Interactive comment on “On retrieving refractive index of dust-like particles using shape distributions of ellipsoids” by O. Kemppinen et al.

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The main (quantitative) discussion of the paper is based on the notion of optimal (best-fit) refractive index. This is of limited informative value since such best-fit value is always a random variable affected by many different factors. Although it does allow one to conclude that various problems are possible, the discussion would be much clearer in terms of confidence regions for the refractive index. The authors do make some steps in this direction by Figs.3-6 and using the term “good-fit region”, but that is all purely qualitative (it doesn’t say which fit values are rather probable and which are not). If such confidence region is used, the main question would be not whether optimal m is close to the real one, but whether confidence region for m contains the real one.
For instance, if the latter is true, then the ellipsoidal model would be “adequate” at estimating the refractive index of the irregular particles (in terms of the confidence region). And the practical applicability of such estimation would be quantitatively described by the width of this confidence region (or of that for any derived quantity).

While the confidence region is the basic quantity commonly derived during the least-square fit, it is usually based on assumption that the fit residuals are due to some random noise. Here the situation is markedly different, since the residual is mostly due to “model errors”, i.e. the fact that the realistic model is more complicated than the ones used to fit it. As far as I know, no rigorous statistical analysis is possible in this case, however, a semi-empirical approach was proposed and successfully used for a similar problem of fitting light-scattering patterns of biological cells using simple shape models. See: D. I. Strokotov et al., “Is there a difference between T- and B-lymphocyte morphology?,” J. Biomed. Opt. 14, 064036 (2009) [doi:10.1117/1.3275471]. A. E. Moskalensky et al., “Accurate measurement of volume and shape of resting and activated blood platelets from light scattering,” J. Biomed. Opt. 18, 017001 (2013) [doi:10.1117/1.JBO.18.1.017001].

Another related issue is that of DDA accuracy. Since the discussion of confidence region (be it qualitative or quantitative) is heavily based on fit residuals, it is important to have some estimate of what part of it is due to inaccuracy of the DDA. This can be estimated for a couple of representative cases using refined discretization. An instructive exercise would be to perform the whole workflow (DDA simulation + fitting) for an ellipsoid – this will immediately lead to refractive index uncertainty due to the DDA.

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