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Identification and deconvolution of overlapped peaks derived from raw 2D PAGE images

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A standard approach for the analytical separation of proteins in the field of proteomics is the use of two-dimensional polyacrylamide gel electrophoresis (2D-PAGE), which separates a complex crude protein samples from a given cellular or organellar sample based upon charge and size in separate perpendicular dimensions. However, often separation is incomplete, leaving gel spots (or peaks) that are overlapped spatially in not one but often both dimensions. We are attempting to ameliorate these instances by mathematically deconvoluting these peaks de novo from raw 2D-PAGE images. It is our overarching goal to engineer algorithms that will be applicable to global sets of proteomics data where pre-sample conditions have been varied and individual protein levels can be reasonably quantified for even the most overlapped of peptide species. This will greatly increase the quality and speed of information gleaned from a given proteome gained visualized via standard 2D-PAGE analysis. As a first step and proof of principle, we have begun to formulate an image process and analysis method, which utilizes a novel nonlinear least squares algorithm (NLLS) to fit and quantify the spots on a single gel image. The first step of this process is to digitize the 2D image data, creating a three-dimensional densiometric image, roughly creating a data matrix of the JPEG or TIFF file of the original gel. This 3D data matrix is then fit through the application of a nonlinear least squares algorithm modified with a chemically relevant constraint. Specifically, we have imposed a voight line profile, composed of a combination of gaussian and lorentzian functions, on the 3D data matrix. Limiting these functions with convergence criteria based upon the error of the areas of cross-sections of the nonlinear least squares fit compared to that of the original data have yielded the promising preliminary results that will be discussed.