Fishing Net Algorithm:
an original approach for quantitative spectral analysis of undefined mixtures

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The quantitative analysis of ***s*** *component mixture in the molecular spectroscopy is based on the additivity principle:*

$$\varepsilon_j(z_k) = l_j \cdot \sum_{i=1}^{s} c_{i,j} \cdot \varepsilon_i^o(z_k) \qquad (1)$$

where: ***k****=1 to* ***m****;* ***j****=1 to* ***p****;* ***m****-number of the spectral co-ordinates (points);* ***p****-number of the absorption spectra (solutions);* ***z*** *- wavelength or wavenumber;* $\varepsilon_j(z_k)$ *-measured molar absorptivity of* j^{th} *solution at* z_k*;* $\varepsilon_i^o(z_k)$ *-individual absorbance of* i^{th} *component at* z_k*;* $c_{i,j}$ *-concentration of* i^{th} *component in* j^{th} *solution;* ***l****-path width.*

Evidently if the individual spectrum of any component is unknown the analysis is impossible in general using the known methods for data processing.

On the other hand each individual spectrum can be described as superposition of the individual bands (n_i*) composing it:*

$$\varepsilon_i^o(z_k) = \sum_{q=1}^{n_j} F(z_k, \varepsilon_{max}^{j,q}, z_{max}^{i,q}, \Delta\nu_{1/2}^{j,q}) \qquad (2)$$

where: ***F****-analytical contour of the bands,* $\varepsilon_{max}, z_{max}, \Delta\nu_{1/2}$ *- basic spectral parameters.*

From Eqs (1) & (2) follows:

$$\frac{\varepsilon_j(z_k)}{l_j} = \sum_{i=1}^{s^*} c_{i,j} \cdot \sum_{q=1}^{n_j} F(z_k, \varepsilon_{max}^{j,q}, z_{max}^{i,q}, \Delta\nu_{1/2}^{j,q}) + \sum_{i=s^*+1}^{s} c_{i,j} \cdot \varepsilon_i^o(z_k) \qquad (3)$$

where ***s**** *is the number of the components with unknown spectra.*

Eq (3) describes an optimization function characterized by unknown $p.s + 3.\sum_{i=1}^{s^*} n_j$ *parameters and* ***p.m*** *experimental points and the concentrations and the individual spectra of the components can be obtained after two step (simplex+gradient procedure) nonlinear optimization procedure. The optimization is quite fast and results obtained are with high precision, what can be explained with the fact that the parameters depending on* ***s*** *(the concentrations), but independing on* ***z*** *and the parameters depending on* ***z*** *(the individual spectral parameters), but independing on* ***s*** *are connected in a common optimization function and like a fishing net help each other to find the optimization minimum.*

General Description of The Method:

RESOLUTION OF OVERLAPPING UV-VIS ABSORPTION BANDS AND QUANTITATIVE ANALISYS.
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Mathematical Background and Applications:

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