27. Model validation and improved determination of chromophore concentrations in quantitative tissue spectrophotometry

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Abstract:
Improved models based on Kubelka-Munk theory, as well as improved algorithms, for the quantification of chromophore concentrations in tissues based on optical multi-wavelength measurements, recorded in the visible range, are presented. The usefulness of principal component analysis (PCA) and canonical correlation analysis (CCA) for model validation is investigated and proven by many examples. It is shown how PCA is able to detect the number of independent components with variable contribution. A subsequent CCA points out these components, which should be included in the model function. Furthermore, three different methods for estimating the model parameters are presented: a nonlinear least squares (NLLS) algorithm, an ordinary least squares (LS) algorithm and a mixed LS-total least squares algorithm wLS-TLS with appropriate weights. The wLS-TLS algorithm offers the best compromise since it is almost as efficient as ordinary LS and almost as accurate as NLLS fitting.