# Matrix Formulas That Is Useful In Least Square Analysis

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

# 1 Difference of Quadratic Forms - The Regression Improvement by Introducing a Variate

For invertible  $(n_1 + n_2 + n_3) \times (n_1 + n_2 + n_3)$  matrix R (no need symmetric), define Q

$$Q = \begin{bmatrix} Q^{(xx)} & Q^{(xy)} & Q^{(xz)} \\ Q^{(yx)} & Q^{(yy)} & Q^{(yz)} \\ Q^{(zx)} & Q^{(zy)} & Q^{(zz)} \end{bmatrix} = R^{-1} = \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{bmatrix}^{-1}.$$
 (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 quadratic forms  $SS_{R[x,z]}$  and  $SS_{R[x,y,z]}$ , solutions  $\begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{bmatrix}$  and  $\begin{bmatrix} \vec{a}^{(11)}_T & \vec{a}^{(12)}_T & \vec{a}^{(13)}_T \end{bmatrix}$  as (replace transpose  $\cdot^T$  to conjugate transpose  $\cdot^H$  for matrix with complex entries)

$$SS_{R[x,z]} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xz)} \\ R^{(zx)} & R^{(zz)} \end{bmatrix}^{-1} \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{bmatrix}^{T},$$

$$SS_{R[x,y,z]} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} \end{bmatrix} \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix}^{T},$$

$$\begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} \end{bmatrix} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix},$$

$$\begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \end{bmatrix}^{T} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix}.$$

Then the difference of the quadratic forms is

(Assume the inverse matries in the expressions are all valid. Pseudo-inverse might 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 in R blocks as (Swap index x and z will give another expression)

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

# 2 Difference of Solutions - The Correction to Coefficients When Introducing a Variate

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)

$$b^{(12)} = a^{(12)} - a^{(13)} \left( Q^{(zz)} \right)^{-1} Q^{(zy)} \tag{4}$$

$$a^{(12)} \left( I - \left( Q^{(yy)} \right)^{-1} Q^{(yz)} \left( Q^{(zz)} \right)^{-1} Q^{(zy)} \right) = b^{(12)} + b_{[xz]}^{(13)} \left( Q^{(zz)} \right)^{-1} Q^{(zy)}$$
 (5)

Define P

$$P = \begin{bmatrix} P^{(xx)} & P^{(xy)} \\ P^{(yx)} & P^{(yy)} \end{bmatrix} \triangleq \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1}.$$

There are relations between P, Q and R

$$P = \begin{bmatrix} Q^{(xx)} & Q^{(xy)} \\ Q^{(yx)} & Q^{(yy)} \end{bmatrix} - \begin{bmatrix} Q^{(xz)} \\ Q^{(yz)} \end{bmatrix} (Q^{(zz)})^{-1} \begin{bmatrix} Q^{(zx)} & Q^{(zy)} \end{bmatrix}$$
(6)

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

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

$$= -\left[ R^{(zx)} \quad R^{(zy)} \right] \left[ P^{(xy)} \right]$$

$$I - \left(Q^{(yy)}\right)^{-1} Q^{(yz)} \left(Q^{(zz)}\right)^{-1} Q^{(zy)} = \left(Q^{(yy)}\right)^{-1} P^{(yy)}$$

Sometimes  $\vec{b}^{(11)}$  is also wanted

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

In matrix form

$$\begin{bmatrix} \vec{b}^{(11)} & \vec{b}^{(12)} \\ \vec{b}^{(21)} & \vec{b}^{(22)} \end{bmatrix} = \begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} \\ \vec{a}^{(21)} & \vec{a}^{(22)} \end{bmatrix} - \begin{bmatrix} a^{(13)} \\ a^{(23)} \end{bmatrix} \left( Q^{(zz)} \right)^{-1} \left[ Q^{(zx)} & Q^{(zy)} \right]$$

$$\begin{bmatrix} \vec{b}^{(11)} & \vec{b}^{(12)} \\ \vec{b}^{(21)} & \vec{b}^{(22)} \end{bmatrix} = \begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} \\ \vec{a}^{(21)} & \vec{a}^{(22)} \end{bmatrix} + \begin{bmatrix} a^{(13)} \\ a^{(23)} \end{bmatrix} \left[ R^{(zx)} & R^{(zy)} \right] \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1}$$

$$\begin{bmatrix} a^{(13)} \\ a^{(23)} \end{bmatrix} \left[ R^{(zx)} & R^{(zy)} \right] = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} \\ \vec{r}^{(y|x)} & \vec{r}^{(y|y)} \end{bmatrix} - \begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} \\ \vec{a}^{(21)} & \vec{a}^{(22)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}$$

$$\begin{bmatrix} a^{(13)} \\ a^{(23)} \end{bmatrix} \left[ R^{(zx)} & R^{(zy)} \right] \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} \\ \vec{r}^{(y|x)} & \vec{r}^{(y|y)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} \\ R^{(yx)} & R^{(yy)} \end{bmatrix}^{-1} - \begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} \\ \vec{a}^{(21)} & \vec{a}^{(22)} \end{bmatrix}$$

## 3 Relation to Linear Regression and Granger Causality For Time Series

Assume  $E(x_t) = E(y_t) = E(y_t) = O$ , as usual, let's do a 3-var AR of order m:

$$\begin{cases} x_{t} = \sum_{j=1}^{m} a_{j}^{(11)} x_{t-j} + \sum_{j=1}^{m} a_{j}^{(12)} y_{t-j} + \sum_{j=1}^{m} a_{j}^{(13)} z_{t-j} + \epsilon_{t}^{(1)} & \text{(a)} \\ y_{t} = \sum_{j=1}^{m} a_{j}^{(21)} x_{t-j} + \sum_{j=1}^{m} a_{j}^{(22)} y_{t-j} + \sum_{j=1}^{m} a_{j}^{(23)} z_{t-j} + \epsilon_{t}^{(2)} & \text{(b)} \\ z_{t} = \sum_{j=1}^{m} a_{j}^{(31)} x_{t-j} + \sum_{j=1}^{m} a_{j}^{(32)} y_{t-j} + \sum_{j=1}^{m} a_{j}^{(33)} z_{t-j} + \epsilon_{t}^{(3)} & \text{(c)} \end{cases}$$

The least square solution for  $\vec{a}^{(11)}$   $\vec{a}^{(12)}$   $\vec{a}^{(13)}$  in min var  $\epsilon_t^{(1)}$   $(E(\epsilon_t^{(u)}x_{t-k}^{(v)T})=0, \ \forall k=1\ldots m)$  satisfies

$$\begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{bmatrix} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix},$$
 (9)

where (here  $\mathbb{E}$  can be expectation operator or  $\frac{1}{L}\sum_{t=1}^{L}$ )

$$\begin{split} \vec{a}^{(uv)} &= \left(a_j^{(uv)}\right)_{j=1...m}^{\text{row}}, \ (u,v \in \{1,2,3\}), \\ R^{(uv)} &= \left(\mathbb{E}(x_{t-j}^{(u)}x_{t-k}^{(v)T})\right)_{j,k=1...m}, \ (u,v \in \{x,y,z\}), \\ \vec{r}^{(u|v)} &= \left(\mathbb{E}(x_t^{(u)}x_{t-k}^{(v)T})\right)_{k=1...m}^{\text{row}}, \ (u,v \in \{x,y,z\}). \end{split}$$

 $(a_j)_{j=1...m}^{\text{row}}$  means tiling  $a_j$  in a row:  $(a_j)_{j=1...m}^{\text{row}} = \begin{bmatrix} a_1 & \cdots & a_m \end{bmatrix}$ , and  $(a_{jk})_{j,k=1...m}$  is a matrix which its j row k column is  $a_{jk}$ .

The residual variance of Eq. (8) can be obtained by

$$var(x_t) = \vec{a}^{(11)} \vec{r}^{(x|x)T} + \vec{a}^{(12)} \vec{r}^{(x|y)T} + \vec{a}^{(13)} \vec{r}^{(x|z)T} + var(\epsilon_t^{(1)})$$

or

$$\operatorname{var}(\epsilon_t^{(1)}) = \operatorname{var}(x_t) - \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & R^{(xz)} \\ R^{(yx)} & R^{(yy)} & R^{(yz)} \\ R^{(zx)} & R^{(zy)} & R^{(zz)} \end{bmatrix}^{-1} \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & \vec{r}^{(x|z)} \end{bmatrix}^{T}.$$
(10)

Similarly for least square min var  $\epsilon_t^{(1|3)}$  in (regression of x without y)

$$x_{t} = \sum_{j=1}^{m} c_{j}^{(11)} x_{t-j} + \sum_{j=1}^{m} c_{j}^{(13)} z_{t-j} + \epsilon_{t}^{(1|3)},$$

$$(11)$$

that is

$$\operatorname{var}(\epsilon_t^{(1|3)}) = \operatorname{var}(x_t) - \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xz)} \\ R^{(zx)} & R^{(zz)} \end{bmatrix}^{-1} \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|z)} \end{bmatrix}^T.$$
(12)

Conditional Granger causality  $F_{y\to x|z}$  is defined as

$$F_{y\to x|z} = \ln \frac{\operatorname{var}(\epsilon_t^{(1|3)})}{\operatorname{var}(\epsilon_t^{(1)})} = \ln \left( 1 + \frac{\operatorname{var}(\epsilon_t^{(1|3)}) - \operatorname{var}(\epsilon_t^{(1)})}{\operatorname{var}(\epsilon_t^{(1)})} \right). \tag{13}$$

With help of Eq.(2), we get

$$F_{y \to x|z} = \ln \left( 1 + \frac{\vec{a}^{(12)} \left( Q^{(yy)} \right)^{-1} \left( \vec{a}^{(12)} \right)^T}{\operatorname{var}(\epsilon_t^{(1)})} \right)$$
(14)

#### 3.1 Conditional GC and pairwise GC

Due to expression Eq.(14), the pairwise GC can be expressed as

$$F_{y \to x|z} = \ln \left( 1 + \frac{\vec{b}^{(12)} \left( P^{(yy)} \right)^{-1} \left( \vec{b}^{(12)} \right)^{T}}{\operatorname{var}(\epsilon_t^{(1|2)})} \right)$$
(15)

where (recall Eq.(4) (2) and (6))

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

$$\operatorname{var}(\epsilon_t^{(1|2)}) = \operatorname{var}(\epsilon_t^{(1)}) + \vec{a}^{(13)} \left( Q^{(zz)} \right)^{-1} \left( \vec{a}^{(13)} \right)^T,$$

$$P^{(yy)} = Q^{(yy)} - Q^{(yz)} \left( Q^{(zz)} \right)^{-1} Q^{(zy)}.$$

The related regression is

$$\begin{cases} x_{t} = \sum_{j=1}^{m} b_{j}^{(11)} x_{t-j} + \sum_{j=1}^{m} b_{j}^{(12)} y_{t-j} + \epsilon_{t}^{(1|2)} & \text{(a)} \\ y_{t} = \sum_{j=1}^{m} b_{j}^{(21)} x_{t-j} + \sum_{j=1}^{m} b_{j}^{(22)} y_{t-j} + \epsilon_{t}^{(2|1)} & \text{(b)} \end{cases}$$

$$(16)$$

From Eq.(15), one can know that the pairwise GC can be expressed by joint regression coefficients and residuals, and Q matrix.

## 3.2 Application in Frequency Domain Conditional GC

The equation is

$$\begin{cases} x_{t} = \sum_{j=1}^{m} c_{j}^{(11)} x_{t-j} + \sum_{j=1}^{m} c_{j}^{(13)} z_{t-j} + \epsilon_{t}^{(1|3)} & \text{(a)} \\ z_{t} = \sum_{j=1}^{m} c_{j}^{(31)} x_{t-j} + \sum_{j=1}^{m} c_{j}^{(33)} z_{t-j} + \epsilon_{t}^{(3|1)} & \text{(b)} \end{cases}$$

$$(17)$$

Similarly to Eq. (7), we have

$$\left[ \begin{array}{cc} \vec{c}^{(11)} & \vec{c}^{(13)} \\ \vec{c}^{(31)} & \vec{c}^{(33)} \end{array} \right] = \left[ \begin{array}{cc} \vec{a}^{(11)} & \vec{a}^{(13)} \\ \vec{a}^{(31)} & \vec{a}^{(33)} \end{array} \right] - \left[ \begin{array}{cc} a^{(12)} \\ a^{(32)} \end{array} \right] \left( Q^{(yy)} \right)^{-1} \left[ \begin{array}{cc} Q^{(yx)} & Q^{(yz)} \end{array} \right]$$

And with help of Eq. (2)

$$\operatorname{var}(\epsilon_t^{(1,3)}) - \operatorname{var}(\epsilon_t^{(1,3|2)}) = \left[ \begin{array}{c} \vec{a}^{(12)} \\ \vec{a}^{(32)} \end{array} \right] \left( Q^{(yy)} \right)^{-1} \left[ \begin{array}{c} \vec{a}^{(12)} \\ \vec{a}^{(32)} \end{array} \right]^T$$

#### 3.3 Approximation of GC

Due to Taylor expansion, we have approximation

$$\ln(1+x) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1} x^k}{k} \approx x, \quad \text{for } x \ll 1.$$
 (18)

From Eq. (13) get

$$F_{y \to x|z} \approx \frac{\vec{a}^{(12)} \left(Q^{(yy)}\right)^{-1} \left(\vec{a}^{(12)}\right)^{T}}{\operatorname{var}(\epsilon_{+}^{(1)})}.$$
(19)

Or, one might choose a different definition of "GC":

$$F_{y \to x|z}^{\text{(linear)}} = \exp(F_{y \to x|z}) - 1 = \frac{\vec{a}^{(12)} \left(Q^{(yy)}\right)^{-1} \left(\vec{a}^{(12)}\right)^{T}}{\operatorname{var}(\epsilon_t^{(1)})}$$
(20)

For whitened signal and a weak GC, we might even get a reasonable approximation

$$F_{y \to x|z} \approx \frac{\text{var}(\epsilon_t^{(2)})}{\text{var}(\epsilon_t^{(1)})} \vec{a}^{(12)} \vec{a}^{(12)T}$$
 (21)

#### 3.4 Partial correlation coefficient (seems useless)

$$\begin{bmatrix} \vec{a}^{(11)} & \vec{a}^{(12)} & \vec{a}^{(13)} \end{bmatrix} \begin{bmatrix} R^{(xx)} & R^{(xy)} & O \\ R^{(yx)} & R^{(yy)} & O \\ O & O & R^{(zz)} \end{bmatrix} = \begin{bmatrix} \vec{r}^{(x|x)} & \vec{r}^{(x|y)} & 0 \end{bmatrix}$$

$$\begin{pmatrix} Q^{(yy)} \end{pmatrix}^{-1} = R^{(yy)} - R^{(yx)} \begin{pmatrix} R^{(xx)} \end{pmatrix}^{-1} R^{(xy)}$$

$$x'_t = x_t - \alpha Y$$

What if z is totally whitened? i.e.

$$R^{(zz)} = I$$

not verified

$$c^{(33)} = a^{(33)} - \begin{bmatrix} a^{(31)} & a^{(32)} \end{bmatrix} \begin{bmatrix} Q^{(xx)} & Q^{(xy)} \\ Q^{(yx)} & Q^{(yy)} \end{bmatrix}^{-1} \begin{bmatrix} Q^{(xz)} \\ Q^{(yz)} \end{bmatrix}$$

## 4 Spectral Approximation

The  $Q^{(uv)}$  and  $R^{(uv)}$  can be approximated by circulant matrix. Hence, their related operations can be approximated by operations of spectrum.

#### 4.1 Definitions

The Fourier transform used here is (Discrete-time Fourier transform)

$$\mathscr{F}_{\text{DTFT}}\left[\left\{x_j\right\}_{j\in\mathbb{Z}}\right] = \sum_{j=-\infty}^{\infty} x_j e^{-ijw},\tag{22}$$

$$\mathscr{F}_{\mathrm{DTFT}}^{-1}\left[f(w)\right] = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(w)e^{\mathrm{i}jw} \mathrm{d}w. \tag{23}$$

Note in Eq. (22) and (23) both  $x_j$  and f(w) can be matrix. And the convolution theorem still works. The frequency domain quantities we will use include

$$\hat{a} = \mathscr{F}_{DTFT} [\{a_j\}_{j=0..m}], \quad \hat{b} = \mathscr{F}_{DTFT} [\{b_j\}_{j=0..m}], \quad \hat{c} = \mathscr{F}_{DTFT} [\{c_j\}_{j=0..m}],$$

$$\hat{Q} = \hat{a}^H \Sigma^{-1} \hat{a}$$

where  $\Sigma = \text{var}\left(\begin{bmatrix} \epsilon_t^{(1)T} & \epsilon_t^{(2)T} & \epsilon_t^{(3)T} \end{bmatrix}^T\right)$  is the residual variance.

We use  $\hat{Q}_{uv}$  to denote the *u*-th row *v*-th column block of  $\hat{Q}$ , and similarly  $\hat{a}^{(uv)}$  to  $\hat{a}$ ,  $a_j^{(uv)}$  to  $a_j$ , (and also b, c, see Eq. (16) and (17)). Also note the time lag for coefficients are starting from 0,  $a_0^{(uv)} = \delta_{uv}I$ . The block parts of  $\hat{Q}$ , explicitly write down is:

$$\hat{Q}_{uv} = \sum_{j,k=1}^{3} (\hat{a}^{(ju)})^{H} (\Sigma^{-1})^{(jk)} \hat{a}^{(kv)}$$

where  $(\Sigma^{-1})^{(jk)}$  means the j-th row k-th column block of  $\Sigma^{-1}$ .

Sometimes we need the operator  $[\cdot]_+$  to extract the positive time part (work in frequency domain):

$$[f(w)]_{+} = \mathscr{F}_{\text{DTFT}} \left[ u(t) \mathscr{F}_{\text{DTFT}}^{-1} \left[ f(w), t \right](t), w \right]$$
$$u(t) = \begin{cases} 1 & t > 0 \\ 0 & t \le 0 \end{cases}.$$

#### 4.2 The Approximations

The conditions of these approximations to work good will be discussed later. Roughly speaking, that condition is weak conditional GC.

The x-y regression coefficient formula Eq. (4) can be approximated by

$$\hat{b}^{(12)} \approx \hat{a}^{(12)} - \left[\hat{a}^{(13)}\hat{Q}_{zz}^{-1}\hat{Q}_{zy}\right]_{+}.$$
(24)

GC is

$$F_{y \to x|z} \approx F_{y \to x|z}^{\text{(linear)}} \approx \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\hat{a}^{(12)} \hat{Q}_{yy}^{-1} \left(\hat{a}^{(12)}\right)^H}{\text{var}(\epsilon_t^{(1)})} dw.$$
 (25)

See Eq.(20) for definition of  $F_{u \to r^{\dagger}r}^{(linear)}$ 

Actually the frequency domain GC can also be approximated

$$f_{y \to x|z} \approx f_{y \to x|z}^{\text{(linear)}} \approx f_{y \to x|z}^{\text{(app freq)}} = \frac{\hat{a}^{(12)} \hat{Q}_{yy}^{-1} \left(\hat{a}^{(12)}\right)^H}{\text{var}(\epsilon_t^{(1)})}.$$
 (26)

One beauty thing is that the frequency domain GC approximation Eq. (26) does not involve complicated "renormalization" operations discussed in Geweke [2] when the residual variance  $\Sigma$  is non-diagonal.

#### 4.3 Approximations Under Certain (Restricted) Conditions

#### 4.3.1 Assumptions and approximation to GC

(Assumption #1) Under the assumption that the variance of residual is blocked diagonal matrix

$$\Sigma = \operatorname{diag} \left( \left[ \begin{array}{ccc} \Sigma_{xx} & \Sigma_{yy} & \Sigma_{zz} \end{array} \right] \right)$$

We have

$$\hat{Q}_{yy} = \left(\hat{a}^{(12)}\right)^{H} \left(\Sigma^{-1}\right)^{(11)} \hat{a}^{(12)} + \left(\hat{a}^{(22)}\right)^{H} \left(\Sigma^{-1}\right)^{(22)} \hat{a}^{(22)} + \left(\hat{a}^{(32)}\right)^{H} \left(\Sigma^{-1}\right)^{(33)} \hat{a}^{(32)}$$

(Assumption #2) To further simplify, the next assumption is:  $\Sigma$  is diagonal matrix (i.e. each block is also diagonal). With this assumption, and the invariant property of GC under scalar transform to variates, we can assume  $\Sigma = I$ . This leads to

$$\hat{Q}_{yy} = \left(\hat{a}^{(12)}\right)^{H} \hat{a}^{(12)} + \left(\hat{a}^{(22)}\right)^{H} \hat{a}^{(22)} + \left(\hat{a}^{(32)}\right)^{H} \hat{a}^{(32)}, \tag{27}$$

Note the coefficients here (Eq. (27), and later this sub-section) are properly scaled to reflect the normalization of  $\Sigma = I$ :

$$a^{(uv)(\text{normalized})} = \frac{\sum^{(vv)}}{\sum^{(uu)}} a^{(uv)(\text{original})}.$$
 (28)

Under these assumptions, the expressions Eq. (26) now become more clean (When we calculate GC, x and y are scalars, so the matrix inversion become division)

$$f_{y \to x|z}^{\text{(app freq)}} = \frac{\hat{a}^{(12)} \left(\hat{a}^{(12)}\right)^{H}}{\left(\hat{a}^{(12)}\right)^{H} \hat{a}^{(12)} + \left(\hat{a}^{(22)}\right)^{H} \hat{a}^{(22)} + \left(\hat{a}^{(32)}\right)^{H} \hat{a}^{(32)}}.$$
(29)

(Assumption #3) After that, an aggressive approximation would be to drop high order terms in Eq. (29), usually (for small system and weak GC) that is  $(\hat{a}^{(12)})^H \hat{a}^{(12)}$  and  $(\hat{a}^{(32)})^H \hat{a}^{(32)}$ :

$$f_{y\to x|z}^{\text{(app freq)}} \approx \frac{\hat{a}^{(12)} \left(\hat{a}^{(12)}\right)^H}{\left(\hat{a}^{(22)}\right)^H \hat{a}^{(22)}}.$$
 (30)

Note, for system involves hundreds of neurons,  $(\hat{a}^{(32)})^H \hat{a}^{(32)}$  might not be drop.

#### 4.3.2 Comparison to exact frequency domain GC

The exact bivariate frequency domain GC is

$$\exp(f_{y\to x}) - 1 = \frac{1 - \Upsilon^2}{\left|\frac{1}{r} - \Upsilon\right|^2} = \frac{1 - \Upsilon^2}{\frac{1}{rr^H} - \frac{\Upsilon}{r^H} - \frac{\Upsilon}{r} + \Upsilon^2}$$
(31)

where  $\Upsilon = \Sigma^{(12)}$ ,  $r = \hat{a}^{(12)}/\hat{a}^{(22)}$ . In Eq. (31), normalization to residual variance Eq. (28) is applied, but none of the assumptions #1, #2 and #3 is used.

Case 1:  $\Upsilon = 0$ 

In this case,

$$\exp(f_{y\to x}) - 1 = rr^H$$

which is exactly the Eq.(30). One might also start from Eq.(29), and apply the function

$$g(f) = \frac{1}{1/f - 1}$$

to get a exact "approximation"  $\exp(f_{y\to x}) - 1 = g(f_{y\to x|z}^{\text{(app freq)}})$ .

Case 2:  $\Upsilon \neq 0$  (no instantaneous correlation)

Still, the  $f_{y\to x|z}^{(app \text{ freq})}$  without assumptions (Eq. (26)) (but with the residual variance normalization) is a good approximation

$$f_{y \to x|z}^{\text{(app freq)}} = \hat{a}^{(12)} \left( \hat{a}^{(12)H} \hat{a}^{(12)} + \hat{a}^{(22)H} \hat{a}^{(22)} - (\hat{a}^{(22)H} \hat{a}^{(12)} + \hat{a}^{(12)H} \hat{a}^{(22)}) \frac{\Upsilon}{1 - \Upsilon^2} \right)^{-1} \left( \hat{a}^{(12)} \right)^{H}$$

$$= \frac{1}{\frac{1}{rr^{H}} - \frac{\Upsilon/(1 - \Upsilon^2)}{r^{H}} - \frac{\Upsilon/(1 - \Upsilon^2)}{r} + 1} = \frac{1}{\left| \frac{1}{r} - \frac{\Upsilon}{1 - \Upsilon^2} \right|^2 + 1 - \left( \frac{\Upsilon}{1 - \Upsilon^2} \right)^2}$$

If apply the function

$$g_{\Upsilon}(f) = \frac{1 - \Upsilon^2}{1/f - \frac{1}{1 - \Upsilon^2}}$$

The approximation can be more accurate:  $\exp(f_{y\to x}) - 1 \approx g_{\Upsilon}(f_{y\to x|z}^{\text{(app freq)}}) < \text{TODO: pic to show that} >$ 

#### 4.3.3 Approximation to "auto"-regression coefficients

Recall Eq.(24)

$$\hat{b}^{(12)} \approx \hat{a}^{(12)} - \left[\hat{a}^{(13)}\hat{Q}_{zz}^{-1}\hat{Q}_{zy}\right]_{+}.$$

Follow the same assumptions in Sec 4.3.1, we get:

• Apply assumptions #1 and #2:

$$\hat{Q}_{zz} = \left(\hat{a}^{(13)}\right)^{H} \hat{a}^{(13)} + \left(\hat{a}^{(23)}\right)^{H} \hat{a}^{(23)} + \left(\hat{a}^{(33)}\right)^{H} \hat{a}^{(33)}, \tag{32}$$

$$\hat{Q}_{zy} = \left(\hat{a}^{(13)}\right)^H \hat{a}^{(12)} + \left(\hat{a}^{(23)}\right)^H \hat{a}^{(22)} + \left(\hat{a}^{(33)}\right)^H \hat{a}^{(32)}. \tag{33}$$

• Apply also assumption #3:

$$\hat{b}^{(12)} \approx \hat{a}^{(12)} - \left[ \hat{a}^{(13)} \left( \left( \hat{a}^{(33)} \right)^H \hat{a}^{(33)} \right)^{-1} \left( \left( \hat{a}^{(23)} \right)^H \hat{a}^{(22)} + \left( \hat{a}^{(33)} \right)^H \hat{a}^{(32)} \right) \right]_+ .$$

$$= \hat{a}^{(12)} - \left[ \hat{a}^{(13)} \left( \hat{a}^{(33)} \right)^{-1} \left( \left( \hat{a}^{(33)H} \right)^{-1} \left( \hat{a}^{(23)} \right)^H \hat{a}^{(22)} + \hat{a}^{(32)} \right) \right]_+ .$$

(assumption #4) If further, y and z been jointly whiten before, i.e.  $\hat{a}^{(33)} \approx I$  and  $\hat{a}^{(22)} \approx I$ . then

$$\hat{b}^{(12)} \approx \hat{a}^{(12)} - \left[\hat{a}^{(13)} \left(\hat{a}^{(23)H} + \hat{a}^{(32)}\right)\right]_{+}.$$

Full matrix form

$$\begin{bmatrix} O & A_{xy} & A_{xz} \\ & O & \\ & A_{zy} \end{bmatrix} + \begin{bmatrix} A_{xy} & O & A_{yz} \\ & A_{zy} \end{bmatrix}^{*T} = A(A + A^*)$$

## 5 Approximation of Toeplitz Matrix Operations (not useful)

Mul of band toeplitz matrix

$$\begin{bmatrix} a_0 & a_1 \\ a_{-1} & a_0 & a_1 \\ a_{-1} & a_0 \end{bmatrix} \begin{bmatrix} b_0 & b_1 \\ b_{-1} & b_0 & b_1 \\ b_{-1} & b_0 \end{bmatrix} = \begin{bmatrix} c_0 - a_{-1}b_1 & c_1 & c_2 \\ c_{-1} & c_0 & c_1 \\ c_{-2} & c_{-1} & c_0 - a_1b_{-1} \end{bmatrix}$$
(34)

where  $c_0 = a_{-1}b_1 + a_0b_0 + a_1b_{-1}$ ,  $c_{-1} = a_{-1}b_0 + a_0b_{-1}$ ,  $c_1 = a_0b_1 + a_1b_0$ . Inverse of band toeplitz ??????????

$$R(Q+G) = I$$

$$GR = I - QR$$

$$GRQ = Q - QRQ$$

since

$$RQ \approx I$$

so

$$G \approx Q - QRQ$$
$$R^{-1} \approx Q + Q - QRQ$$

In summary, that is

$$K = I - QR$$
$$R^{-1} = (I - K)^{-1}Q$$

Bad.....since it possible that ||K|| > 1. Indeed, there is a 10 neuron case that ||K|| = 8.34 (for non-whitenned covz). But seems work for whitened signal and p < 40.

## 6 Appendix: Formulas Used to Derive Above Results

#### 6.1 Binomial inverse theorem

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

Specially

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

## **6.2** Inverse of $(n_1 + n_2) \times (n_1 + n_2)$ matrix

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

$$\left(R^{(zy)} - R^{(zx)}\left(R^{(xx)}\right)^{-1}R^{(xy)}\right)\left(R^{(yy)} - R^{(yx)}\left(R^{(xx)}\right)^{-1}R^{(xy)}\right)^{-1}$$

Use row elimination, get

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

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

#### 6.2.1 Known inverse matrix, get inverse of sub matrix

Known

$$\left[\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right]^{-1} = \left[\begin{array}{cc} b_{11} & b_{12} \\ b_{21} & b_{22} \end{array}\right]$$

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

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

## **6.3** Inverse of $(n_1 + n_2 + n_3) \times (n_1 + n_2 + n_3)$ matrix

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

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

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

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

Note:

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

## 7 Useful Theorems

## 7.1 Spectral Representation of Multivariate Stationary Time Series [1]

For X(h) widesense stationary, for its covariance R(h), there exist F(w) such that

$$R(h) = \int_{-\pi}^{\pi} e^{ihw} dF(w), \quad h = 0, \pm 1, \dots$$

 $F(-\pi) = 0$ , F is right-continuous,  $F(\mu) - F(\lambda)$  non-negative define for all  $\lambda < \mu$ . And satisfies

- $E(Z(\lambda)Z^*(\lambda))$  finite
- $E(Z(\lambda)) = 0$ , for  $-\pi < \lambda < \pi$
- $E(Z(\lambda_4) Z(\lambda_3))(Z(\lambda_2) Z(\lambda_1))^* = 0$ , for  $(\lambda_1, \lambda_2] \cap (\lambda_3, \lambda_4] = \phi$
- $E(Z(\lambda + \delta) Z(\lambda))(Z(\lambda + \delta) Z(\lambda))^* \to 0$ , as  $\delta \downarrow 0$ .

unique matrix distribution F,  $F(\mu) - F(\lambda) = E((Z(\mu) - Z(\lambda))(Z(\mu) - Z(\lambda))^*)$ ,  $\lambda \leq \mu$ . o

$$E\left(\mathrm{d}Z(\lambda)\mathrm{d}Z^*(\lambda)\right) = \begin{cases} \mathrm{d}F(\lambda) & \mu = \lambda\\ 0 & \text{otherwise} \end{cases}$$

$$X_t = \int_{-\pi}^{\pi} e^{itv} dZ(v), \quad t = 0, \pm 1, \dots$$
 with probability 1

## References

- [1] Peter J. Brockwell and Richard A. Davis. *Time Series: Theory and Methods*. Springer Science & Business Media, November 2013.
- [2] John F. Geweke. Measures of Conditional Linear Dependence and Feedback between Time Series. *Journal of the American Statistical Association*, 79(388):907–915, 1984.