5.2.4.1 Least Squares Approach

For illustrative purposes, suppose $N = 2$ and $J = 4$ so that

$$
\begin{aligned}
y_{11} &= \theta_1\phi_1 + \varepsilon_{11} \quad ; \quad y_{21} = \theta_2\phi_1 + \varepsilon_{21} \\
y_{12} &= \theta_1\phi_2 + \varepsilon_{12} \quad ; \quad y_{22} = \theta_2\phi_2 + \varepsilon_{22} \\
y_{13} &= \theta_1\phi_3 + \varepsilon_{13} \quad ; \quad y_{23} = \theta_2\phi_3 + \varepsilon_{23} \\
y_{14} &= \theta_1\phi_4 + \varepsilon_{14} \quad ; \quad y_{24} = \theta_2\phi_4 + \varepsilon_{24}
\end{aligned}
$$

<u>Step (a):</u> Treating ϕ_j as known, we can re-write model (1) in matrix form

$$\mathbf{y} = \mathbf{x}^T\boldsymbol{\theta} + \boldsymbol{\varepsilon} \qquad (2)$$

Where $\mathbf{y} = \begin{pmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{14} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{24} \end{pmatrix}$, $\mathbf{x} = \begin{pmatrix} \phi_1 & 0 \\ \phi_2 & 0 \\ \phi_3 & 0 \\ \phi_4 & 0 \\ 0 & \phi_1 \\ 0 & \phi_2 \\ 0 & \phi_3 \\ 0 & \phi_4 \end{pmatrix}$, and $\boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}$

$\boldsymbol{\varepsilon}$ is a vector of random errors

The least squares system of normal equations yields

$$\hat{\boldsymbol{\theta}} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y}$$

$$\mathbf{x}^T\mathbf{x} = \begin{bmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{bmatrix} \begin{bmatrix} \phi_1 & 0 \\ \phi_2 & 0 \\ \phi_3 & 0 \\ \phi_4 & 0 \\ 0 & \phi_1 \\ 0 & \phi_2 \\ 0 & \phi_3 \\ 0 & \phi_4 \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{4} \phi_j^2 & 0 \\ 0 & \sum_{j=1}^{4} \phi_j^2 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{y} = \begin{bmatrix} \phi_1 y_{11} + \phi_2 y_{12} + \phi_3 y_{13} + \phi_4 y_{14} \\ \phi_1 y_{21} + \phi_2 y_{22} + \phi_3 y_{23} + \phi_4 y_{24} \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{4} \phi_j y_{1j} \\ \sum_{j=1}^{4} \phi_j y_{2j} \end{bmatrix}$$

So $\hat{\boldsymbol{\theta}} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y} = \frac{1}{\sum_{j=1}^{4} \phi_j^2} \begin{bmatrix} \sum_{j=1}^{4} \phi_j y_{1j} \\ \sum_{j=1}^{4} \phi_j y_{2j} \end{bmatrix}$

$$Var(\hat{\boldsymbol{\theta}}) = \sigma^2(\mathbf{x}^T\mathbf{x})^{-1} = \frac{\sigma^2}{\sum_{j=1}^{4} \phi_j^2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

<u>Step (b):</u> Now treating $\boldsymbol{\theta}_i$ as known, we can re-write model (1) in matrix form

$$\mathbf{y} = \mathbf{x}\boldsymbol{\varphi} + \boldsymbol{\varepsilon} \qquad (3)$$

Where $\mathbf{y} = \begin{bmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{14} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{24} \end{bmatrix}$, $\mathbf{x} = \begin{bmatrix} \theta_1 & 0 & 0 & 0 \\ 0 & \theta_1 & 0 & 0 \\ 0 & 0 & \theta_1 & 0 \\ 0 & 0 & 0 & \theta_1 \\ \theta_2 & 0 & 0 & 0 \\ 0 & \theta_2 & 0 & 0 \\ 0 & 0 & \theta_2 & 0 \\ 0 & 0 & 0 & \theta_2 \end{bmatrix}$, and $\boldsymbol{\varphi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix}$

$\boldsymbol{\varepsilon}$ is a vector of random errors

The least squares system of normal equations is

$$(\mathbf{x}^T\mathbf{x})\hat{\boldsymbol{\varphi}} = \mathbf{x}^T\mathbf{y}$$

$$\mathbf{x}^T\mathbf{x} = (\theta_1^2 + \theta_2^2)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{y} = \begin{bmatrix} \theta_1 y_{11} + \theta_2 y_{21} \\ \theta_1 y_{12} + \theta_2 y_{22} \\ \theta_1 y_{13} + \theta_2 y_{23} \\ \theta_1 y_{14} + \theta_2 y_{24} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{2} \theta_i y_{i1} \\ \sum_{i=1}^{2} \theta_i y_{i2} \\ \sum_{i=1}^{2} \theta_i y_{i3} \\ \sum_{i=1}^{2} \theta_i y_{i4} \end{bmatrix}$$

So $$\hat{\boldsymbol{\varphi}} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y} = \frac{1}{\sum_{i=1}^{2}\theta_i^2}\begin{bmatrix} \sum_{i=1}^{2}\theta_i y_{i1} \\ \sum_{i=1}^{2}\theta_i y_{i2} \\ \sum_{i=1}^{2}\theta_i y_{i3} \\ \sum_{i=1}^{2}\theta_i y_{i4} \end{bmatrix}$$

$$Var(\hat{\boldsymbol{\varphi}}) = \sigma^2(\mathbf{x}^T\mathbf{x})^{-1} = \frac{\sigma^2}{\sum_{i=1}^{2}\theta_i^2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Using step (a) to estimate $\boldsymbol{\theta}$ followed by step (b) to estimate $\boldsymbol{\varphi}$ iteratively are the basis of computing the least square estimates of the parameters using iterative fitting.

From $\hat{\boldsymbol{\theta}} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y} = \frac{1}{\sum_{j=1}^{4}\phi_j^2}\begin{bmatrix} \sum_{j=1}^{4}\phi_j y_{1j} \\ \sum_{j=1}^{4}\phi_j y_{2j} \end{bmatrix}$, making the constraint that the sum squares of ϕs be equal to J does not seem to make the model identifiable. It is seen that, in order to iteratively fit the set of θs and ϕs, regarding the other set as known (as stated in the paper), we at least need starting values of the set of ϕs (or the starting values of the set of θs).

Li and Wong stated that a large number (>10) of arrays are needed for the probe sensitivity index ϕs to be estimated accurately, otherwise the uncertainty in the estimation must be taken into account in the standard error computation.