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

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Some questions

• I would like a description of how to interpret the models.
• What do all of Greek letters mean?
• Which fit statistics are most important?
• What are the rules of thumb for the fit statistics?
• What are paths and how are the path statistics interpreted?
Some questions

• What are the advantages/disadvantages of using the measurement models (PLS or SEM) as compared to using factor analysis (exploratory and confirmatory) and item reliability analysis?
• Is it possible to use the measurement models to understand construct validity (discriminant validity and convergent validity)?

Some questions

• How much impact does sample size have? I am aware of the 7-10 observations per item rule of thumb, but how sensitive are the statistics to variations in this rule of thumb? (i.e., as a reviewer, when should I question the use of one of the techniques?)
• When to use PLS v. LISREL etc. What are the advantages of PLS?
Some questions

• How to interpret results - I'm a little more familiar with LISREL, but with many of these approaches there are multiple indicators of the quality of the solution (i.e., fit indices in LISREL, etc.) which makes it difficult to know which ones to report? Also, when do I have a "good" solution?
• What do I look for when I am reviewing a paper that uses these techniques? What things should be reported, how might I evaluate what is reported.

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. Gain some understanding of causal diagrams and go over the LISREL approach.
5. Go over the PLS algorithm - implications for sample size, data distributions & epistemological relationships between measures and concepts.
6. Cover notions of formative and reflective measures.
7. See how PLS and LISREL compare and compliment one another.
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.
Do any of the following pertain to you?

- 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?

Do any of the following pertain to you? (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,
- 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 companies such as IBM, Ford, ATT and GM.
Background of the PLS-Graph methodology (continued)

- The PLS-Graph software has been under development for the past 9 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

<table>
<thead>
<tr>
<th>Constructs</th>
<th>Source</th>
<th>Original Definition</th>
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<tbody>
<tr>
<td>Perceived Usefulness</td>
<td>Davis (1989)</td>
<td>The degree to which a person believes that using a particular system would enhance his or her job performance.</td>
</tr>
<tr>
<td>Perceived Ease of Use</td>
<td>Davis (1989)</td>
<td>The degree to which a person believes that using a particular system would be free of effort.</td>
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<tr>
<td>Compatibility</td>
<td>Moore and Benbasat (1991)</td>
<td>The degree to which an innovation is perceived as being consistent with the existing values, needs, and past experiences of potential adopters.</td>
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<tr>
<td>Voluntariness</td>
<td>Moore and Benbasat (1991)</td>
<td>The degree to which use of the innovation is perceived as being voluntary, or of free will.</td>
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<td>Result Demonstrability</td>
<td>Moore and Benbasat (1991)</td>
<td>The degree to which the results of an innovation are communicable to others.</td>
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<tr>
<td>Adoption intention</td>
<td>authors</td>
<td>A measure of the strength of one’s intention to perform a behavior (e.g., use voice mail).</td>
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</tbody>
</table>
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.
PERCEIVED USEFULNESS

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

VRA2 Using Voice Mail improves (would improve) 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.
ATTITUDE

All things considered, my using Voice Mail is (would be):

- pleasant  unpleasant
- good  bad
- likable  dislikable
- harmful  beneficial
- wise  foolish
- negative  positive
- valuable  worthless

“We’re getting the wrong results. ... Ask the question differently.”
Introduction To Structural Equation Modeling

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 auxiliary theory which relates empirical measures and methods for measurement to theoretical concepts
- constant interplay between theory and data based on interpretation of data via one's 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 modeling flexibility include:

- Modeling multiple predictors and criterion variables
- Construct latent (unobservable) variables
- Model errors in measurement for observed variables due to noise and other unique factors
- Confirmatory analysis - Statistically test prior substantive/theoretical and measurement assumption against empirical data

Viewed as an extension or generalization of first generation techniques - SEM can be used to perform the following analyses:

- Factor or component based analysis
- Discriminant analysis
- Multiple regression
- Canonical correlation
- MANOVA
At this point, I’d like to:

- Provide a non-technical introduction to the logic behind structural equation modeling (SEM) - both covariance and partial least squares based
- Introduce the casual diagramming approach and concepts underlying it
- Contrast SEM to other methods (in particular multiple regression) and demonstrate why accounting for measurement error using SEM is very important
Postivistic Mechanistic Choo Choo Train Model

Holistic, gwounded (as in living-in-the-hole-in-the-gwound), "wabbit" model
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.

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.

Relationships:
- 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.

Multiple regression with two independent variables

\[ y = b_1 X_1 + b_2 X_2 + \text{error} \]
Simple Regression

Multiple Regression

Path Analysis
Causal Chain System
(Recursive)

Path Analysis
Interdependent System
(Non-recursive)
Impact of Measurement error on correlation coefficients

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<th>$r$</th>
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Correlated Two Factor Model

\[ \rho \]

\[ \xi_1 \]

\[ \xi_2 \]

\[ \lambda_1, \lambda_2, \lambda_1 \]

\[ \lambda_2, \lambda_3, \lambda_3 \]

\[ X_{11}, X_{12}, X_{13} \]

\[ X_{21}, X_{22}, X_{23} \]

\[ \varepsilon_{11}, \varepsilon_{12}, \varepsilon_{13} \]

\[ \varepsilon_{21}, \varepsilon_{22}, \varepsilon_{23} \]

Correlation matrix of indicators

\[
\begin{pmatrix}
X_{11} & X_{12} & X_{13} & X_{22} \\
X_{11} & 1.000 & & \\
X_{12} & 0.810 & 1.000 & \\
X_{21} & 0.576 & 0.576 & 1.000 \\
X_{22} & 0.576 & 0.675 & 0.640 & 1.000
\end{pmatrix}
\]

Fit Function = \( \ln|\Sigma| + tr(\Sigma^{-1}) - \ln|\Sigma| - p \)
More Graphical Representations

More Graphical Representations
Two-block model with reflective indicators.

Two-block model with reflective indicators.

\[
\begin{array}{cccc}
\xi & p & \eta \\
\xi_1 & a & x_1 & b & x_2 & c & y_1 & d & y_2 \\
\varepsilon_1 &  & \varepsilon_2 &  & \varepsilon_3 &  & \varepsilon_4 &  \\
\end{array}
\]

\[
\begin{array}{cccc}
x_1 & 1.00 \\
x_2 & .81 & 1.00 \\
y_1 & .576 & .586 & 1.00 \\
y_2 & .576 & .576 & .64 & 1.00 \\
\end{array}
\]
### Results using LISREL

**Diagram:**

- Nodes: $\zeta$, $\eta$.
- Edges:
  - $\zeta$ to $\eta$: 0.83
  - $x_1$ to $\zeta$: 0.33
  - $x_2$ to $\zeta$: 0.59
  - $x_2$ to $x_1$: 0.25
  - $x_2$ to $x_2$: 0.26
  - $y_1$ to $\eta$: 0.46
  - $y_2$ to $\eta$: 0.59
  - $y_1$ to $y_1$: 0.14
  - $y_2$ to $y_2$: 0.14

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Results using Partial Least Squares

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<th>x2</th>
<th>y1</th>
<th>y2</th>
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<td></td>
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<td>y1</td>
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<td>y2</td>
<td>.152</td>
<td>.143</td>
<td>.272</td>
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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
\[ \nu_{ji} = \begin{cases} \text{sign} \text{cov}(Y_j; Y_i) & \text{if } Y_i \text{ and } Y_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases} \]

#2 Inside approximation
\[ \tilde{Y}_j = \sum_i \nu_{ji} Y_i \]

#3 Outer weights; solve for \( \omega_{kj} \)
\[ y_{kjn} = \bar{\omega}_{kj} \tilde{Y}_{jn} + e_{kjn} \quad \text{in a Mode A block} \]
\[ \tilde{Y}_{jn} = \sum_k \omega_{kj} y_{kjn} + d_{jn} \quad \text{in a Mode B block} \]

#4 Outside approximation
\[ Y_{jn} = f_j \sum_k \bar{\omega}_{kj} y_{kjn} \]
Multiblock model (mode C).
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

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

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.
Test - Latent or Emergent Construct?

Stressful Change Events
• Been sexually attacked
• Family and parental stress
• Accident and illness events
• Family relocation events

Mother’s Ability to Interact and Monitor a Child
• Number of children in a family
• Health of the Mother
• Hours of Maternal Employment

Illness
• Number of illnesses
• Respiratory problems or illnesses
• Cardiovascular or circulatory problems

(Examples from Cohen, Cohen, Teresi, Marchi, & Velex, 1990)

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.

Table 4. 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).
Behavioral Intention to Use IT 
(R^2 = 0.402)

Attitude Towards Using IT 
(R^2 = 0.673)

Ease of Use 
(R^2 = 0.260)

Usefulness 
(R^2 = 0.222)

Resources (reflective)
Testing Fit

• Examine individual reliability of factor loadings (are most greater than .7?)
• Calculate composite reliability - similar to alpha without assumption of equal weighting
• Calculate average variance extracted - measures average variance of measures accounted for by the construct - should be greater than .5. Can be used to test discriminant validity.

Composite Reliability

\[ \rho_c = \frac{\left( \sum \lambda_i \right)^2 \text{var} F}{\left( \sum \lambda_i \right)^2 \text{var} F + \sum \Theta_{ii}} \]

where \( \lambda_i \), \( F \), and \( \Theta_{ii} \) are the factor loading, factor variance, and unique/error variance respectively. If \( F \) is set at 1, then \( \Theta_{ii} \) is the 1-square of \( \lambda_i \).
Average Variance Extracted

\[ AVE = \frac{\sum \lambda_i^2 \text{var } F}{\sum \lambda_i^2 \text{var } F + \sum \Theta_{ii}} \]

where \( \lambda_i \), F, and \( \Theta_{ii} \), are the factor loading, factor variance, and unique/error variance respectively. If F is set at 1, then \( \Theta_{ii} \) is the 1-square of \( \lambda_i \).

<table>
<thead>
<tr>
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<th>Ease of use</th>
<th>Resources</th>
<th>Attitude</th>
<th>Intention</th>
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Correlation Among Construct Scores (AVE extracted in diagonals).
Loadings and Cross-Loadings for the Measurement (Outer) Model:

<table>
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<tr>
<th>USEFUL</th>
<th>EASE OF USE</th>
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<th>ATTITUDE</th>
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Are the results presented confirmatory or exploratory?

- If initial exploratory analysis were performed on the same data set - possible capitalization of chance may occur.
- Need to provide cross-validation on a new sample.
Initial Model or set of competing models

Item measures and data gathering design developed with Model in mind; data gathered

Does the model fit the data?

Tentative Confirmation (i.e., fail to reject)

YES

Modifying Model

YES

NO

Rejected Model

Pure confirmatory mode using SEM

Exploratory mode using SEM

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.

\[
\frac{Path_{sample,1} - Path_{sample,2}}{\sqrt{\frac{(m-1)}{(m+n-2)} * S.E_{sample1}^2 + \frac{(n-1)}{(m+n-2)} * S.E_{sample2}^2}} * \sqrt{\frac{1}{m} + \frac{1}{n}}
\]

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)

Results from Monte Carlo Simulation

<table>
<thead>
<tr>
<th>Sample size</th>
<th>Indicators per construct</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>one item per construct</td>
</tr>
<tr>
<td>20</td>
<td>0.1458 (0.2852)</td>
</tr>
<tr>
<td>50</td>
<td>0.1133 (0.1604)</td>
</tr>
<tr>
<td>100</td>
<td>0.1012 (0.0989)</td>
</tr>
<tr>
<td>150</td>
<td>0.0953 (0.0843)</td>
</tr>
<tr>
<td>200</td>
<td>0.0962 (0.0785)</td>
</tr>
<tr>
<td>500</td>
<td>0.0965 (0.0436)</td>
</tr>
</tbody>
</table>

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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

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

### SUMMARIZING

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


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### Additional Questions?