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New Perspectives in Partial Least Squares and Related Methods

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Foreword

This book contains write-ups of presentations at PLS 2012 which was the 7th meeting in the series of PLS conferences and chaired by Professors Wynne Chin and David Francis at the University of Texas at Houston. Here PLS stands for partial least squares projection to latent structures. It is an approach for modeling relations between data matrices of different types of variables measured on the same set of objects (cases, individuals, chemical or biological samples, businesses, etc.).

The series was started in Paris in 1999 by Michel Tenenhaus, Vincenzo Vinci, et al., with two objectives: (a) to present interesting developments and applications of the PLS approach and (b) bring together PLS users from a wide range of fields in social, economic, natural sciences, and engineering.

It was a privilege and a joy to attend this 7th conference, listening to interesting talks, experiencing Houston and the hospitality of Wynne Chin and his team, including a fascinating visit to NASA to hear the story of the American space program.

In the tradition of the PLS-*nn* meetings, we were entertained by a great variety of PLS developments (e.g., PLS metamodels, variable selection, sparse PLS regression, distance-based PLS, significance vs. reliability, nonlinear PLS, and much more) and applications on a wide range of data, from the traditional econometric/economic data to data from genomics, brain images, epidemiology, and chemical spectroscopy. All this gave rise to numerous interesting discussions and new scientific contacts spanning the world.

It is now about 50 years since Herman Wold, my dear late father, started to look into multivariate analysis and its potential for analyzing and interpreting multidimensional econometric data. He started with principal component analysis (PCA), in computer science often called singular value decomposition (SVD). PCA can be seen as the simplest PLS model with a single block $\mathbf{X}$. One of Herman's first accomplishments in this field was to make PCA handle missing data, and he soon realized that PCA was a wonderful tool to reduce a block of data (a matrix) to something much smaller. This could then, with some modifications, be used as building blocks in complex schemes of information flow, so-called PLS path models. The PLS path

models grew in different directions as summarized in the second volume of the book *Systems under Indirect Observation* (edited by KG Jöreskog and H Wold, Amsterdam, North Holland 1982).

Around 1975 some chemists—Bruce Kowalski in Seattle, and myself in Umeå, Sweden—started to be interested in PLS-modeling. Bruce successfully tried PLS path modeling on water samples from the “Trout Creek” area in Colorado, with the same 11 ions measured at 5 sites along the creek. Myself (Svante), I investigated the simplest two-block PLS model and its use for multiple regression problems with one or several responses (y or Y). This turned out to be a powerful approach. Suddenly we could do regression-like modeling with arbitrary many X -variables even for data sets with a small number of observations. And PLS provided a model also of the X -space, greatly facilitating the chemical (or biological, or, etc.) interpretation of the results and prediction of new events. In collaboration with Harald Martens in Oslo, this was further developed to an approach of multivariate calibration where the whole spectra of samples were related to concentrations of interest, instead of the traditional calibration using data at a single wavelength.

The two-block PLS, or PLS regression, became the core of a toolbox of data mining, long before the latter term was coined, and today this has expanded to PLS-discriminant analysis, time-series PLS, hierarchical PLS, PLS-trees, three-way PLS, batch-PLS, nonlinear PLS, and more.

So, before 1999, we had two apparently dissimilar PLS camps, one in social-economic science with complex multiblock PLS path models and one in chemistry-biology and engineering limiting themselves to the simplest two-block PLS model (PLS regression). Then, at the first PLS-*nn* conference in Paris in 1999, these two camps were brought together, discussed the PLS approach in its different flavors, and considered interesting applications in various fields. The present PLS 12 conference had the same format and scope. The expansion on the natural science side is noticeable, especially what concerns biological applications, but the integration of the two approaches is still limited (see, however, the article by Löfstedt, Hanafi, and Trygg). Given the close connection between the two PLS approaches, this is somewhat strange, and with time we can hope that this division will disappear, much helped by this series of PLS-*nn* conferences.

Some interesting connections between the two approaches are seen by considering the relations between:

- (a) The simplest two-block PLS model
- (b) A hierarchical PLS model where matrix X is split into blocks—a “star-formed” path model where each X -block is connected to Y and only to Y
- (c) A PLS path model, where the blocks in (b) are arranged in a path structure, all applied to the same data, (X, Y) , and using the same Mode A for the estimation of all score vectors (LVs)

Going from (a) to (b) corresponds to installing restrictions on the model since implicit interactions between variables in different blocks are forced to be zero. Similarly, going from (b) to (c) installs further restrictions since only a few of the inner relations between the score vectors have coefficients different from zero.

Hence, by comparing the amount of explained and cross-validated variances for the **Y**-block (R^2 and Q^2 , respectively) for the three models, one will have Model (a) be “better” than Model (b), which in turn will be “better” than Model (c). This occurs because a nonrestricted model always fits data better than a restricted one, but not necessarily predicts better. If the differences in fit or predictivity are large, this indicates a misspecification of Model (c) and/or of Model (b), which can then be diagnosed further by means of the residual variances of blocks and individual variables, for both fitted and cross-validated and other residuals.

So, to conclude this brief foreword, I wish once more to thank and congratulate the organizers to an excellent and most interesting conference. And second, I would like to see—hopefully already at the next PLS-*nn* conference (i.e., PLS 2014 in Paris)—more cases where different types of PLS models (e.g., path models, hierarchical PLS regression, and ordinary PLS regression) are run on the same data, including discussions of similarities and differences.

Thanks a million.

Umeå, Sweden

Svante Wold

Preface

In 1999 the first meeting dedicated to partial least squares methods (abbreviated as PLS and also, sometimes, expanded as *projection to latent structures*) took place in Paris. Other meetings in this series took place in various cities, and in 2012, from the 19th to the 22nd of May, the seventh meeting of the partial least squares (PLS) series took place for the first time in the United States (in Houston, Texas). This *première* was a superb success with roughly 120 authors presenting 44 papers during these 4 days. These contributions were all very impressive by their quality and by their breadth. They covered the multiple dimensions of partial least squares-based methods, ranging from partial least squares regression and correlation to component-based path modeling, regularized regression, and subspace visualization. In addition several of these papers presented exciting new theoretical developments. This diversity was also expressed in the large number of domains of application presented in these papers: brain imaging, genomics, chemometrics, marketing, management, and information systems to name only but a few.

After the conference, we decided that a large number of the papers presented in the meeting were of such an impressive high quality and originality that they deserved to be made available to a wider audience and we asked the authors of the best papers if they would like to prepare a revised version of their paper. Most of the authors contacted shared our enthusiasm, and the papers that they submitted were then read and commented by anonymous reviewers, revised, and finally edited for inclusion in this volume. These 22 papers (including three invited contributions from our keynote speakers), included in *New perspectives in Partial Least Squares and Related Methods*, provide a comprehensive overview of the current state of the most advanced research related to PLS and cover all domains of PLS and related domains.

Each paper was overviewed by one editor who took charge of having the paper reviewed and edited (Hervé was in charge of the papers of Martens et al., Maroulides and Chin, Beaton et al., Ciampi et al., Krishnan et al., Le Floch et al., Kovacecic et al., and Churchill et al.; Wynne was in charge of the papers of Chin et al., Cepeda et al., Murray et al., and Newman et al.; Vincenzo was in charge of the papers of Magidson and Aluja-Banet et al.; Giorgio was in charge of the papers

of Sharma and Kim, Liu et al., Löfstedt et al., and Eslami et al.; Laura was in charge of the papers of Mehmood and Snipen, Farooq et al., and Martinez-Ruiz and Aluja-Banet). The final production of the L^AT_EX version of the book was mostly the work of Laura, Giorgio, and Hervé.

We are particularly grateful to Professor Svante Wold—one of the creators of PLS—who opened the seventh PLS meeting with an outstanding opening keynote that presented an overview of the field from its creation to its most recent developments and wrote the foreword presenting this book. We are also particularly grateful to our (anonymous) reviewers for their help and dedication.

Finally, this meeting would not have been possible without the generosity, help, and dedication of several persons, and we would like to specifically thank John Antel, Thierry Fahmy, David Francis, Michele Hoffman, Jennifer James, Yong Jin Kim, Ken Nieser, Blair Stauffer, Doug Steel Sarah J. Sweaney, Reza Vaezi, and Sean Woodward.

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