Comments on "Near-Infrared Hyperspectral Unmixing Based on a Minimum Volume Criterion for Fast and Accurate Chemometric Characterization of Counterfeit Tablets".

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For illustration that the conceptions used by Lopes et al. are not always proper, i.e., the methods used by them are not always optimal; let us use the data published by Henry and Kim (Table 1 in their paper).[1] Figure 1 depicts the so called Borgen plot[1,3,4,5] of the data; this concrete plot is the abstract concentration space (the points can be retransformed into concentration profiles). All the three vertices of the simplices, here triangles (which have to cover the data points, i.e., the red-lined inner polygon), lying on the three feasible regions (blue-colored areas), respectively, are equally optimal solutions of the unmixing process without regarding any particular unmixing algorithms. The sizes of the feasible regions indicate the magnitude of the rotational ambiguity for the three components/endmembers, respectively. The vertices of the dashed green-lined triangle are the true solutions. The two dash-dot black-colored triangles form the Borgen triangles (they role to determine the limitations) which are necessary to construct the feasible regions.

The dash-dot and dashed magenta-lined triangles are the SISAL and MVSA solutions, respectively. It can be seen that one or two of the vertices are outside the outer polygon, thus the non-negativity is violated. Well, the vertices are rather far from the true values as well. At this point, the main conclusion can be drawn, i.e., there exists no general algorithm which is the best (optimal) for all data sets.
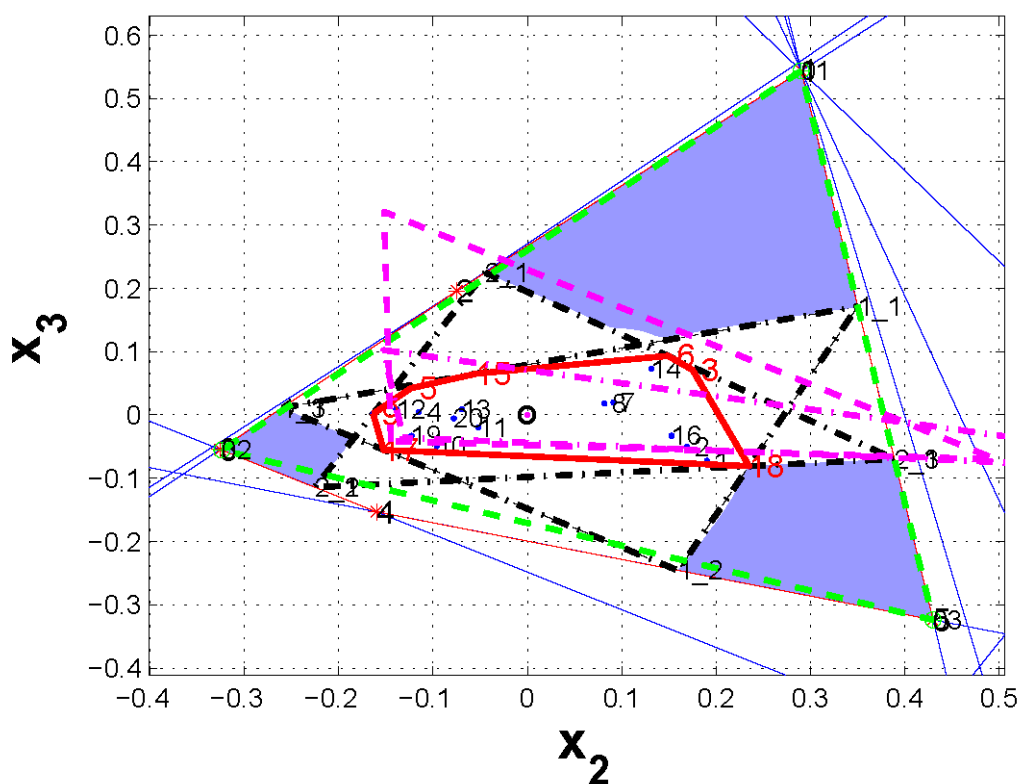
Figure 1. Borgen plot of Henry and Kim's data (for more information see the text).

References

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