Estimation of truncated spline in nonlinear structural equation modeling using weighted least squares method

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Abstract. Structural equation modeling (SEM) consists of two parts, the measurement model and the structural model. In this paper, we develop a SEM model that the measurement model is linear and the structural model is nonlinear. Structural model explain about relationship between latent variables. Truncated spline is used for modeling the nonlinear relationship between the latent variables. Through weighted least squares (WLS) method, it is found that estimation of parameter truncated spline in nonlinear SEM for two exogen and an endogen latent variables is resulted by optimizing

$$\min_\gamma \{ \| \Sigma^{-\frac{1}{2}} (\omega_\eta - \Gamma_\xi \gamma) \|^2 \}$$

and it gave an estimator

$$\hat{\gamma} = (\Gamma'_\xi \Sigma^{-1} \Gamma_\xi)^{-1} \Gamma'_\xi \Sigma^{-1} \omega_\eta$$

The estimator influenced by the location and some knot points $\kappa_1$ and $\kappa_2$.

1. Introduction

Structural equation modeling (SEM), is one of the statistical approaches used for research that uses a variable that cannot be measured directly (latent variable) but it is conducted through indicators. In general, studies with SEM approach which assumes that the relationship between the variables is linear, while it is known that the application in the field there is a phenomenon that cannot be enforced because the actual relationship is nonlinear.

For certain cases, linearity in structural models can be modified into nonlinear in order to clarify the relationship between the latent variables that are not linear [1], [2], [3], [4], and [5].

Therefore, this work aims to investigating the parameter estimation of nonlinear structural model by using weighted least squares method (WLS). The nonlinear is indicated with a change the relation pattern between latent variables, which differs in the certain range.

2. Structural Equation Modelling (SEM)

Research variable in SEM is a vector $h$ dimension $p$ with $h = (\eta_j, \xi_j)'$ that can not be measured directly, but through an indicator $z = (z_1, z_2, ..., z_p)'$, it can be stated with the relationship $z =$
\( \tau + A h + e \), a vector for the intercept \( \tau \) and factor loading matrix \( A \), as well as measurement error models \( e \). Wall and Amemiya [2] formulated the measurement model in general form i.e.

\[
z = Ah + e
\]  

(1)

where \( z \) was a vector \( p + q \) of observed variable which was called indicator, \( A \) was a loading factor matrix, \( h = (\eta, \xi)' \) was the vector of latent variables and \( e \) was error, with \( e \sim N(0, \Theta_e) \). Bollen [6] defined the general structural model following

\[
\eta = \Gamma \xi + \zeta
\]

(2)

where \( \eta \) and \( \xi \) were the vectors of endogenous and exogenous latent variables respectively, \( \Gamma \) was coefficient matrix that measured the linear relation of latent variables.

In many cases vector \( z \) as described in Equation (1) is divided in two parts, the exogenous indicators \( x \) and the endogenous indicators \( y \). Figure 1 shows the path diagram for two exogenous latent variables and one endogenous latent variable. Measurement model for two exogenous and one endogenous latent variable respectively are written as follow:

\[
\begin{bmatrix}
x_{11} \\
x_{21} \\
\vdots \\
x_{p1} \\
x_{12} \\
x_{22} \\
\vdots \\
x_{p2}
\end{bmatrix}
\begin{bmatrix}
\lambda_{x11}I_n & 0 \\
\lambda_{x21}I_n & 0 \\
\vdots & \vdots \\
\lambda_{xp1}I_n & 0 \\
0 & \lambda_{x12}I_n \\
0 & \lambda_{x22}I_n \\
\vdots & \vdots \\
0 & \lambda_{xp2}I_n
\end{bmatrix}
\begin{bmatrix}
\xi_1 \\
\xi_2 \\
\vdots \\
\delta_{p1} \\
\delta_{p2}
\end{bmatrix}
\]

(3)

and

\[
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_q
\end{bmatrix}
= \begin{bmatrix}
\lambda_{y1}I_n \\
\lambda_{y2}I_n \\
\vdots \\
\lambda_{yq}I_n
\end{bmatrix}
\begin{bmatrix}
\xi \\
\xi \\
\vdots \\
\xi
\end{bmatrix}
+ \begin{bmatrix}
\epsilon_1 \\
\epsilon_2 \\
\vdots \\
\epsilon_q
\end{bmatrix}
\]

(4)

In matrix notation the Confirmatory Factor Analysis (CFA) model can be written as:

a. variance-covariance matrix among the indicators \( x \)

\[
\Sigma_{xx}(\theta) = E[(A_x \xi + \delta)(A_x \xi + \delta')]
= E(A_x \xi \xi' A_x' + A_x \xi \delta' + \delta \xi' A_x' + \delta')
= A_x \Phi A_x' + \Theta_\delta
\]

(5)

where the matrix \( \Phi \) represents the correlation matrix between the factors.

b. variance-covariance matrix among the indicators \( y \)

\[
\Sigma_{yy}(\theta) = E[(A_y \eta + \epsilon)(A_y \eta + \epsilon')]
= A_y E(\eta \eta') A_y' + A_y \epsilon \epsilon' + \epsilon \eta' A_y' + \epsilon' \epsilon
= A_y E(\eta \eta') A_y' + \Theta_\epsilon
\]

(6)

In order to determine the covariance matrix for the endogenous variables \( \eta \) it is necessary to use the reduce form \( \eta = (I - B)^{-1}(\Gamma \xi + \zeta) \)

\[
E(\eta \eta') = E[((I - B)^{-1}(\Gamma \xi + \zeta))(I - B)^{-1}(\Gamma \xi + \zeta)]'
= (I - B)^{-1}E[\Gamma \xi \xi' \Gamma' + \Gamma \xi \zeta' + \zeta \xi' \Gamma + \zeta \zeta'](I - B)^{-1}E
= (I - B)^{-1}(\Gamma \Phi \Gamma' + \Psi)(I - B)^{-1}
\]

(7)
So, the covariance matrix among the $y$'s is
\[
\mathbf{E}(yy') = \Lambda_y[(I - B)^{-1}(\Gamma \Phi \Gamma' + \Psi)(I - B)^{-1}]\Lambda_y' + \Theta_e \tag{8}
\]
c. covariance matrix between $x$'s and $y$'s
\[
\Sigma_{xy}(\theta) = \mathbf{E}[(A_x \xi + \delta)(A_y \eta + \varepsilon)'] = \mathbf{E}((A_x \xi + \delta)(\eta' \Lambda_y' + \varepsilon)) = \Lambda_x \mathbf{E}(\xi \eta') \Lambda_y' + \Lambda_x \mathbf{E}(\xi \varepsilon') + \mathbf{E}(\delta \eta') \Lambda_y' + \mathbf{E}(\delta \varepsilon') \tag{9}
\]
Substituting $\eta$ by reduced form we have
\[
\mathbf{E}(xy) = \Lambda_x \mathbf{E}[\xi [(I - B)^{-1}(\Gamma \xi + \zeta)]I \Lambda_y' + \Lambda_x \mathbf{E}(\xi \varepsilon') + \mathbf{E}(\delta \eta') \Lambda_y' + \mathbf{E}(\delta \varepsilon') = \Lambda_x \mathbf{E}(\xi \eta') \Lambda_y' + \Lambda_x \mathbf{E}(\xi \varepsilon') + \mathbf{E}(\delta \eta') \Lambda_y' + \mathbf{E}(\delta \varepsilon') \tag{10}
\]
d. covariance matrix between $y$'s and $x$'s
\[
\Sigma_{yx}(\theta) = \mathbf{E}[(A_y \eta + \varepsilon)(A_x \xi + \delta)'] = \mathbf{E}[(A_y \eta + \varepsilon)(\xi' \Lambda_x' + \varepsilon' \Lambda_x' + \varepsilon') = \Lambda_y \mathbf{E}(\eta \xi') \Lambda_x' + \Lambda_y \mathbf{E}[\eta \delta'] + \mathbf{E}[\varepsilon \xi'] \Lambda_x' + \mathbf{E}[\varepsilon \delta'] \tag{11}
\]
Substituting $\eta$ by reduced form we have
\[
\mathbf{E}(yx) = \Lambda_y \mathbf{E}[[I - B)^{-1}(\Gamma \xi + \zeta)]I \Lambda_x' + \Lambda_y \mathbf{E}[[I - B)^{-1}[(\Gamma \xi + \zeta) \delta']] + \mathbf{E}[\varepsilon \xi'] \Lambda_x' + \mathbf{E}[\varepsilon \delta'] = \Lambda_y (I - B)^{-1}[(\Gamma \xi + \zeta)] \Lambda_x' + \mathbf{E}[\varepsilon \xi'] \Lambda_x' \tag{12}
\]
If structured equation of (5), (8), (10) and (12) in a matrix form $\Sigma = \Sigma(\theta)$ than we will obtain the covariance matrix for the observation variables $x$ and $y$ as a function of the model parameters
\[
\Sigma(\theta) = \begin{bmatrix}
\Lambda_y (I - B)^{-1}F & \Lambda_y (I - B)^{-1}G \\
\Lambda_x (I - B)^{-1} \Gamma \Phi \Lambda_x'
\end{bmatrix} \tag{13}
\]
where
\[
F = (\Gamma \Phi \Gamma' + \Psi) ((I - B)^{-1})' \Lambda_y' + \Theta_e; \\
G = \Phi \Gamma' \Lambda_y'
\]
For null B model (one endogenous latent variable), matrix in equation (13) became
\[
\begin{bmatrix}
\Lambda_y (\Gamma \Phi \Gamma' + \Psi) \Lambda_y' + \Theta_e & \Lambda_y \Gamma \Phi \Lambda_x' \\
\Lambda_x \Phi \Gamma' \Lambda_y' & \Lambda_x \Phi \Lambda_x'
\end{bmatrix}
\]
Furthermore,
\[
\eta = f(\xi_1, \xi_2) + \zeta \tag{14}
\]
$\eta$ is vector $n \times 1$ of endogenous latent variable, $f(\xi_1, \xi_2)$ is functions of exogenous latent variables $\xi_1$ and $\xi_1$ and then $\zeta$ is vector $n \times 1$ which contains the error structural model.
3. Nonlinear SEM

The lives of children with Cystic Fibrosis by using quadratic and interaction SEM approach can be found in [2]. Nonlinear SEM suggest by dramatically increased feelings of dejection come at a sort of tipping point or breaking point. That is, after a certain level of stress or a certain lack of self-esteem, the feelings of dejection are much higher. The main investigation of this work is to estimate parameters and functions in structural model as mentioned in Equation (14) using WLS. Ruliana, et al. [1] had written down the factor scores for $\xi$ and $\omega_1$, and the score factor for $\eta$ is $\omega_2$ . Model nonlinear SEM for two variables of latent exogenous is written down as follows:

$$\omega_{\eta i} = \sum_{r=0}^{m_1} \alpha_1 r \omega_{\xi i}^r + \sum_{s=1}^{K_1} \beta_1 s (\omega_{\xi i} - \kappa_1)^{m_1} + \sum_{t=0}^{m_2} \alpha_2 t \omega_{\xi 2}^t + \sum_{u=1}^{K_2} \beta_2 u (\omega_{\xi 2} - \kappa_u)^{m_2} + \zeta_i$$

(15)

Model in Equation (15) can be written as

$$\zeta_i = \omega_{\eta i} - A$$

(16)

where

$$A = \sum_{r=0}^{m_1} \alpha_1 r \omega_{\xi i}^r + \sum_{s=1}^{K_1} \beta_1 s (\omega_{\xi i} - \kappa_1)^{m_1} + \sum_{t=0}^{m_2} \alpha_2 t \omega_{\xi 2}^t + \sum_{u=1}^{K_2} \beta_2 u (\omega_{\xi 2} - \kappa_u)^{m_2}$$

In the form of matrix model (16) can be written down such as the following:

$$\zeta = \omega_{\eta} - \Gamma_{\xi \kappa} \gamma$$

(17)

Furthermore, given the function

$$Q(\gamma) = \zeta^{\prime} \Sigma^{-1} \zeta$$

$$= (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma)^{\prime} \Sigma^{-1} (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma)$$

$$= \omega_{\eta}^{\prime} \Sigma^{-1} \omega_{\eta} - \omega_{\eta}^{\prime} \Sigma^{-1} \Gamma_{\xi \kappa} \gamma + \gamma^{\prime} \Gamma_{\xi \kappa}^{\prime} \Sigma^{-1} \Gamma_{\xi \kappa} \gamma$$

(18)

where $\Sigma^{-1}$ is variance covariance matrix or weighted matrix, $\Gamma_{\xi \kappa}$ is the function-based containing exogenous latent variable and knot [1].

In order to modelling nonlinear relationship between latent variable in structural equation modeling (SEM), it is necessary to find the parameter estimation. The method applied for the estimation parameter was a weighted least square (WLS) that minimized the sum of quadratics error, which was weighted by a matrix inverse of error variance. Ordinary least square (OLS) method, was assumed that all elements of $\Theta^{-1}$ should be similar. In WLS It was weighted by matrix inverse of error variance whose the objective was to solve if the assume was not fulfilled.

A theorem of parameter estimation was given with WLS method for latent variables following:

**Theorem 1** If model is given as described in Equation (15), and the error term in Equation (17) then estimator of parameter $\gamma$ with method of weighted least square (WLS) is given by

$$\hat{\gamma} = (\Gamma_{\xi \kappa} \Sigma^{-1} \Gamma_{\xi \kappa})^{-1} \Gamma_{\xi \kappa} \Sigma^{-1} \omega_{\eta}$$

with $\gamma = [\gamma_1, \gamma_2]^\prime$, with

$$\gamma_1' = [\alpha_{10} \, \alpha_{11} \, \cdots \, \alpha_{1m_1} \, \beta_{11} \, \cdots \, \beta_{1K_1}]'$$

(19)

$$\gamma_2' = [\alpha_{20} \, \alpha_{21} \, \cdots \, \alpha_{2m_2} \, \beta_{21} \, \cdots \, \beta_{2K_2}]'$$

(20)

and

$$\Gamma_{\xi \kappa} = [\Gamma_{\xi \kappa(1)} \Gamma_{\xi \kappa(2)}]$$
The application of this estimator in data concentration CO$_2$ in rainy season (January, 2013) of ambient air in Surabaya, Indonesia. The concentration of CO$_2$ influenced by two latent variables, they are meteorology and environment. The indicators of meteorology are wind speed (Kec$_A$), wind direction (Ar$_A$), solar radiation (Rad$_M$), temperature (Temp), humidity (Kelemb), and the indicators of environment are: elevation (elev), green space (GS), and non green space (NGS).

The result of the measurement model is given in the Table 1 below. From the table, it clear that the indicators to measure latent variables meteorological i.e. wind speed, wind direction, solar radiation, temperature and humidity are significant at P value $< 0.05$. The indicators that measure the latent variables environment i.e. green space and non green space are significant at P values $< 0.05$. CO$_2$ variable is measured directly by concentration CO$_2$ (kon$_{CO_2}$).

4. Data Applications

Proof:

Based on model as mentioned in Equation (15) is obtained a measurement $\hat{\zeta} = \omega_{\eta} - \Gamma_{\xi \kappa} \eta$ with using WLS method, then estimator for $\gamma$ was resulted by optimizing:

$$\min_{\gamma} \{ \| \Sigma^{-\frac{1}{2}} (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma) \|^2 \} = \min_{\gamma} \{ (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma) \Sigma^{-1} (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma) \}$$

$$= \min_{\gamma} \{ (\omega_{\eta}^\prime - \gamma^\prime \Gamma_{\xi \kappa}^\prime) \Sigma^{-1} (\omega_{\eta} - \Gamma_{\xi \kappa} \gamma) \}$$

$$= \min_{\gamma} \{ (\omega_{\eta}^\prime \Sigma^{-1} \omega_{\eta} - \omega_{\eta}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta} + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma) \}$$

$$= \min_{\gamma} \{ Q(\gamma) \}$$

where

$$Q(\gamma) = \{(\omega_{\eta}^\prime \Sigma^{-1} \omega_{\eta} - \omega_{\eta}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma)\}$$

Derivation of Equation (21) with respect to $\gamma$ is obtained

$$\frac{\partial Q(\gamma)}{\partial \gamma} = \frac{\partial}{\partial \gamma} \{(\omega_{\eta}^\prime \Sigma^{-1} \omega_{\eta} - \omega_{\eta}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma)\}$$

$$= \frac{\partial}{\partial \gamma} \{(\omega_{\eta}^\prime \Sigma^{-1} \omega_{\eta} - (\omega_{\eta}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma)^\prime + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta} + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma)\}$$

$$= \frac{\partial}{\partial \gamma} \{(\omega_{\eta}^\prime \Sigma^{-1} \omega_{\eta} - 2 \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta} + \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} \gamma)\} - 2 \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta}$$

$$+ 2 \gamma \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa}$$

Equation (23) is similar to zero and then the estimation for parameter $\gamma$ is gave

$$\hat{\gamma} \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa} = \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta}.$$  

Because $\Gamma_{\xi \kappa}$ is full matrix rank, we have

$$\hat{\gamma} = (\Gamma_{\xi \kappa}^\prime \Sigma^{-1} \Gamma_{\xi \kappa})^{-1} \Gamma_{\xi \kappa}^\prime \Sigma^{-1} \omega_{\eta}$$

(24)
Table 1. Combined loadings and cross-loadings

| Indicator | Meteo | Ling | $CO_2$ | Type | SE  | P-value |
|-----------|-------|------|--------|------|-----|---------|
| kec_A     | -0.709 | -0.33 | -0.03  | reflect | 0.068  | < 0.001 |
| Ar_A      | 0.34   | -0.286 | 0.458  | reflect | 0.068  | < 0.001 |
| Rad_M     | -0.159 | 0.132 | -0.22  | reflect | 0.068  | < 0.001 |
| Temp      | 0.757  | 0.047 | -0.217 | reflect | 0.068  | < 0.001 |
| kelemb    | 0.789  | -0.192 | -0.059 | reflect | 0.068  | < 0.001 |
| elev      | -0.284 | 0.538 | -0.319 | reflect | 0.068  | < 0.001 |
| GS        | 0.065  | 0.971 | 0.067  | reflect | 0.068  | < 0.001 |
| NGS       | -0.093 | -0.963 | -0.11  | reflect | 0.068  | < 0.001 |
| kon_CO_2  | 0      | 0     | 1      | reflect | 0.068  | < 0.001 |

Plots of score factor are shown in Fig. 1 and Fig. 2.

Figure 1. a. Scatterplot of Score Factor $CO_2$ and Meteo, b. Scatterplot of Score Factor $CO_2$ and Ling

Figure 2. Surface Plot of $CO_2$ vs Meteo and Ling
From the Figure 1 and Figure 2, we can see that the relation between laten variable is nonlinear, and by using the estimator in the Theorem 1 for $\Sigma = I$, we get the structural model estimation in the Table 2 and Path Diagram 3 as follows:

**Table 2. Structural Model**

| Coef  | SE Coef | T     | Pvalue |
|-------|---------|-------|--------|
| 2.2990| 0.9240  | 2.4881| 0.0141 |
| -3.0147| 0.9319 | -3.2351| 0.0015 |
| 4.1882| 1.4418  | 2.9048| 0.0043 |
| -3.8396| 1.4810 | -2.5925| 0.0106 |
| -6.8345| 2.1936 | -3.1157| 0.0023 |
| 6.7444| 2.2190  | 3.0393| 0.0029 |

Minimum GCV : 0.0000417
Knot Optimum : -2.453; 0.0324; 0.21; -1.014

**Figure 3. Path Diagram of CO$_2$, Meteorology, and Environment**

From the table above, the estimation of structural model of nonlinear SEM by using spline truncated is:

$$CO_2 = 2.2990\, Meteo - 3.0147(Meteo + 2.453) + 4.1882(Meteo - 0.0324) + 3.8396(Meteo + 0.21) + 6.8345\, Ling + 6.7444(\text{Ling} + 1.014)$$

All of parameter in structural model estimation are significant for P value < 0.05 [7], [8] with minimum GCV is 0.0000417. The plot of CO$_2$ model with the estimator are given in Figure 4.
5. Conclusion
By using confirmatory factor analysis for measurement model and weighted least squares (WLS) method for the estimation parameter of spline truncated in nonlinear SEM $\omega_\eta = \Gamma \xi \gamma + \zeta$ with respect to $Q(\gamma) = \zeta \Sigma^{-1} \zeta$ can be concluded as follow:

a. variance-covariance matrix among the indicators $x$ is $\Lambda_x \Phi \Lambda_x' + \Theta_x$, among the indicators $y$ is $\Lambda_y [(I - B)^{-1}(\Gamma \Phi' + \Psi)(I - B)^{-1}] \Lambda_y' + \Phi_x$, covariance matrix between $x$ and $y$ is $\Lambda_x \Phi \Gamma_y' (I - B)^{-1} \Lambda_y'$ and matrix between $y$ and $x$ is $\Lambda_y (I - B)^{-1} \Gamma \Phi \Lambda_x'$.

b. Estimation parameter $\gamma$ of spline truncated in nonlinear SEM $\omega_\eta = \Gamma \xi \gamma + \zeta$ is $\hat{\gamma} = (\Gamma_{\xi \eta} \Sigma^{-1} \Gamma_{\xi \eta})^{-1} \Gamma_{\xi \eta} \Sigma^{-1} \omega_\eta$

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