Estimation of solution uncertainties for parametric inverse light-scattering problems

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Direct simulation of light scattering by single particles of arbitrary shape and composition in a wide range of sizes has become a routine endeavor due to both the development of numerically exact simulation methods and the increase of raw computer power. However, most practical applications of light scattering require one to solve the inverse problem, i.e., to characterize particles from the measured 1D or 2D light-scattering patterns (LSPs). This problem is much more challenging both conceptually and computationally; its solution currently seems feasible only if one assumes a specific particle model limiting the variation to several shape parameters. The parametric inverse problem boils down to a non-linear regression, which can be solved by standard local or global optimization techniques. However, the resulting best-fit parameters are rather meaningless without an estimate of their uncertainties. While standard statistical (e.g., Bayesian) methods exist for such estimation, they are based on strong assumptions about experimental noise, typically Gaussian errors with the same amplitude and mutually independent for all data points, i.e., for different scattering angles. There are two major limitations of these assumptions. First, many single-particle measurement techniques incur complicated distortions and do not allow repeated measurements to construct a rigorous model of the experimental noise. Second, the real particle shape can be significantly different from the simplified shape model used for the retrieval.

In my talk I will discuss an approximate method to handle both these issues, namely a concept of an effective number of degrees of freedom, calculated from the autocorrelation of the fit residuals. This concept is based on an approximate equivalence of correlated residuals (experimental errors) and a smaller number of uncorrelated ones, for which standard statistical methods are applicable. In particular, I will review the application of this concept to estimating uncertainties during the characterization of biological cells from the LSPs measured with scanning flow cytometry. I will also present a new theoretical analysis of this concept providing more rigorous justification of its usage and pinpointing remaining inherent limitations.