Partial Least Squares For Researchers: An overview and presentation of recent advances using the PLS approach

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Slides will be available after December 20th at:
http://disc-nt.cba.uh.edu/chin/indx.html

Agenda

1. List conditions that may suggest using PLS.
2. See where PLS stands in relation to other multivariate techniques.
3. Demonstrate the PLS-Graph software package for interactive PLS analyses.
4. Go over the LISREL approach.
5. Go over the PLS algorithm - implications for sample size, data distributions & epistemological relationships between measures and concepts.
6. Show a situation where PLS & LISREL results can differ.
7. Cover notions of **formative** and **reflective** measures.
8. Cover statistical re-sampling techniques for significance testing.
9. Look at second order factors, interaction effects, and multi-group comparisons.
10. Recap of the issues and conditions for using PLS.

Conditions when you might consider using PLS

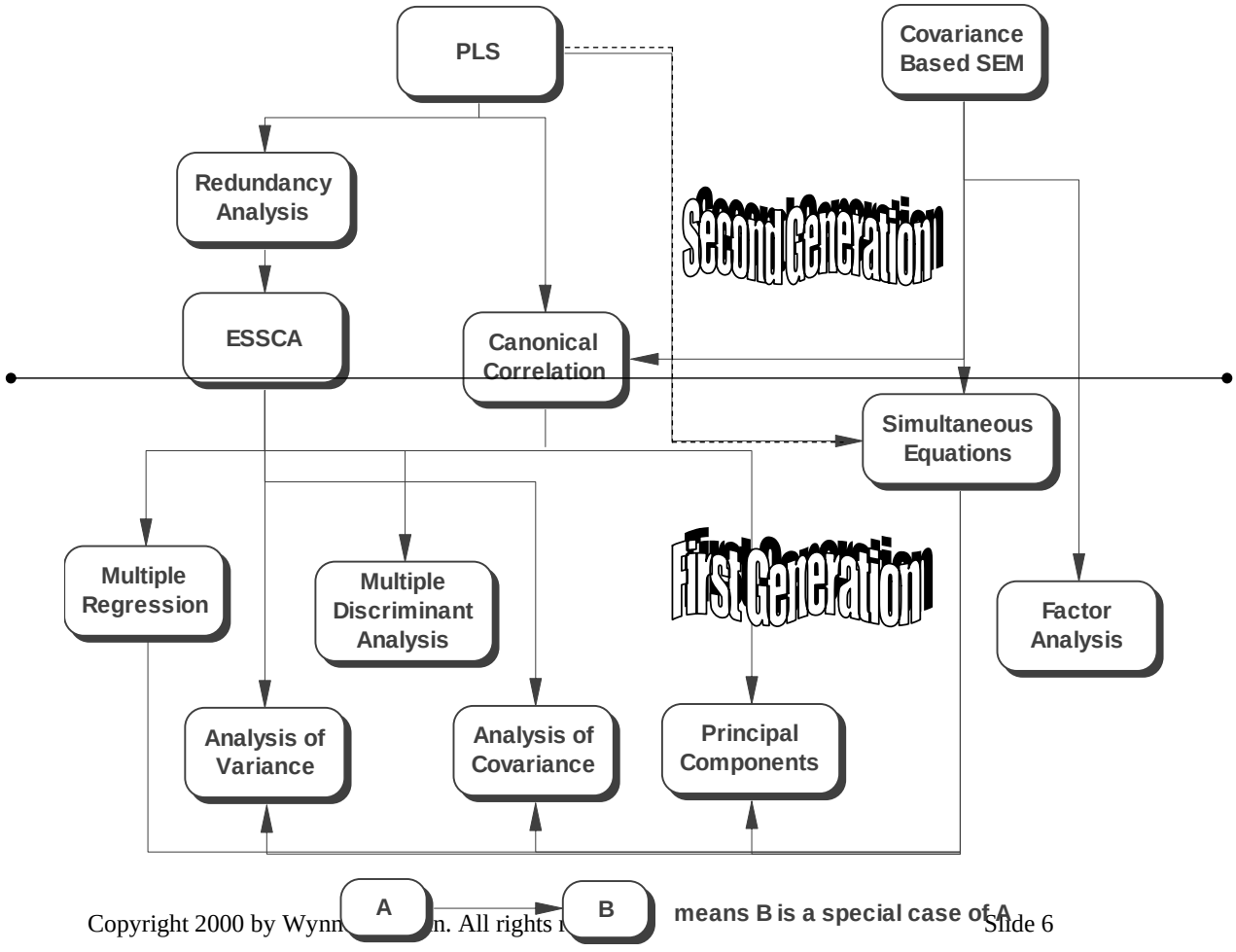
- Do you work with theoretical models that involve latent constructs?
- Do you have multicollinearity problems with variables that tap into the same issues?
- Do you want to account for measurement error?
- Do you have non-normal data?

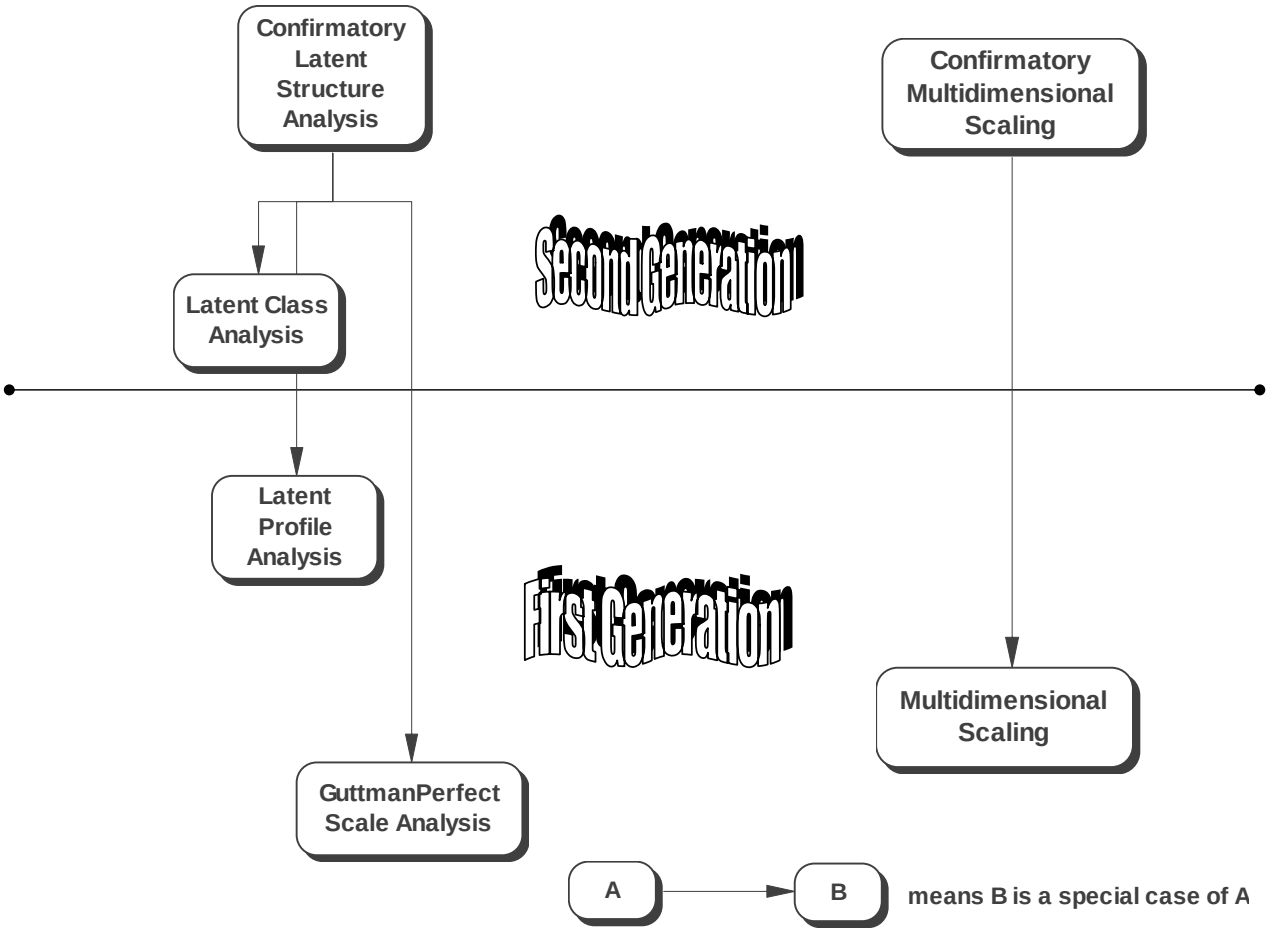
Conditions when you might consider using PLS?(continued)

- Do you have a small sample set?
- Do you wish to determine whether the measures you developed are valid and reliable within the context of the theory you are working in?
- Do you have formative as well as reflective measures?

Being a component approach, PLS covers:

- principal component,
- multiple regression
- canonical correlation,
- redundancy,
- inter-battery factor,
- multi-set canonical correlation, and
- correspondence analysis as special cases





Background of the PLS-Graph methodology

- Statistical basis initially formed in the late 60s through the 70s by econometricians in Europe.
- A Fortran based mainframe software created in the early 80s. PC version in mid 80s.
- Has been used by businesses internationally.

Background of the PLS-Graph methodology (continued)

- The PLS-Graph software has been under development for the past 8 years. Academic beta testers include Queens University, Western Ontario, UBC, MIT,UCF, AGSM, U of Michigan, U of Illinois, Florida State, National University of Singapore, NTU, Ohio State, Wharton, UCLA, Georgia State, the University of Houston, and City U of Hong Kong.

"But we just don't have the technology to carry it out."

Let's See How It Works

INTENTION

VINT1	I presently intend to use Voice Mail regularly:
VINT2	My actual intention to use Voice Mail regularly is:
VINT3	Once again, to what extent do you at present intend to use Voice Mail regularly:

VOLUNTARINESS

VVLT1	My superiors expect (would expect) me to use Voice Mail.
VVLT2	My use of Voice Mail is (would be) voluntary (as opposed to required by my superiors or job description).
VVLT3	My boss does not require (would not require) me to use Voice Mail.
VVLT4	Although it might be helpful, using Voice Mail is certainly not (would not be) compulsory in my job.

COMPATIBILITY

VCPT1	Using Voice Mail is (would be) compatible with all aspects of my work.
VCPT2	Using Voice Mail is (would be) completely compatible with my current situation.
VCPT3	I think that using Voice Mail fits (would fit) well with the way I like to work.
VCPT4	Using Voice Mail fits (would fit) into my work style.

RELATIVE ADVANTAGE

VRA1	Using Voice Mail in my job enables (would enable) me to accomplish tasks more quickly.
VRA2	Using Voice Mail improves (would imporve) my job performance.

EASE OF USE

VEOU1	Learning to operate Voice Mail is (would be) easy for me.
VEOU2	I find (would find) it easy to get Voice Mail to do what I want it to do.

RESULT DEMONSTRABILITY

VRD1	I would have no difficulty telling others about the results of using Voice Mail.
VRD2	I believe I could communicate to others the consequences of using Voice Mail.
VRD3	The results of using Voice Mail are apparent to me.
VRD4	I would have difficulty explaining why using Voice Mail may or may not be beneficial.

SEM approach

Structural Equation Modeling (SEM) represents an approach which integrates various portions of the research process in an holistic fashion. It involves:

- development of a theoretical frame where each concept draw its meaning partly through the nomological network of concepts it is embedded,
- specification of the auxillary theory which relates empirical measures and methods for measurement to theoretical concepts
- constant interplay between theory and data based on interpretation of data via ones objectives, epistemic view of data to theory, data properties, and level of theoretical knowledge and measurement.

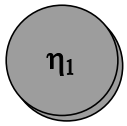
Statistically - SEM represents a second generation analytical technique which:

- Combines an econometric perspective focusing on prediction and
- a psychometric perspective modeling latent (unobserved) variables inferred from observed - measured variables.
- Resulting in greater flexibility in modeling theory with data compared to first generation techniques

SEM with causal diagrams involve three primary components:

- indicators (often called manifest variables or observed measures/variables)
- latent variable (or construct, concept, factor)
- path relationships (correlational, one-way paths, or two way paths).

indicators are normally represented as squares. For questionnaire based research, each indicator would represent a particular question.



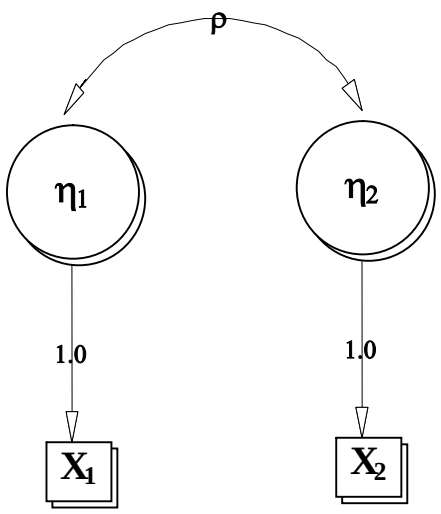
ε11

Latent variables are normally drawn as circles. In the case of error terms, for simplicity, the circle is left off. Latent variables are used to represent phenomena that cannot be measured directly. Examples would be beliefs, intention, motivation.

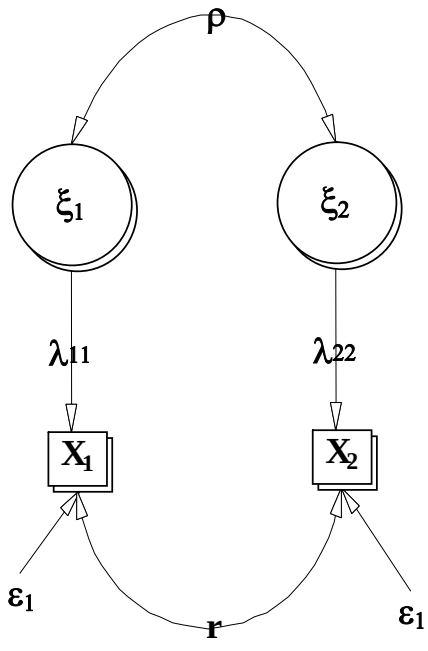
correlational relationship

recursive relationship

non-recursive relationship

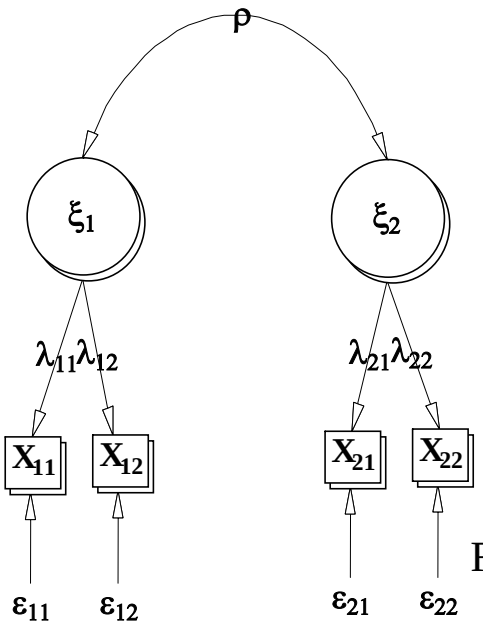


Correlation between two variables. We assume that the indicator is a perfect measure for the construct of interest.



λ_{11}	λ_{22}	ρ	r
0.90	0.90	1.00	0.81
0.90	0.90	0.79	0.64
0.90	0.90	0.62	0.50
0.80	0.80	1.00	0.64
0.80	0.80	0.78	0.50
0.80	0.80	0.63	0.40
0.70	0.70	1.00	0.49
0.70	0.70	0.82	0.40
0.70	0.70	0.61	0.30

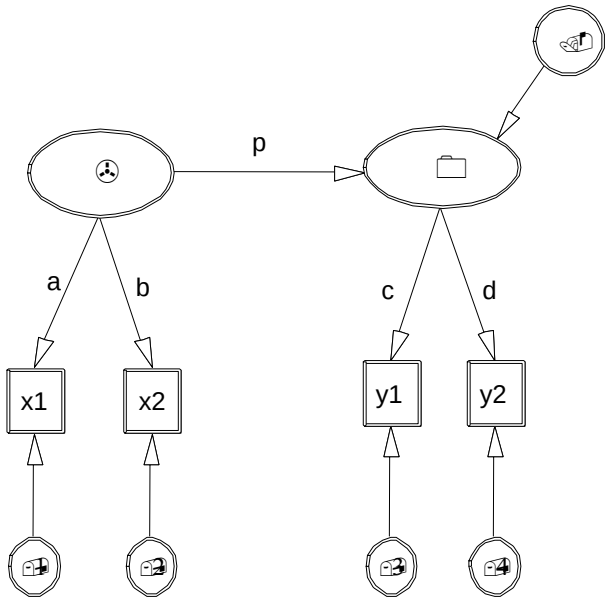
Impact of Measurement error on correlation coefficients



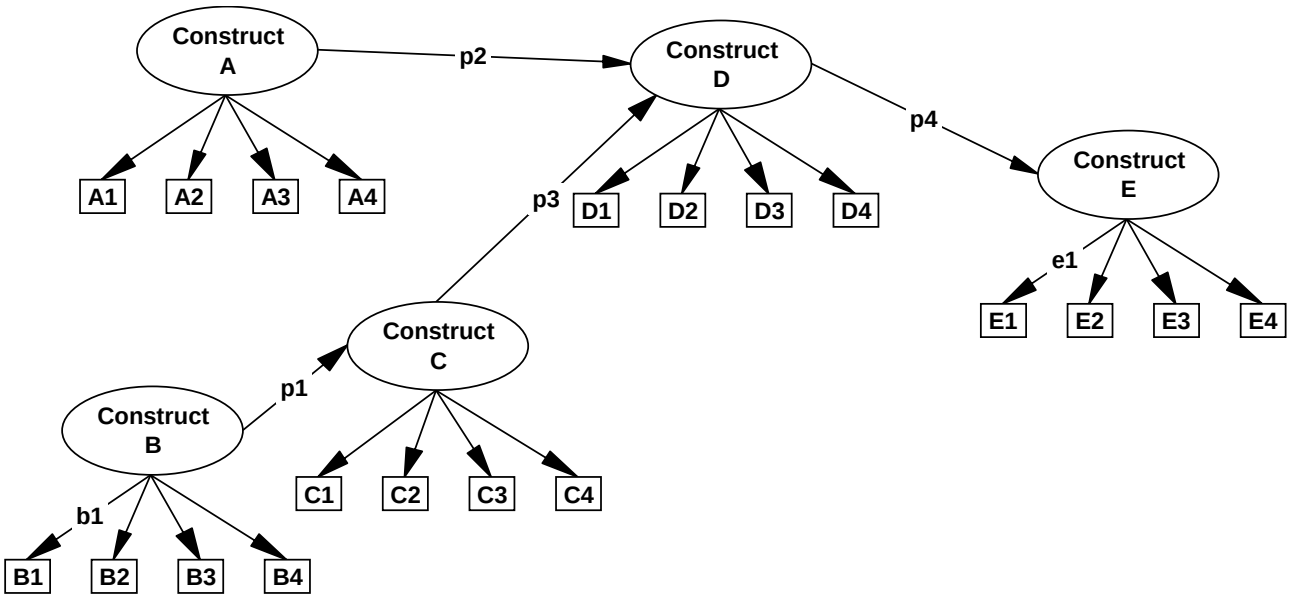
	X_{11}	X_{12}	X_{21}	X_{22}
X_{11}	1.000			
X_{12}	0.810	1.000		
X_{21}	0.576	0.576	1.000	
X_{22}	0.576	0.675	0.640	1.000

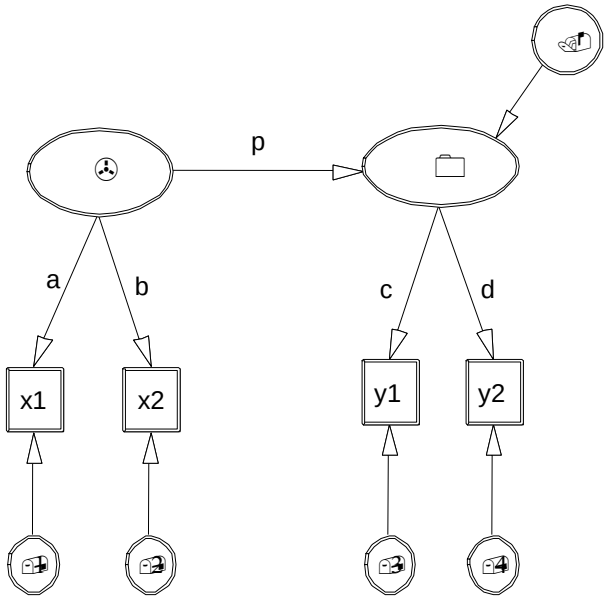
correlation matrix of indicators

$$\text{Fit Function} = \ln|\Sigma| + tr(S\Sigma^{-1}) - \ln|S| - p$$



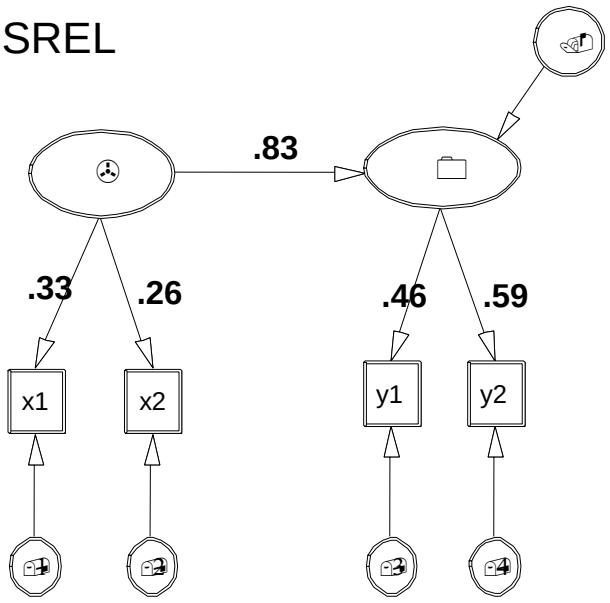
	x1	x2	y1	y2
x1	var(a) a² + var(1) = a² + var(1)			
x2	a*var(b) = a*b	var(b) b² + var(2) = b² + var(2)		
y1	a*var(p)*c =a*p*c	b*var(p)*c = b*p*c	var(c) c² + var(3)	
y2	a*var(p)*d =a*p*d	b*var(p)*d	c*var(d)	var(d) d² + var(4)





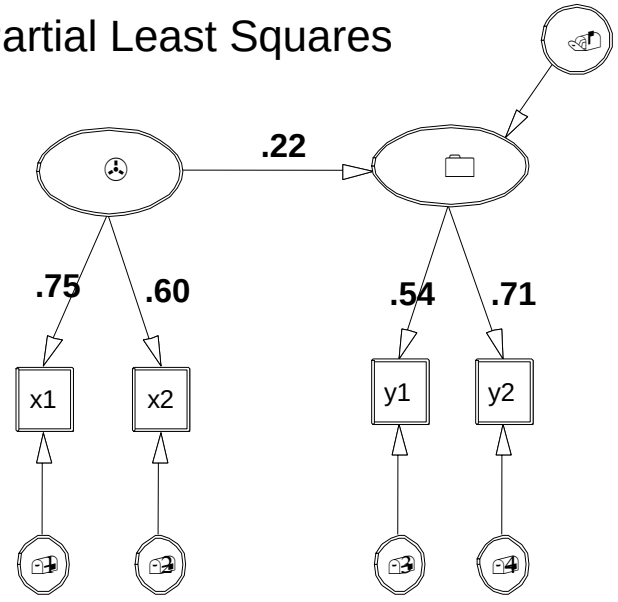
	x1	x2	y1	y2
x1	**1.00**			
x2	**.087**	**1.00**		
y1	**.140**	**.080**	**1.00**	
y2	**.152**	**.143**	**.272**	**1.00**

Results using LISREL

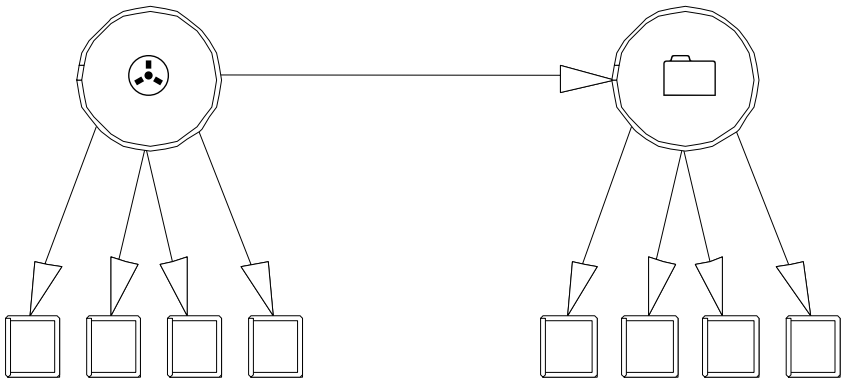


	x1	x2	y1	y2
x1	**1.00**			
x2	**.087**	**1.00**		
y1	**.140**	**.080**	**1.00**	
y2	**.152**	**.143**	**.272**	**1.00**

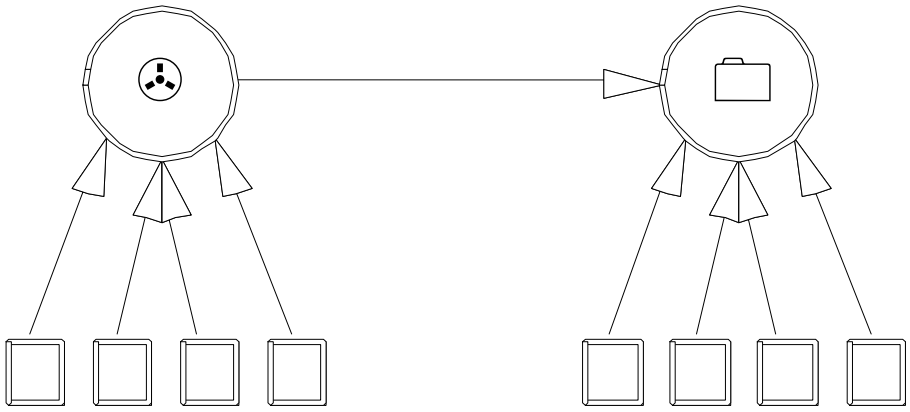
Results using Partial Least Squares



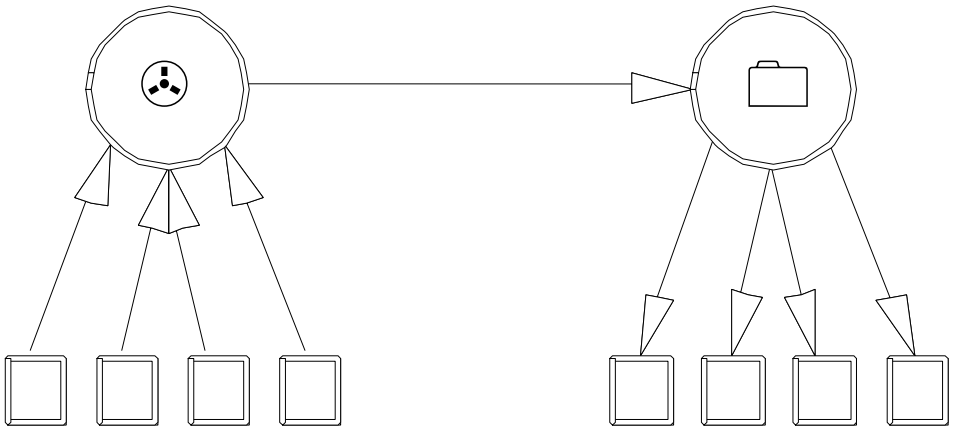
	x1	x2	y1	y2
x1	**1.00**			
x2	**.087**	**1.00**		
y1	**.140**	**.080**	**1.00**	
y2	**.152**	**.143**	**.272**	**1.00**



Interbattery factor analysis (mode A)



Canonical correlation analysis (mode B)



Redundancy Analysis (Mode C).

The basic PLS algorithm for Latent variable path analysis

- Stage 1: Iterative estimation of weights and LV scores starting at step #4,repeating steps #1 to #4 until convergence is obtained.
- Stage 2: Estimation of paths and loading coefficients.
- Stage 3: Estimation of location parameters.

#1 Inner weights

$$\upsilon_{ji} = \begin{cases} sign\,\mathrm{cov}(Y_j; Y_i) & if\ Y_i\ and\ Y_j\ are\ adjacent \\ 0 & otherwise \end{cases}$$

#2 Inside approximation

$$\tilde{Y}_j = \sum_i \upsilon_{ji} Y_i$$

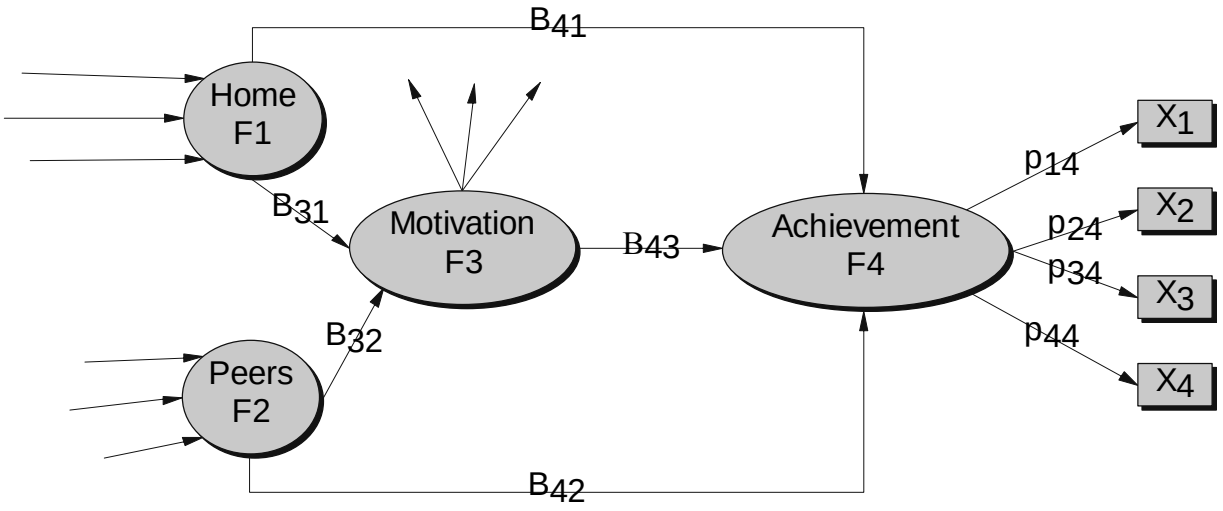
#3 Outer weights; solve for ω_{kj}

$$y_{kjn} = \tilde{\omega}_{kj} \tilde{Y}_{jn} + e_{kjn} \quad in\ a\ Mode\ A\ block$$

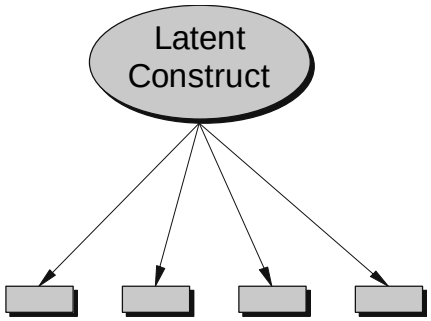
$$\tilde{Y}_{jn} = \sum_{kj} \tilde{\omega}_{kj} y_{kjn} + d_{jn} \quad in\ a\ Mode\ B\ block$$

#4 Outside approximation

$$Y_{jn} = f_j \sum_{kj} \tilde{\omega}_{kj} y_{kjn}$$

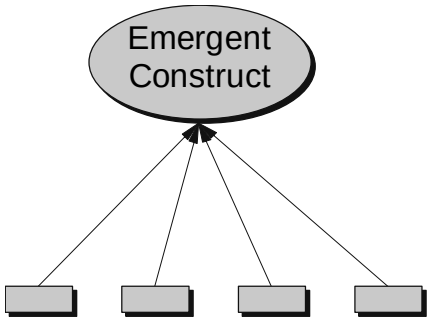


Latent or Emergent Constructs?



Reflective indicators

Parental Monitoring Ability
- self-reported evaluation
- video taped measured time
- child's assessment
- external expert



Formative indicators

Parental Monitoring Ability
- eyesight
- overall physical health
- number of children being monitored
- motivation to monitor

Latent or Emergent Constructs?

Reflective indicators

Parental Monitoring Ability
- self-reported evaluation
- video taped measured time
- child's assessment
- external expert

These measures should covary.
- If a parent behaviorally increased their monitoring ability - each measure should increase as well.

Formative indicators

Parental Monitoring Ability
- eyesight
- overall physical health
- number of children being monitored
- motivation to monitor

These measures need not covary.
- A drop in health need not imply any change in number of children being monitored.
- Measures of internal consistency do not apply.

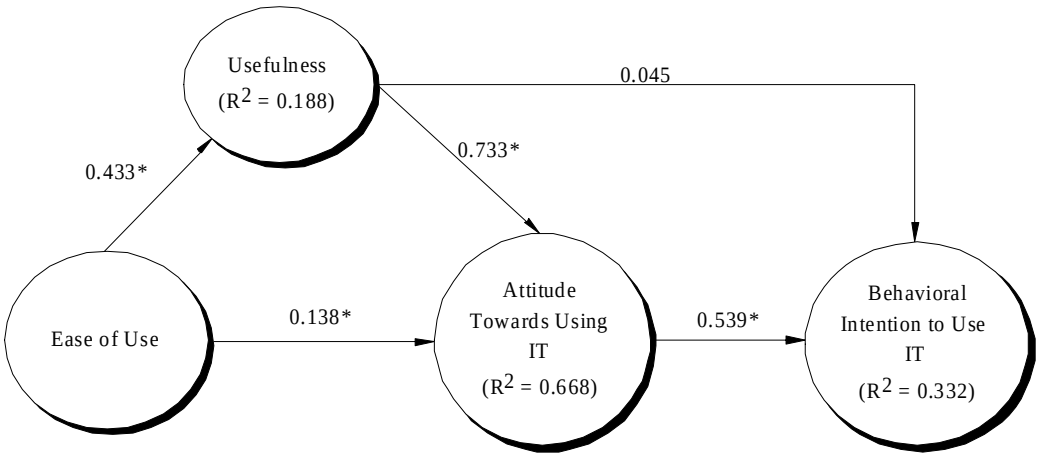
Reflective Items

R1. I have the resources, opportunities and knowledge I would need to use a database package in my job.
R2. There are no barriers to my using a database package in my job.
R3. I would be able to use a database package in my job if I wanted to.
R4. I have access to the resources I would need to use a database package in my job.

Formative Items

R5. I have access to the hardware and software I would need to use a database package in my job.
R6. I have the knowledge I would need to use a database package in my job.
R7. I would be able to find the time I would need to use a database package in my job.
R8. Financial resources (e.g., to pay for computer time) are not a barrier for me in using a database package in my job.
R9. If I needed someone's help in using a database package in my job, I could get it easily.
R10. I have the documentation (manuals, books etc.) I would need to use a database package in my job.
R11. I have access to the data (on customers, products, etc.) I would need to use a database package in my job.

Table4. The Resource Instrument
Fully anchored Likert scales were used. Responses to all items ranged from Extremely likely (7) to Extremely unlikely (1).



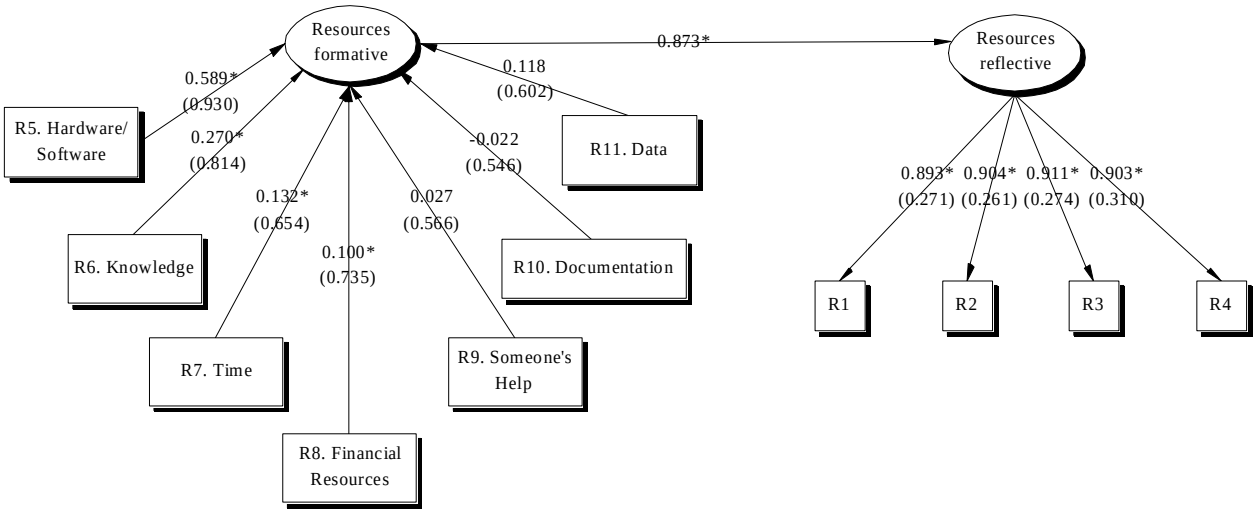
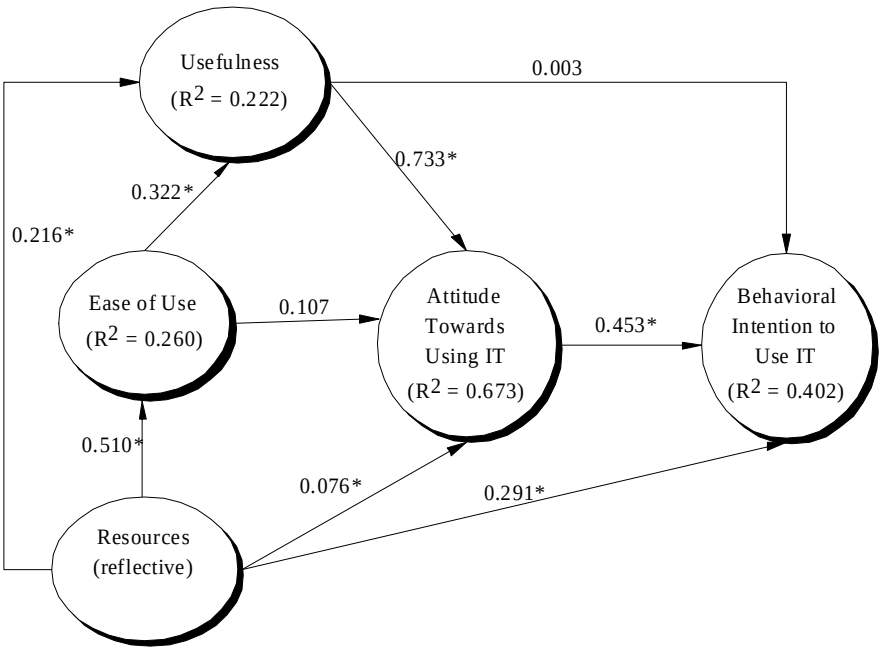
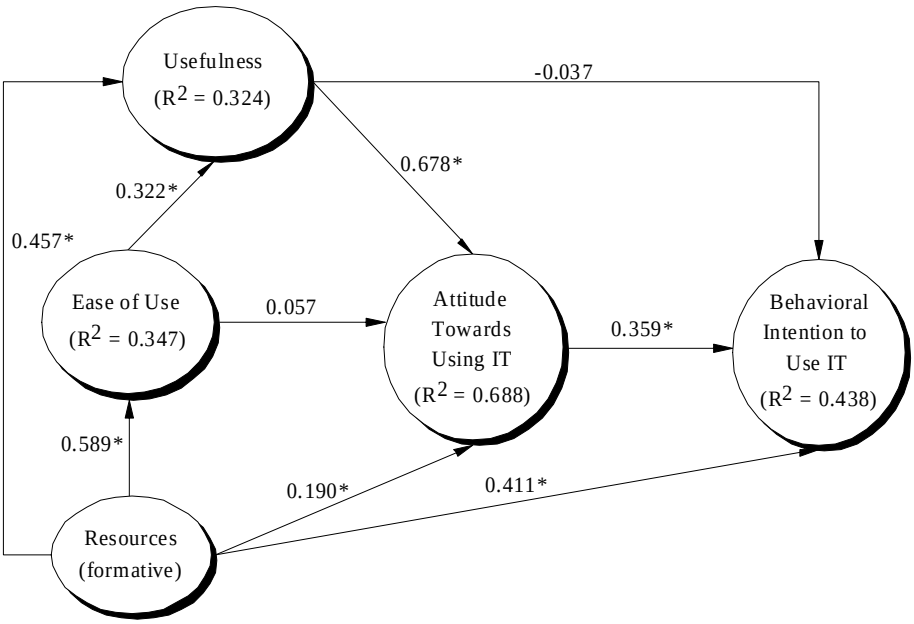


Figure 7. Redundancy analysis of perceived resources (* indicates significant estimates).





	USEFUL	EASE OF USE	RESOURCES	ATTITUDE	INTENTION
U1	**0.95**	0.40	0.37	0.78	0.48
U2	**0.96**	0.41	0.37	0.77	0.45
U3	**0.95**	0.38	0.35	0.75	0.48
U4	**0.96**	0.39	0.34	0.75	0.41
U5	**0.95**	0.43	0.35	0.78	0.45
U6	**0.96**	0.46	0.39	0.79	0.48
EOU1	0.35	**0.86**	0.53	0.42	0.35
EOU2	0.40	**0.91**	0.44	0.41	0.35
EOU3	0.40	**0.94**	0.46	0.40	0.36
EOU4	0.44	**0.90**	0.43	0.44	0.37
EOU5	0.44	**0.92**	0.50	0.46	0.36
EOU6	0.37	**0.93**	0.44	0.42	0.33
R1	0.42	0.51	**0.90**	0.41	0.42
R2	0.37	0.50	**0.91**	0.38	0.46
R3	0.31	0.46	**0.91**	0.35	0.41
R4	0.28	0.38	**0.90**	0.33	0.44
A1	0.80	0.47	0.39	**0.98**	0.54
A2	0.80	0.44	0.41	**0.99**	0.57
A3	0.78	0.45	0.41	**0.98**	0.58
I1	0.48	0.38	0.46	0.58	**0.97**
I2	0.47	0.37	0.48	0.56	**0.99**
I3	0.47	0.37	0.48	0.56	**0.99**

Loadings and Cross-Loadings for the Measurement (Outer) Model.

Composite Reliability

$$\rho_c = \frac{(\sum \lambda_i)^2 \operatorname{var} F}{(\sum \lambda_i)^2 \operatorname{var} F + \sum \Theta_{ii}}$$

where λ_i, F, and Θ_{ii}, are the factor loading, factor variance, and unique/error variance respectively. If F is set at 1, then Θ_{ii} is the **1-square of λ_i.**

Average Variance Extracted

$$AVE = \frac{\sum \lambda_i^{\,2} \operatorname{var} F}{\sum \lambda_i^{\,2} \operatorname{var} F + \sum \Theta_{ii}}$$

where λ_i, F, and Θ_{ii}, are the factor loading, factor variance, and unique/error variance respectively. If F is set at 1, then Θ_{ii} is the **1-square of λ_i.**

	Useful	Ease of use	Resources	Attitude	Intention
Useful	**0.91**				
Ease of use	0.43	**0.83**			
Resources	0.38	0.51	**0.82**		
Attitude	0.81	0.46	0.41	**0.97**	
Intention	0.48	0.38	0.48	0.58	**0.97**

Correlation Among Construct Scores (AVE extracted in diagonals).

Resampling Procedures

- Bootstrapping the Data Set
- Cross-validation - Q square
- Jackknifing

Multi-Group comparison

Ideally do permutation test.

Pragmatically, run bootstrap re-samplings for the various groups and treat the standard error estimates from each re-sampling in a parametric sense via t-tests.

$$\frac{Path_{sample\_1} - Path_{sample\_2}}{\left[\sqrt{\frac{(m-1)^2}{(m+n-2)} * S.E._{sample1}^2 + \frac{(n-1)^2}{(m+n-2)} * S.E._{sample2}^2}\right] * \left[\sqrt{\frac{1}{m} + \frac{1}{n}}\right]}$$

This would follow a t-distribution with m+n-2 degrees of freedom.
(ref: http://disc-nt.cba.uh.edu/chin/plsfaq.htm)

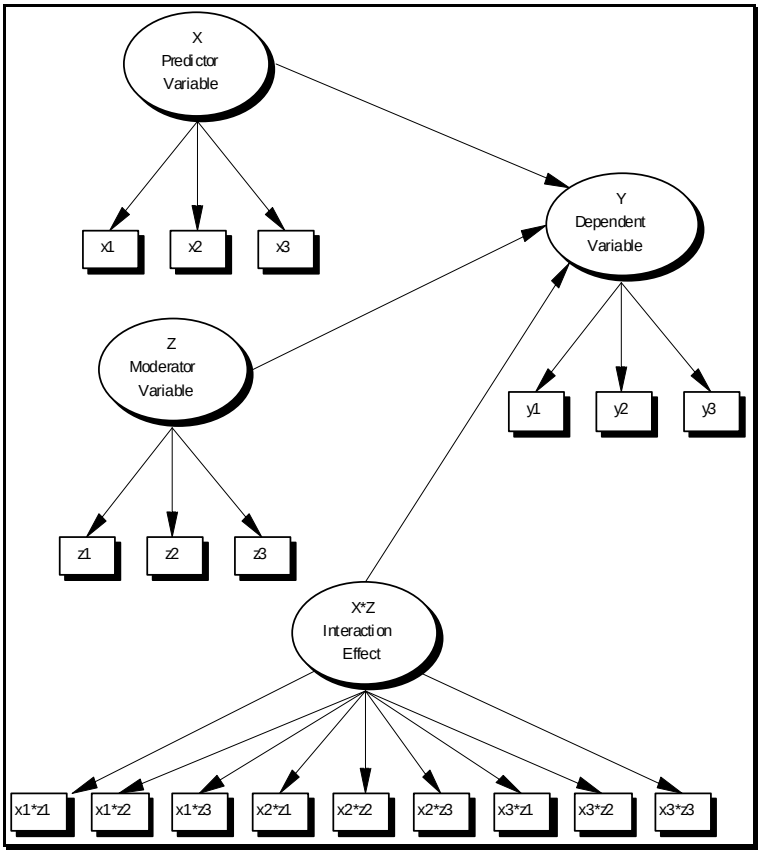
Interaction Effects with reflective indicators

Step 1: Standardize or center indicators for the main and moderating constructs.

Step 2: Create all pair-wise product indicators where each indicator from the main construct is multiplied with each indicator from the moderating construct.

Step 3: Use the new product indicators to reflect the interaction construct.

(Chin, Marcolin, & Newsted, 1996)
Paper available at: http://disc-nt.cba.uh.edu/chin/icis96.pdf



Results from Monte Carlo Simulation

	Indicators per construct						
Sample size	one item per construct	two per construct (4 for interaction)	four per construct (16 for interaction)	six per construct (36 for interaction)	eight per construct (64 for interaction)	ten per construct (100 for interaction)	twelve per construct (144 for interaction)
20	0.1458 (0.2852)	0.1609 (0.3358)	0.2708 (0.3601)	0.1897 (0.4169)	0.1988 (0.4399)	0.2788 (0.3886)	0.3557 (0.3725)
50	0.1133 (0.1604)	0.1142 (0.2124)	0.2795 (0.1873)	0.2403 (0.2795)	0.3066 (0.2183)	0.3083 (0.2707)	0.3615 (0.1848)
100	0.1012 (0.0989)	0.1614 (0.1276)	0.2472 (0.1270)	0.2669 (0.1301)	**0.3029** (0.0916)	**0.3029** (0.0805)	0.3008 (0.1352)
150	0.0953 (0.0843)	0.1695 (0.0844)	**0.2427** (0.0778)	**0.2834** (0.0757)	**0.2805** (0.0916)	**0.3040** (0.0567)	**0.2921** (0.0840)
200	0.0962 (0.0785)	**0.1769** (0.0674)	**0.2317** (0.0543)	**0.2730** (0.0528)	**0.2839** (0.0606)	**0.2843** (0.0573)	**0.3018** (0.0542)
500	0.0965 (0.0436)	**0.1681** (0.0358)	**0.2275** (0.0419)	**0.2448** (0.0379)	**0.2637** (0.0377)	**0.2659** (0.0353)	**0.2761** (0.0375)

The Impact of Heterogeneous Loadings on the Interaction Estimate (PLS vs. Regression – sample size = 100)

Factor Loading Patterns for 8 items - pattern repeated for both X and Z constructs[a]	PLS Product Indicator Estimates[b]	Regression Estimates Using Averaged Scores[b]
4 at .80 2 at .70 2 at.60	x*z--> y **0.307** (0.0970)	x*z--> y **0.2562** (0.0831)
4 at .80 4 at .70	x*z--> y **0.3043** (0.0957)	x*z--> y **0.2646** (0.0902)
4 at .80 4 at .60	x*z--> y **0.3052** (0.1004)	x*z--> y **0.2542** (0.0795)
4 at .80 2 at .60 2 at .40	x*z--> y **0.3068** (0.0969)	x*z--> y **0.2338** (0.0801)
6 at .80 2 at .40	x*z--> y **0.3012** (0.1048)	x*z--> y **0.2461** (0.0886)
4 at .70 4 at.60	x*z--> y **0.2999** (0.1277)	x*z--> y **0.2324** (0.0806)
4 at.70 2 at .60 2 at .30	x*z--> y **0.3193** (0.1298)	x*z--> y **0.2209** (0.0816)

Interaction with formative indicators

Follow a two step construct score procedure.

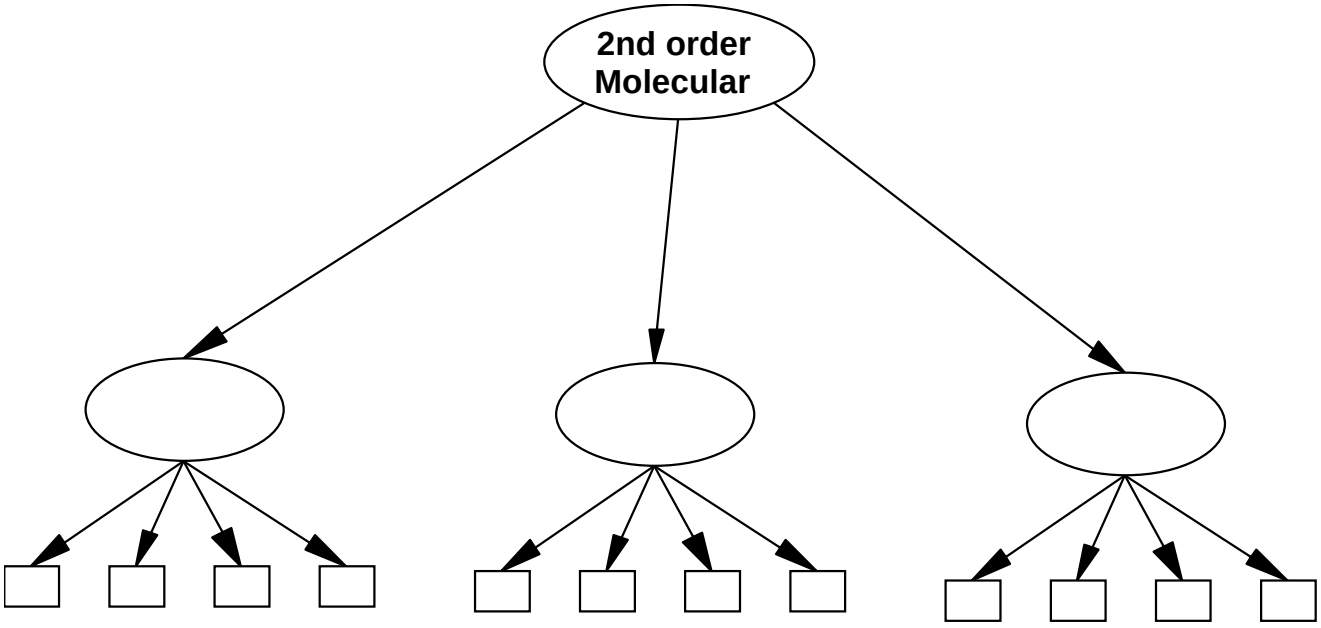
Step 1: Use the formative indicators in conjunction with PLS to create underlying construct scores for the predictor and moderator variables.

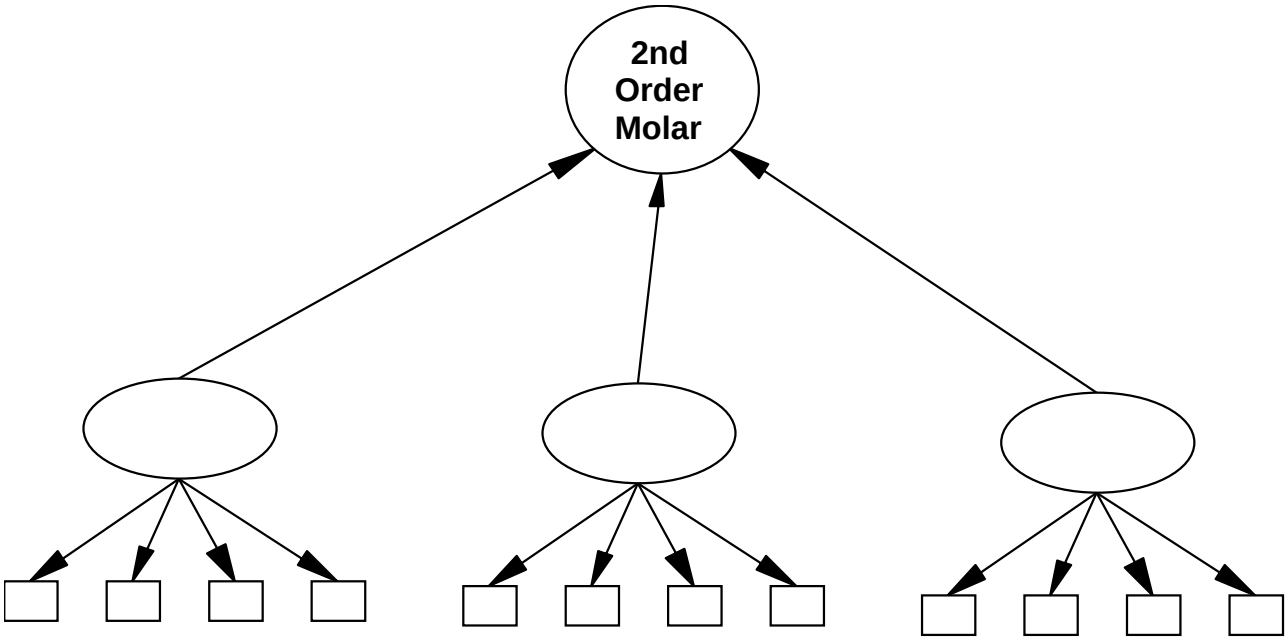
Step 2: Take the single composite scores from PLS to create a single interaction term.

Caveat: This approach has yet to be tested in a Monte Carlo simulation.

Second Order Factors

- Second order factors can be approximated using various procedures.
- The method of repeated indicators known as the hierarchical component model suggested by Wold (cf. Lohmöller, 1989, pp. 130-133) is easiest to implement.
- Second order factor is directly measured by observed variables for all the first order factors that are measured with reflective indicators.
- While this approach repeats the number of manifest variables used, the model can be estimated by the standard PLS algorithm.
- This procedure works best with equal numbers of indicators for each construct.





Considerations when choosing between PLS and LISREL

- Objectives
- Theoretical constructs - indeterminate vs. defined
- Epistemic relationships
- Theory requirements
- Empirical factors
- Computational issues - identification & speed

Objectives

- Prediction versus explanation

Theoretical constructs - Indeterminate versus defined

- For PLS - the latent variables are estimated as linear aggregates or components. The latent variable scores are estimated directly. If raw data is used, scoring coefficients are estimated.
- For LISREL - Indeterminacy

Epistemic relationships

- Latent constructs with reflective indicators - LISREL & PLS
- Emergent constructs with formative indicators - PLS
- By choosing different weighting “modes” the model builder shifts the emphasis of the model from a structural causal explanation of the covariance matrix to a prediction/reconstruction forecast of the raw data matrix

Theory requirements

- LISREL expects strong theory (confirmation mode)
- PLS is flexible

Empirical factors

- Distributional assumptions
  - PLS estimation is a “rigid” technique that requires only “soft” assumptions about the distributional characteristics of the raw data.
  - LISREL requires more stringent conditions.

Empirical factors (continued)

- Sample Size depends on power analysis, but much smaller for PLS
  - PLS heuristic of ten times the greater of the following two (ideally use power analysis)
    - construct with the greatest number of formative indicators
    - construct with the greatest number of structural paths going into it
  - LISREL heuristic - at least 200 cases or 10 times the number of parameters estimated.

Empirical factors (continued)

- Types of measures
  - PLS can use categorical through ratio measures
  - LISREL generally expects interval level, otherwise need PRELIS preprocessing.

Computational issues - Identification

- Are estimates unique?
- Under recursive models - PLS is always identified
- LISREL - depends on the model. Ideally need 4 or more indicators per construct to be over determined, 3 to be just identified. Algebraic proof for identification.

Computational issues - Speed

- PLS estimation is fast and avoids the problem of negative variance estimates (i.e., Heywood cases)
- PLS needs less computing time and memory. The PLS-Graph program can handle up to 400 indicators. Models with 50 to 100 are estimated in a matter of seconds.

SUMMARIZING

Criterion	PLS	CBSEM
Objective	Prediction oriented	Parameter oriented
Approach	Variance based	Covariance based
Assumptions	Predictor Specification (non parametric)	Typically multivariate normal distribution and independent observations (parametric)
Parameter estimates	Consistent as indicators and sample size increase (i.e., consistency at large)	Consistent
Latent Variable scores	Explicitly estimated	Indeterminate

(ref: Chin & Newsted, 1999 In Rick Hoyle (Ed.), Statistical Strategies for Small Sample Research, Sage Publications, pp. 307-341)

SUMMARIZING

Criterion	PLS	CBSEM
Epistemic relationship between a latent variable and its measures	Can be modeled in either formative or reflective mode	Typically only with reflective indicators
Implications	Optimal for prediction accuracy	Optimal for parameter accuracy
Model Complexity	Large complexity (e.g., 100 constructs and 1000 indicators)	Small to moderate complexity (e.g., less than 100 indicators)
Sample Size	Power analysis based on the portion of the model with the largest number of predictors. Minimal recommendations range from 30 to 100 cases.	Ideally based on power analysis of specific model - minimal recommendations range from 200 to 800.

(ref: Chin & Newsted, 1999 In Rick Hoyle (Ed.), Statistical Strategies for Small Sample Research, Sage Publications, pp. 307-341)

Additional Questions?

Slides will be available after December 20th at:
http://disc-nt.cba.uh.edu/chin/indx.html

