_3c_{32} & b_3 \end{bmatrix}$$