Conjugate Gradient Regularization - a Statistical Framework for Partial Least Squares Regression

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Partial Least Squares Regression comprises a large class of methods for dimensionality reduction, model interpretation, and prediction. It has proven to be successful in a wide range of applications. However, the derivation of its statistical properties often remains a challenging task. This is due to the fact that Partial Least Squares constructs latent components that also depend on the response. While this typically leads to good performance and interpretable models in practice, it makes the statistical analysis more involved. The main goal of my talk is to motivate the equivalence of Partial Least Squares to conjugate gradient regularization as a statistical framework. I will illustrate that conjugate gradient techniques allow us to study important statistical properties of Partial Least Squares in a concise way. In particular, I will present two recent results that are based on this framework.

1. The definition of its intrinsic complexity in terms of Degrees of Freedoms.

2. Its universal prediction consistency.

Further, I will discuss two applications of Partial Least Squares to problems that arise from chemistry. These include the incorporation of time-course information in near-infrared spectroscopy and the efficient classification/regression of chemical compounds.