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So, you do not need a fit through the data points, but to obtain the boundaries of your data, do you?

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Abstract

In many astronomical problems one often needs to determine the upper and/or lower boundary of a given data set. An automatic approach consists in fitting the data using a generalized least-squares method, where the function to be minimized is defined to handle asymmetrically the data at both sides of the boundary. Since, depending on the functional form of the sought boundary, the minimization cannot always be performed analytically, a numerical approach, based on the popular downhill simplex method, is employed. The procedure is valid for any numerically computable function. Simple polynomials provide good boundaries in common situations. For data exhibiting a complex behaviour, the use of adaptive splines gives excellent results. Since the described method is sensitive to extreme data points, the simultaneous introduction of error weighting and the flexibility of allowing some points to fall outside of the fitted frontier, supplies the parameters that help to tune the boundary fitting depending on the nature of the considered problem.