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On the equivalence between null space and orthogonal space in latent variable modeling

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The concepts of null space (NS) and orthogonal space (OS) have been developed in independent contexts and with different purposes.
The former arises in the inversion of Partial Least Squares (PLS) regression models, as first proposed by Jaeckle & MacGregor [1], and represents a subspace in the latent space within which variations in the inputs do not affect the prediction of the outputs. The NS is particularly useful in tackling engineering problems such as process design, process scale-up, product formulation, and product transfer.
The second arises in orthogonal PLS (O-PLS) modeling, which was originally proposed by Trygg & Wold [2] as a preprocessing method for multivariate data. O-PLS provides a way to remove systematic variation from the inputs that is not correlated to the outputs. The OS is, therefore, defined as the space that contains the combinations of inputs that do not produce systematic variations in the outputs. Its most important role is in multivariate calibration.
In this study, we bridge PLS model inversion and O-PLS modeling by proving that the NS and the OS are, in fact, the same space (for the univariate response case). We also provide a graphical interpretation of the equivalence between the two spaces.

[1] C. M. Jaeckle and J. F. MacGregor, 'Industrial applications of product design through the inversion of latent variable models', Chemom. Intell. Lab. Syst., 50(2):199–210, 2000.
[2] J. Trygg and S. Wold, 'Orthogonal projections to latent structures (O-PLS)', J. Chemom, 16(3):119–128, 2002.

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