Professor Yanai and Multivariate Analysis

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Professor Yanai in 1992 (Puntanen, Styan, and Isotalo, 2011, p. 307)





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Professor Yanai and Multivariate Analysis

Common threads running through them are:

• projectors,

• singular value decomposition (SVD),

which are main subject matters of Yanai, Takeuchi, and Takane (2011).

Takeuchi, Yanai, and Mukherjee (1982): The Foundations of Multivariate Analysis



Yanai, Takeuchi, and Takane (2011): Projection matrices, generalized inverse matrices, and singular value decomposition



- (1) Constrained principal component analysis (CPCA)
- (2) Khatri's lemma
- (3) The Wedderburn-Guttman theorem
- (4) Ridge operators
- (5) Constrained canonical correlation analysis
- (6) Causal inferences

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- Sp(X): The space spanned by column vectors of X.
- Ker(X'): The orthogonal complement subspace to Sp(X).
- Orthogonal projectors onto $Sp(\mathbf{X})$: $\mathbf{P}_X = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$.
- Orthogonal projectors onto $Ker(\mathbf{X}')$: $\mathbf{Q}_X = \mathbf{I} \mathbf{P}_X$.
- Basic properties:

$$\begin{split} \mathbf{P}'_X &= \mathbf{P}_X, \ \mathbf{Q}'_X = \mathbf{Q}_X \ (\text{symmetric}). \\ \mathbf{P}^2_X &= \mathbf{P}_X, \ \mathbf{Q}^2_X = \mathbf{Q}_X \ (\text{idempotent}). \\ \mathbf{P}_X \mathbf{Q}_X &= \mathbf{Q}_X \mathbf{P}_X = \mathbf{O} \ (\text{orthogonal}). \end{split}$$

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- Let **K** be an *nnd* matrix such that rank(KX) = rank(X).
- K-orthogonal projectors: $\mathbf{P}_{X/K} = \mathbf{X}(\mathbf{X}'\mathbf{K}\mathbf{X})^{-}\mathbf{X}'\mathbf{K}$, and $\mathbf{Q}_{X/K} = \mathbf{I} \mathbf{P}_{X/K}$.
- Basic properties:

 $\begin{aligned} (\mathsf{KP}_{X/K})' &= \mathsf{KP}_{X/K}, \ (\mathsf{KQ}_{X/K})' = \mathsf{KQ}_{X/K} \ (\text{K-symmetric}). \\ \mathsf{P}_{X/K}^2 &= \mathsf{P}_{X/K}, \ \mathsf{Q}_{X/K}^2 = \mathsf{Q}_{X/K} \ (\text{idempotent}). \\ \mathsf{P}_{X/K}' \mathsf{KQ}_{X/K} &= \mathsf{Q}_{X/K}' \mathsf{KP}_{X/K} = \mathsf{O} \ (\text{K-orthogonal}). \end{aligned}$

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- External Analysis and Internal Analysis.
- External Analysis: Decomposes the main data matrix according to the external information abut the row and columns of the data matrix \implies projection.
- Internal Analysis: Further analyses of decomposed matrices into components ⇒ SVD (singular value decomposition

- Y: The main data matrix.
- G: The row (left-hand) side information matrix.
- H: The column (right-hand) side information matrix.
- The basic decomposition:

$\mathbf{Y} = \mathbf{P}_{G}\mathbf{Y}\mathbf{P}_{H} + \mathbf{Q}_{G}\mathbf{Y}\mathbf{P}_{H} + \mathbf{P}_{G}\mathbf{Y}\mathbf{Q}_{H} + \mathbf{Q}_{G}\mathbf{Y}\mathbf{Q}_{H}.$

• A similar decomposition with K-orthogonal projectors.

Finer Decompositions (1)

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$$\mathbf{G} = [\mathbf{M}, \mathbf{N}].$$

• $(1) \mathbf{P}_{G} = \mathbf{P}_{M} + \mathbf{P}_{N} \Leftrightarrow \mathbf{M}'\mathbf{N} = \mathbf{O}.$
• $(2) \mathbf{P}_{G} = \mathbf{P}_{M} + \mathbf{P}_{N} - \mathbf{P}_{M}\mathbf{P}_{N} \Leftrightarrow \mathbf{P}_{M}\mathbf{P}_{N} = \mathbf{P}_{N}\mathbf{P}_{M}.$
• $(3) \mathbf{P}_{G} = \mathbf{P}_{M} + \mathbf{P}_{Q_{M}N} = \mathbf{P}_{N} + \mathbf{P}_{Q_{N}M}.$
• $(4) \mathbf{P}_{G} = \mathbf{P}_{M/Q_{N}} + \mathbf{P}_{N/Q_{M}} \Leftrightarrow \operatorname{rank}(\mathbf{G}) = \operatorname{rank}(\mathbf{M}) + \operatorname{rank}(\mathbf{N}).$
• $(5) \mathbf{P}_{G} = \mathbf{P}_{GA} + \mathbf{P}_{G(G'G)^{-}B} \Leftrightarrow \mathbf{A}'B = \mathbf{O},$
 $\mathrm{Sp}(\mathbf{A}) \oplus \mathrm{Sp}(\mathbf{B}) = \mathrm{Sp}(\mathbf{G}').$

• Analogous decompositions for \mathbf{P}_{H} , $\mathbf{P}_{G/K}$, and $\mathbf{P}_{H/L}$.

- (1) M and N are mutually orthogonal.
- (2) **M** and **N** are mutually orthogonal, except their common space. (ANOVA w/o interactions).
- (3) Fit one first and the other to the residuals.
- (4) **M** and **N** are disjoint. Fit both simultaneously.
- (5) A matrix of regression coefficients **C** constrained by $\mathbf{C} = \mathbf{AC}^*$ or by $\mathbf{B'C} = \mathbf{O}$.

• PCA of terms obtained by the external analysis of \mathbf{Y} , e.g., $\mathbf{P}_{G}\mathbf{Y}\mathbf{P}_{H}$, which amounts to $SVD(\mathbf{P}_{G}\mathbf{Y}\mathbf{P}_{H})$.

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- Constrained Correspondence Analysis (CCA).
- U: The row representation matrix. (We consider only the row side.)
- Two ways of constraining U: (1) $U = AU^*$, and (2) B'U = O.

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$$\mathbf{P}_A = \mathbf{A}(\mathbf{A}'\mathbf{A})^-\mathbf{A}' = \mathbf{I} - \mathbf{B}(\mathbf{B}'\mathbf{B})^-\mathbf{B}' = \mathbf{Q}_B.$$

- What happens if non-identity metric K is used?
- Let $\mathbf{A} (p \times r)$ and $\mathbf{B} (p \times (p r))$ be matrices such that rank $(\mathbf{A}) = r$, rank $(\mathbf{B}) = p - r$, and $\mathbf{A}'\mathbf{B} = \mathbf{O}$. Then $\mathbf{I} = \mathbf{A}(\mathbf{A}'\mathbf{K}\mathbf{A})^{-1}\mathbf{A}\mathbf{K} + \mathbf{K}^{-1}\mathbf{B}(\mathbf{B}'\mathbf{K}^{-1}\mathbf{B})^{-1}\mathbf{B}'$ (Khatri, 1966).

- An alternative expression: $\mathbf{K} = \mathbf{K}\mathbf{A}(\mathbf{A}'\mathbf{K}\mathbf{A})^{-1}\mathbf{A}\mathbf{K} + \mathbf{B}(\mathbf{B}'\mathbf{K}^{-1}\mathbf{B})^{-1}\mathbf{B}'.$
- Useful for rewriting Q-type projectors into P-type.

Some Extensions

- Let A (p × r) and B (p × (p r)) be matrices such that rank(A) = r and rank(B) = p - r, and let M and N be nnd matrices such that
 - (i) $\mathbf{A'MNB} = \mathbf{O}$, (ii) rank(\mathbf{MA}) = rank(\mathbf{A}), (iii) rank(\mathbf{NB}) = rank(\mathbf{B}). Then,

$$\mathbf{I} = \mathbf{A}(\mathbf{A}'\mathbf{M}\mathbf{A})^{-}\mathbf{A}'\mathbf{M} + \mathbf{N}\mathbf{B}(\mathbf{B}'\mathbf{N}\mathbf{B})^{-}\mathbf{B}'.$$

• Reduces to the original lemma when $\mathbf{M} = \mathbf{K}$ and $\mathbf{N} = \mathbf{K}^{-1}$.

The WG Theorem

- Let Y (n × p) be of rank r, and let A (n × s) and B (p × s) be such that A'YB is invertible.
- Then,

$$rank(\mathbf{Y}_1) = rank(\mathbf{Y}) - rank(\mathbf{Y}\mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-1}\mathbf{A}'\mathbf{Y})$$
$$= rank(\mathbf{Y}) - rank(\mathbf{A}'\mathbf{Y}\mathbf{B}) = r - s,$$

where

$$\mathbf{Y}_1 = \mathbf{Y} - \mathbf{Y} \mathbf{B} (\mathbf{A}' \mathbf{Y} \mathbf{B})^{-1} \mathbf{A}' \mathbf{Y}.$$

• Wedderburn (1934) for s = 1. Guttman (1944) for s > 1. Guttman (1957) reverse.

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The Generalized WG Theorem

- When **A'YB** is not invertible, can we replace it by a generalized inverse?
- Yes, but it requires a condition.
- A rank additivity (subtractivity) problem?

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$$\mathbf{Y} - \mathbf{YB}(\mathbf{A}'\mathbf{YB})^{-}\mathbf{A}'\mathbf{Y})$$

= rank(\mathbf{Y}) - rank($\mathbf{YB}(\mathbf{A}'\mathbf{YB})^{-}\mathbf{A}'\mathbf{Y}$). (1)

• Does the following always hold?

$$rank(\mathbf{YB}(\mathbf{A}'\mathbf{YB})^{-}\mathbf{A}'\mathbf{Y}) = rank(\mathbf{A}'\mathbf{YB})$$
(2)

• No. Tian and Styan (2009) showed the following always holds:

$$rank(\mathbf{Y} - \mathbf{Y}\mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-}\mathbf{A}'\mathbf{Y}) = rank(\mathbf{Y}) - rank(\mathbf{A}'\mathbf{Y}\mathbf{B}).$$
 (3)

• (2) requires a condition, as does (1).

The ns Condition

• Let $\mathbf{C} = \mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-}\mathbf{A}'$.

• The *ns* condition for (1)to hold is:

$\mathbf{Y}\mathbf{C}\mathbf{Y}\mathbf{C}\mathbf{Y}=\mathbf{Y}\mathbf{C}\mathbf{Y}.$

- Equivalent conditions: $(\mathbf{Y}\mathbf{C}\mathbf{Y}\mathbf{Y}^{-})^{2} = \mathbf{Y}\mathbf{C}\mathbf{Y}\mathbf{Y}^{-} \Leftrightarrow (\mathbf{Y}^{-}\mathbf{Y}\mathbf{C}\mathbf{Y})^{2} = \mathbf{Y}^{-}\mathbf{Y}\mathbf{C}\mathbf{Y}.$
- $(\mathbf{YC})^2 = \mathbf{YC}$ or $(\mathbf{CY})^2 = \mathbf{CY}$ (sufficient but not necessary).
- **CYC** = **C** (sufficient but not necessary). Even stronger than idempotency of **YC** or **CY**.

The WG Decomposition

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$$\mathbf{Y} = \mathbf{Y}\mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-}\mathbf{A}'\mathbf{Y} + (\mathbf{Y} - \mathbf{Y}\mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-}\mathbf{A}'\mathbf{Y}).$$

• Let $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$ be matrices such that
(i) $\operatorname{Sp}(\tilde{\mathbf{A}}) \subset \operatorname{Sp}(\mathbf{Y}),$
(ii) $\operatorname{Sp}(\tilde{\mathbf{B}}) \subset \operatorname{Sp}(\mathbf{Y}'),$
(iii) $\operatorname{rank}(\mathbf{A}'\mathbf{Y}\mathbf{B}) + \operatorname{rank}(\tilde{\mathbf{B}}'\mathbf{Y}^{-}\tilde{\mathbf{A}}) = \operatorname{rank}(\mathbf{Y}),$
(iv) $\mathbf{A}'\mathbf{Y}\mathbf{Y}^{-}\tilde{\mathbf{A}} = \mathbf{A}'\tilde{\mathbf{A}} = \mathbf{O},$
(v) $\tilde{\mathbf{B}}'\mathbf{Y}^{-}\mathbf{Y}\mathbf{B} = \tilde{\mathbf{B}}'\mathbf{B} = \mathbf{O}.$

• Then, $\mathbf{Y} = \mathbf{Y}\mathbf{B}(\mathbf{A}'\mathbf{Y}\mathbf{B})^{-}\mathbf{A}'\mathbf{Y} + \tilde{\mathbf{A}}(\tilde{\mathbf{B}}'\mathbf{Y}^{-}\tilde{\mathbf{A}})^{-}\tilde{\mathbf{B}}'.$

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- R_X(λ) = X(X'X + λP_{X'})⁻X', where P_{X'} = X'(XX')⁻X is the orthogonal projector onto Sp(X'). (P_{X'} = I if X is columnwise nonsingular.)
- The ridge LS estimation $\min_{\mathbf{c}} = \phi_{\lambda}(\mathbf{c})$, where $\phi_{\lambda}(\mathbf{c}) = SS(\mathbf{e}) + \lambda SS(\mathbf{c})_{P_{X'}}$ and $\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{c}$. (We assume, w/o loss of generality, that $Sp(\mathbf{c}) \subset Sp(\mathbf{X'})$.)

- Let $\mathbf{S}_X(\lambda) = \mathbf{I} \mathbf{R}_X(\lambda)$.
- $\mathbf{R}_X(\lambda)$ and $\mathbf{S}_X(\lambda)$ have properties similar to those of \mathbf{P}_X and \mathbf{Q}_X .
- For example:

$$\begin{aligned} & \mathsf{R}_X(\lambda)\mathsf{K}_X(\lambda)\mathsf{R}_X(\lambda) = \mathsf{R}_X(\lambda) \text{ (i.e., } \mathsf{K}_X(\lambda) = \mathsf{R}_X(\lambda)^+.), \\ & \mathsf{R}_X(\lambda) - \mathsf{R}_X(\lambda)^2 = \mathsf{R}_X(\lambda)\mathsf{S}_X(\lambda) = \mathsf{S}_X(\lambda)\mathsf{R}_X(\lambda) \ge \mathsf{O}. \\ & \mathsf{R}_X(\lambda)\mathsf{K}_X(\lambda) = \mathsf{P}_X, \text{ etc.} \end{aligned}$$

• Similar decompositions of $\mathbf{R}_X(\lambda)$ to those of \mathbf{P}_X .

- Ridge metric matrix: $\mathbf{K}_X(\lambda) = \mathbf{P}_X + \lambda (\mathbf{X}\mathbf{X}')^+$.
- Then, $\mathbf{R}_X(\lambda)$ can be rewritten as:

$$\mathbf{R}_X(\lambda) = \mathbf{X}(\mathbf{X}'\mathbf{K}_X(\lambda)\mathbf{X})^{-}\mathbf{X}'.$$

• Generalized ridge operator:

 $\mathbf{R}_{X}^{(W,L)}(\lambda) = \mathbf{X}(\mathbf{X}'\mathbf{W}\mathbf{X} + \lambda\mathbf{L})^{-}\mathbf{X}'\mathbf{W}$, where **L** is an *nnd* matrix such that $Sp(\mathbf{L}) \subset Sp(\mathbf{X}')$, and **W** is an *nnd* matrix such that rank($\mathbf{W}\mathbf{X}$) = rank(\mathbf{X}).

• Generalized ridge metric matrix: $\mathbf{K}_{X}^{(W,L)}(\lambda) = \mathbf{P}_{X} + \lambda \mathbf{X} (\mathbf{X}'\mathbf{W}\mathbf{X})^{-} \mathbf{L} (\mathbf{X}'\mathbf{W}\mathbf{X})^{-} \mathbf{X}'\mathbf{W}.$

• Then, $\mathbf{R}_X^{(W,L)}(\lambda) = \mathbf{X}(\mathbf{X}'\mathbf{W}\mathbf{K}_X^{(W,L)}(\lambda)\mathbf{X})^-\mathbf{X}'\mathbf{W}.$

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- Total association between **X** and **Y**: $tr(\mathbf{P}_X\mathbf{P}_Y)$.
- $\mathbf{X} = \mathbf{M} + \mathbf{N}$, $\mathbf{M'N} = \mathbf{O}$ does not guarantee $\mathbf{P}_X = \mathbf{P}_M + \mathbf{P}_N$.
- cf. $\mathbf{X} = [\mathbf{M}, \mathbf{N}]$, $\mathbf{M}'\mathbf{N} = \mathbf{O}$ leads to $\mathbf{P}_X = \mathbf{P}_M + \mathbf{P}_N$.
- We need orthogonal decompositions of \mathbf{P}_X and \mathbf{P}_Y to derive additive decompositions of the total association.

Two Orthogonal Decompositions of Projectors

• (1) Let A, B, and W be matrices such that $Sp(A) = Ker(H'X'P_GX)$, $Sp(B) = Ker(H'X'Q_GX)$, and Sp(W) = Ker(X'G). Then,

$$\mathbf{P}_{[X,G]} = \mathbf{P}_{P_G XH} + \mathbf{P}_{P_G XA} + \mathbf{P}_{Q_G XH} + \mathbf{P}_{Q_G XB} + \mathbf{P}_{GW}.$$

• (2) Let \mathbf{K} , \mathbf{U} , and \mathbf{V} be matrices such that $Sp(\mathbf{K}) = Ker(\mathbf{H}'\mathbf{X}'\mathbf{X})$, $Sp(\mathbf{U}) = Ker(\mathbf{G}'\mathbf{X}\mathbf{H})$, and $Sp(\mathbf{V}) = Ker(\mathbf{G}'\mathbf{X}\mathbf{K})$. Then,

$$\mathbf{P}_{[X,G]} = \mathbf{P}_{P_{XH}G} + \mathbf{P}_{XHU} + \mathbf{P}_{P_{XK}G} + \mathbf{P}_{XKV} + \mathbf{P}_{Q_XG}.$$

- Similar decompositions of $\mathbf{P}_{[\mathbf{Y},\mathbf{G}_{Y}]}$.
- Take one term each from a decomposition of $P_{[X,G_{\chi}]}$ and that of $P_{[Y,G_{\gamma}]}$, apply SVD to the product of the two, e.g.,

$$SVD(\mathbf{P}_{\mathbf{Q}_{G_{\chi}}XH_{\chi}}\mathbf{P}_{YH_{Y}U_{Y}}).$$

Confounding Variables

- Causal inferences without randomization. How to eliminate the effects of confounding variables.
- y: The dependent variable.
- x: The independent variable.
- U: The confounding variables.
- Regression analysis (1): y = xa₁ + Uc + e₁. The OLS estimate of xa₁ is given by

$$\mathbf{x}\hat{a}_1 = \mathbf{P}_{\mathbf{x}/Q_u}\mathbf{y} \tag{4}$$

• On the other hand, consider the regression of x onto U, i.e., $x = Ud + e_2$. The OLS estimate of Ud is given by

$$\mathbf{U}\hat{\mathbf{d}} = \mathbf{P}_U \mathbf{x}.$$
 (5)

Linear Propensity Scores

- We call P_Ux linear propensity scores. Residuals from the above regression Q_Ux represent the portions of x left unaccounted for by U.
- We next consider using P_Ux instead of U in the first regression, i.e., y = xa₂ + P_Uxb + e₃. the OLS estimate of xa₂ is given by

$$\mathbf{x}\hat{a}_2 = \mathbf{P}_{x/Q_{P_U^{\times}}}\mathbf{y},\tag{6}$$

where $\mathbf{Q}_{P_{U}x} = \mathbf{I} - \mathbf{P}_{U}\mathbf{x}(\mathbf{x}'\mathbf{P}_{U}\mathbf{x})^{-1}\mathbf{x}'\mathbf{P}_{U}$.

• Since $\mathbf{Q}_{P_U \mathbf{x}} \mathbf{x} = \mathbf{x} - \mathbf{P}_U \mathbf{x} (\mathbf{x}' \mathbf{P}_U \mathbf{x})^{-1} \mathbf{x}' \mathbf{P}_U \mathbf{x} = \mathbf{Q}_U \mathbf{x}$, we obtain

$$\mathbf{P}_{x/Q_{P_Ux}}\mathbf{y} = \mathbf{P}_{x/Q_U}\mathbf{y}.$$
 (7)

This means (4) and (6) are equivalent.

Regression analysis: y = xa₃ + e₄. The IV estimate of xa₃ with z = Q_Ux as the IV is given by

$$\mathbf{x}\hat{a}_3 = \mathbf{P}_{x/P_z}\mathbf{y} = \mathbf{P}_{x/Q_U}\mathbf{y}.$$
 (8)

• Since $\mathbf{P}_z = \mathbf{Q}_U \mathbf{x} (\mathbf{x}' \mathbf{Q}_U \mathbf{x})^{-1} \mathbf{x}' \mathbf{Q}_U$ and $\mathbf{x}' \mathbf{P}_z = \mathbf{x}' \mathbf{Q}_U$, this is identical to (4) and (6).

- It can also be easily verified that z defined above satisfies the following properties required of a IV:
 (i) z'U = 0 (z and U are uncorrelated),
 (ii) z'x ≠ 0 (z and x are correlated),
 (iii) z'Q_[U,x]y = 0 (*i.e.*, z has a predictive power on y only through x).
- (i) and (ii) are trivial. That it also satisfies (3) can be seen from:

$$\mathbf{z}'\mathbf{Q}_{[U,x]}\mathbf{y} = \mathbf{x}'\mathbf{Q}_U\mathbf{Q}_{[U,x]}\mathbf{y} = \mathbf{x}'\mathbf{Q}_{[U,x]}\mathbf{y} = 0.$$
(9)

Thanks for your attention.