

# Partial Least Squares Structural Equation Modeling Ib

## Model estimation

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# Outline

- 1 Introduction
- 2 Inner and outer relations
- 3 Algorithm
- 4 Interpretation and statistical properties
- 5 R example

# Outcome

This lecture will help you to understand

- ▶ The formalisation of the relationships among latent variables as well as between latent and manifest variables
- ▶ The iterative PLS-SEM algorithm
- ▶ How to interpret the model and its statistical properties

# Herman Wold (1908 - 1992) I



- ▶ Swedish Professor of statistics at Uppsala University
- ▶ Considered the “grandfather” of the family of partial least squares methods
- ▶ Also known for Cramer-Wold theorem, Wold decomposition, macro-economics and contributions to utility theory
- ▶ His work on causality has been characterized as being decades ahead of time (see e.g. Judea Pearl’s book “Causality” (2nd edition))
- ▶ Member of Nobel Economic Science Prize Committee from 1968 - 1980

# Herman Wold (1908 - 1992) II



- ▶ The development of the PLS algorithm in 1977 was founded on two other developments he made
  - ▶ Fixed-Point algorithm: Iterative ordinary least squares algorithm to estimate coefficients of a system of simultaneous equations
  - ▶ NIPALS (Non-linear Iterative Partial Least Squares) algorithm: Which among other things can calculate principal components and canonical correlations

# Structural equation modeling (SEM)

- ▶ “Structural”: Each inner equation should represent a hypothesized causal relationships between a set of (latent) variables, and the form of each equation conveys the assumptions that the analyst has asserted
- ▶ Two main ways of estimating SEM models
  - 1 Based on the covariance matrix of the variables: Developed primarily by Karl Jöreskog, a doctoral student of Herman Wold
  - 2 Using the PLS-SEM algorithm (which we will soon visit) developed by Herman Wold

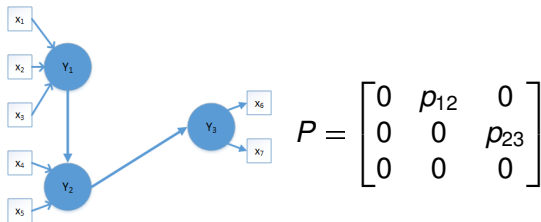
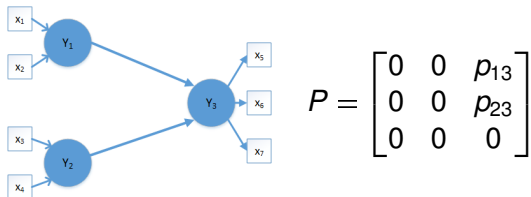
# Inner relations I

Let  $N$  be the sample size,  $K$  the number of indicators/observed variables and  $H$  be the number of latent variables

$$(1) \quad Y = Y \cdot \underbrace{(P + t(P))}_C + v$$

- ▶  $Y$  is a  $N \times H$  matrix of latent variables
- ▶  $P$  is a  $H \times H$  matrix of inner weights/path coefficients
  - ▶ Is upper diagonal
  - ▶ Restrictions on  $P$  determines the inner model
- ▶  $v$  is a  $N \times H$  matrix of inner errors

# Inner relations II



**Figure:** Different constraints on the inner weights

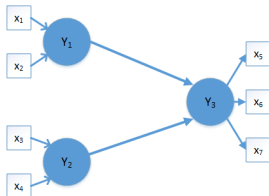


# Outer relations - correlation weights (mode A) I

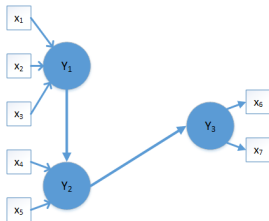
$$(2) \quad X = Y \cdot L + \varepsilon$$

- ▶  $X$  is a  $N \times K$  matrix of standardized indicators
- ▶  $Y$  is a  $N \times H$  matrix of latent variables
- ▶  $L$  is a  $H \times K$  matrix of correlation weights/loadings
- ▶  $\varepsilon$  is a  $N \times K$  matrix of outer errors

# Outer relations - correlation weights (mode A) II



$$L = \begin{bmatrix} l_{11} & l_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & l_{23} & l_{24} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & l_{35} & l_{36} & l_{37} \end{bmatrix}$$



$$L = \begin{bmatrix} l_{11} & l_{12} & l_{13} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & l_{24} & l_{25} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & l_{36} & l_{37} \end{bmatrix}$$

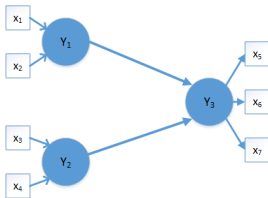
Figure: Different constraints on the correlation weights

# Outer relations - regression weights (mode B) I

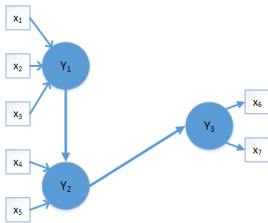
$$(3) \quad Y = X \cdot \Omega + \delta$$

- ▶  $Y$  is a  $N \times H$  matrix of latent variables
- ▶  $X$  is a  $N \times K$  matrix of standardized indicators
- ▶  $\Omega$  is a  $K \times H$  matrix of regression weights/weights
- ▶  $\delta$  is a  $N \times K$  matrix of validity errors

# Outer relations - regression weights (mode B) II



$$\Omega = \begin{bmatrix} \omega_{11} & 0 & 0 \\ \omega_{21} & 0 & 0 \\ 0 & \omega_{32} & 0 \\ 0 & \omega_{42} & 0 \\ 0 & 0 & \omega_{53} \\ 0 & 0 & \omega_{63} \\ 0 & 0 & \omega_{73} \end{bmatrix}$$



$$\Omega = \begin{bmatrix} \omega_{11} & 0 & 0 \\ \omega_{21} & 0 & 0 \\ \omega_{31} & 0 & 0 \\ 0 & \omega_{42} & 0 \\ 0 & \omega_{52} & 0 \\ 0 & 0 & \omega_{63} \\ 0 & 0 & \omega_{73} \end{bmatrix}$$

Figure: Different constraints on the regression weights

# Assumptions

- ▶ The relations in the model are linear (as given in the previous slides)
- ▶ We do not need to assume a specific distribution of our variables
- ▶ For identification we assume
  - ▶  $Var(Y_j) = 1$  for  $j = 1, \dots, H$
  - ▶  $E(Y_j) = 0$  for  $j = 1, \dots, H$

# The PLS-SEM algorithm

- 1 Initialization: Standardize all indicators, and create an initial (poor) approximation of the LV scores
  - 2 Inner approximation: Estimate inner weights (using one of three weighting schemes) and use these weights to approximate the LV's
  - 3 Outer approximation: Estimate temporary correlation and/or regression weights (depending on type of measurement model) to approximate LV's as weighted sums of their indicators
  - 4 Convergence: Iterate step 2 and 3 until there is convergence of temporary correlation and regression weights
  - 5 Final estimates: Estimate correlation weights, regression weights and inner weights using standardized LV's
- See also small R script for illustration

# PLS-SEM algorithm - step 1: initialization

- ▶ Standardize all indicators,  $X$
- ▶ Choose initial weights by setting  $\omega_{ij} = 1$  for all  $i, j$  and let  $W^0 = \Omega$
- ▶ Make approximate LV's,  $\hat{Y}^{*0} = X \cdot W^0$

# PLS-SEM algorithm - step 2: inner approximation

- ▶ We can choose between three different estimates of the inner weighting schemes,  $\hat{P}^{i-1} = f(\hat{Y}^{*(i-1)}), i = 1, \dots$ 
  - ▶ Factorial: The inner weights are the correlation between adjacent approximate LV's
  - ▶ Centroid: The inner weights are the sign of the correlation between adjacent approximate LV's
  - ▶ Path: The inner weights are the regression coefficients in an OLS regression with the endogenous approximate LV as dependent and its exogenous approximate LV' as independent variables (preferred)
- ▶ Update approximate LV's,

$$\hat{Y}^i = \hat{Y}^{*(i-1)} \cdot (\hat{P}^{i-1} + t(\hat{P}^{i-1})) = \hat{Y}^{*(i-1)} \cdot \hat{C}^{i-1}, i = 1, \dots$$

- ▶ Standardize approximate LV's



# PLS-SEM algorithm - step 3: outer approximation

- ▶ Update approximate LV's as a weighted sum

$$\hat{Y}^{*i} = X \cdot \hat{W}^i, i = 1, \dots$$

where  $\hat{W}^i = g(\hat{Y}^i)$  is a  $K \times H$  matrix of temporary weights and  $\hat{Y}^*$  is the approximate LV's

- ▶ When a LV is measured reflectively, it is the estimated correlation weights,  $\hat{L}^i$ , that are used as weights in the weighted sum
- ▶ When a LV is measured formatively, it is the estimated regression weights,  $\hat{\Omega}^i$ , that are used as weights in the weighted sum
- ▶ Standardize approximate LV's

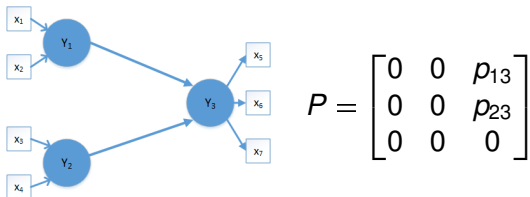
# PLS-SEM algorithm - step 4 and 5

- ▶ Based on the initialization and step 2 and 3 we get the sequence,

$$\hat{Y}^{*0}, \hat{Y}^1, \hat{Y}^{*1}, \hat{Y}^2, \hat{Y}^{*2}, \dots$$

- ▶ When  $\hat{W}^i$  only change by a small amount from one iteration to the next, the iterations stops. We denote the final weights (after convergence) as  $\hat{W}$
- ▶ The final LV scores are calculated as  $\hat{Y} = X \cdot \hat{W}$
- ▶ Using the LV scores,  $\hat{Y}$ , and the indicators,  $X$ , the final parameter estimates,  $\hat{P}$  (using the path weighting scheme),  $\hat{L}$  and  $\hat{\Omega}$  are calculated

## Estimation after convergence – inner relations

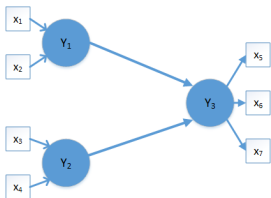


- ▶ We recall that the inner relations are given by  $Y = Y \cdot (P + P') + \nu$
- ▶ The inner weights,  $P$ , are estimated by a range of separate OLS regressions using the estimated LV scores
- ▶ For example, the weights  $p_{13}$  and  $p_{23}$  are estimated from the linear regression

$$\hat{Y}_3 = p_{13} \hat{Y}_1 + p_{23} \hat{Y}_2 + \nu_3$$

- ▶ We use  $\hat{\phantom{x}}$  on the LV, to indicate that we are dealing with the LV approximations from the PLS-SEM algorithm

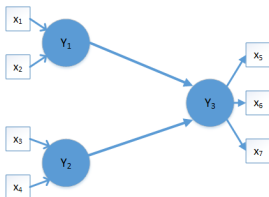
# Estimation after convergence – outer relations I



$$L = \begin{bmatrix} l_{11} & l_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & l_{23} & l_{24} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & l_{35} & l_{36} & l_{37} \end{bmatrix}$$

- ▶ We recall that the outer relations with respect to the correlation weights,  $L$ , are given as  $X = Y \cdot L + \varepsilon$
- ▶ The individual correlation weights in  $L$  are estimated as the OLS regression where the indicator is the dependent variable and its respective LV is the independent variable

## Estimation after convergence – outer relations II



$$L = \begin{bmatrix} l_{11} & l_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & l_{23} & l_{24} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & l_{35} & l_{36} & l_{37} \end{bmatrix}$$

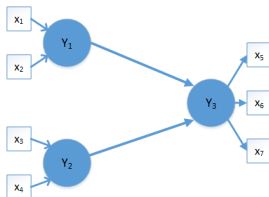
- ▶ For example, the correlation weights,  $l_{11}$  and  $l_{35}$  are estimated from two separate linear regressions:

$$x_1 = l_{11} \hat{Y}_1 + \varepsilon_1$$

$$x_5 = l_{35} \hat{Y}_3 + \varepsilon_5$$

- ▶ The regression estimates are the same as the correlation between an indicator and its LV approximation because the variables are standardized

## Estimation after convergence – outer relations III



$$\Omega = \begin{bmatrix} \omega_{11} & 0 & 0 \\ \omega_{21} & 0 & 0 \\ 0 & \omega_{32} & 0 \\ 0 & \omega_{42} & 0 \\ 0 & 0 & \omega_{53} \\ 0 & 0 & \omega_{63} \\ 0 & 0 & \omega_{73} \end{bmatrix}$$

- ▶ The regression weights are calculated by regressing each LV approximation on its indicators. For example:

$$\hat{Y}_1 = \omega_{11}x_1 + \omega_{21}x_2 + \delta_1$$

$$\hat{Y}_3 = \omega_{53}x_5 + \omega_{63}x_6 + \omega_{73}x_7 + \delta_3$$

# Interpretation

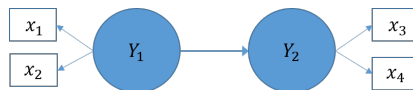
- ▶ With theoretical support of our model, the inner weights are often interpreted as causal effects
- ▶ A correlation weight can be interpreted as the effect of the LV on the indicator
- ▶ When a construct is measured reflectively, the correlation weights are used for interpretation
- ▶ A regression weight can be interpreted as the effect of the indicator on the LV
- ▶ When a construct is measured formatively, the regression weights are used for interpretation

# Model estimation - statistical properties I

- ▶ Focus on maximizing the explained variance in the dependent variables. i.e. focus is on prediction
- ▶ No distributional assumptions → rely on bootstrapping for significance testing
- ▶ Assume that all indicator variance is useful and should be used to estimate LV scores → measurement error of indicators is transferred to latent variables → typically results in overestimation of the parameters in the measurement model and attenuated estimates of the parameters in the structural model (called PLS-SEM bias)



# Model estimation - statistical properties II



- In empirical relevant settings PLS-SEM does not estimate correlations between latent variables,  $cor[Y_1, Y_2]$ , but correlations between conditional expectations of latent variables. For example, in the model given above PLS-SEM will estimate

$$cor[E(Y_1|x_1, x_2), E(Y_2|x_3, x_4)]$$

- Increasing both sample size and number of indicators sufficiently, we will estimate the correlation between the latent variables → consistency of PLS-SEM (called consistency at large)

# PLS-SEM and principal component analysis (PCA)

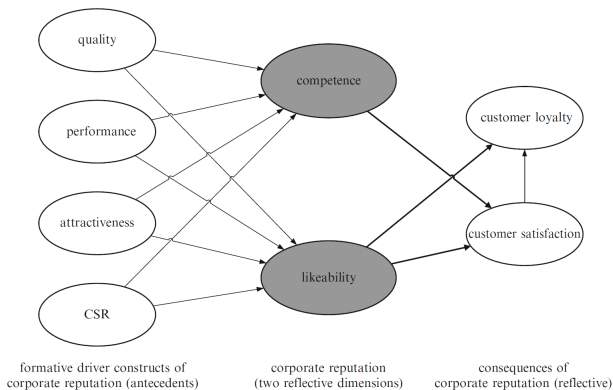
## ▶ PCA

- ▶ In PCA we extract a set of components from the set of observed variables we want to analyze
- ▶ Each component is orthogonal to the other components
- ▶ Each component is constructed as a weighted sum of all observed variables

## ▶ PLS-SEM

- ▶ The set of observed variables we want to analyze is divided in  $H$  sets, where each set only measure a specific latent variable
- ▶ The division of the variables is determined based on *prior theory* or *subject matter knowledge*
- ▶ The components are not orthogonal by construction (the purpose of PLS-SEM is to investigate if the latent variables are related to each other)
- ▶ A latent variable is constructed as a weighted sum of the observed variables intended to measure that latent variable (not all observed variables)

# Corporate reputation model from Eberl (2010)



**Figure:** The extended corporate reputation model. (Source: Eberl 2010, in Handbook of Partial Least Squares: Concepts, Methods and Applications)

# Corporate reputation I

*“(..) a stakeholder’s overall evaluation of a company over time. This evaluation is based on the stakeholder’s direct experiences with the company, any other form of communication and symbolism that provides information about the firm’s actions and/or a comparison with the actions of other leading rivals”*

(Source: Gotsi and Wilson 2001, Corporate reputation: seeking a definition)

# Corporate reputation II

- ▶ The two core dimensions of corporate reputation: Competence (COMP) and likeability (LIKE)
- ▶ Cognitive evaluation: Competence. A more rationally based dimension
- ▶ Affective evaluation: Likeability. A more emotionally based dimension
- ▶ The model aims to explain the effect of corporate reputation on customer satisfaction (CUSA) and customer loyalty (CUSL)

# Antecedent to corporate reputation

- ▶ Drivers of corporate reputation
  - ▶ Quality (QUAL)
  - ▶ Performance (PERF)
  - ▶ Attractiveness (ATTR)
  - ▶ Corporate social responsibility (CSOR)
- ▶ We will look further into these constructs in the lecture concerning the evaluation of the formative measurement model

# Data sample and scales

- ▶ Telephone interviews: asking respondents about four major network providers in German mobile communication market
- ▶ 7-point Likert scales, with higher scores indicating higher levels of agreement with these statements

Competence (COMP)	
comp_1	[The company] is a top competitor in its market.
comp_2	As far as I know, [the company] is recognized worldwide.
comp_3	I believe that [the company] performs at a premium level.
Likeability (LIKE)	
like_1	[The company] is a company that I can better identify with than other companies.
like_2	[The company] is a company that I would regret more not having if it no longer existed than I would other companies.
like_3	I regard [the company] as a likeable company.
Customer loyalty (CUSL)	
cusl_1	I would recommend [company] to friends and relatives.
cusl_2	If I had to choose again, I would choose [company] as my mobile phone service provider.
cusl_3	I will remain a customer of [company] in the future.

Figure: Table 3.1

# Subset of corporate reputation model

- In this lecture we will focus on the subset of the model where we have reflective indicators

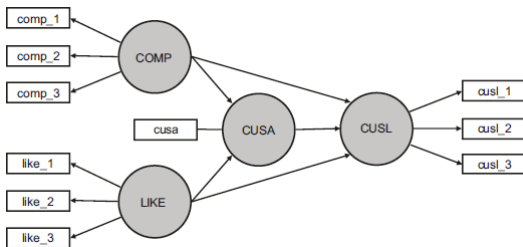


Figure: Figure 3.2



# Corporate reputation model – specification and estimation

- ▶ Data for the corporate reputation model are readily available – either directly from the `seminr` package or via the books homepage
- ▶ Data are basically already cleaned and it is just a matter of following the instructions in Hair et al. 2021
- ▶ To specify the measurement model as well as the structural model follow the instructions in Hair et al. 2021
- ▶ After having estimated the model you can assess its convergence properties – after four iterations we obtained convergence
- ▶ Many of the results from the estimation appear as point estimates – uncertainty can be assessed via bootstrapping

# Exercises

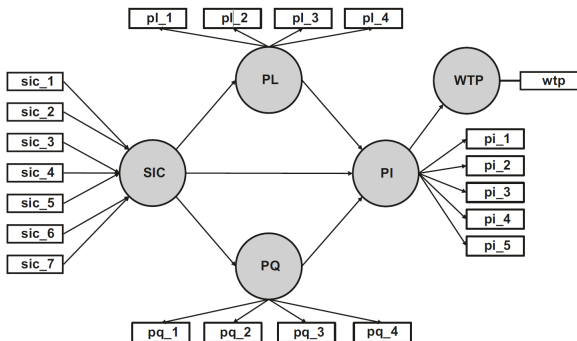


Figure: Fig 3.10

- ▶ The influencer model analyzes if consumers are likely to follow social media influencers' purchase recommendations
- ▶ See also chapter 3 in Hair et al. 2021 for a description
- ▶ Complete exercises 1,2, and 3 on page 71 in Hair et al. 2021