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Mullen, K.M.

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ABSTRACT

Separable nonlinear models: theory, implementation
and applications in physics and chemistry

Katharine M. Mullen

This thesis considers separable nonlinear models with random effects comprised of additive Gaussian white noise and applications thereof in physics and chemistry. Particular attention is devoted to the use of the variable projection algorithm to fit such models under least squares criteria to multiway data. Extensions of variable projection to constrain the conditionally linear parameters are developed, along with methodology to estimate the precision of parameter estimates. Software to fit separable nonlinear models under least squares criteria to data arising in physics and chemistry is implemented as the package **TIMP** for the R language and environment for statistical computing. Applications of separable nonlinear models to data arising in multi-way spectroscopy, time-resolved microscopy and time-resolved mass spectrometry experiments are investigated in-depth.