ELECTRONIC SUPPLEMENTARY INFORMATION

"**Case Based Reasoning (CBR) for Multicomponent Analysis Using Sensor Arrays: Application to Water Quality Evaluation**"

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Case Based Reasoning Cycle:

Classical CBR Cycle, including machine learning when user validates new cases solution. (See for instance, ref. 11 in the paper, i.e. J. L. Kolodner, in *Case-Based Reasoning,* ed. M. Kaufmann, San Mateo, 1993, for details).
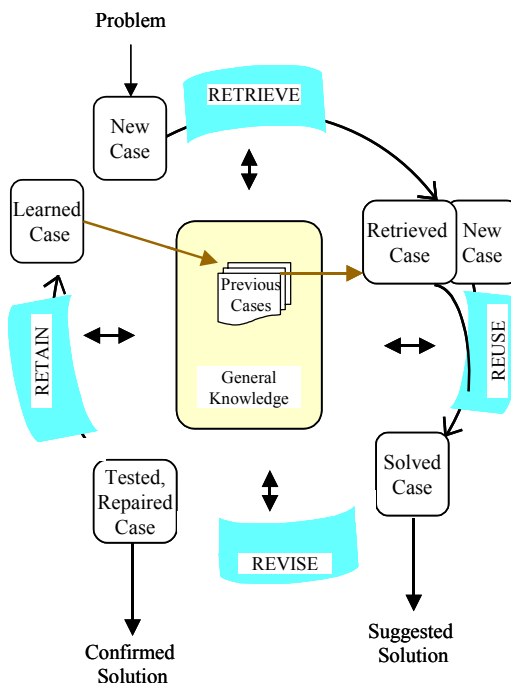
Case Base:

    Case Description:
        6-ISE Sensor Array:
            H^+, Ca^{2+}, Na^+, K^+, NO_3^-, Cl^-.

    Case Solution:
        Water recognition (most similar case, MSC) and ranges of concentrations
        (mg.l^{-1}) of several ionic species HCO_3^-, SO_4^-, Cl^-, Ca^{2+}, Mg^{2+}, Na^+, K^+

Similitude function:

Normalized distance in a 6-dimensional space:

$$fs = \sum_{i=1}^{6} 1 - Abs\left(\frac{(d_{1i} - d_{2i})}{max(d_{in})}\right)$$

where 'fs' is the case similitude function, and d_1 and d_2 the array data of the case descriptions to compare.

Initial Case Base Data Set:

Table 3 Full Data-Set for Mineral water samples named W1-W20. Values of Electronic potential in mV

Water	H^+- ISE	Ca^{2+}-ISE	Na^+-ISE	K^+-ISE	NO_3^--ISE	Cl^--ISE
W1	228.1	-3.3	72.5	-71.9	129.8	188.6
W2	213.9	8.0	184.7	-52.8	158.6	140.0
W3	235.9	16.2	167.5	-72.4	158.6	179.3
W4	203.9	15.2	64.9	-91.0	162.5	204.8
W5	203.2	13.3	45.0	-89.9	156.4	207.8
W6	173.3	1.8	174	-57.6	145.6	148.0
W7	210.4	13.1	72.6	-86.6	156.2	199.9
W8	238.2	-2.8	184.1	-57.6	147.0	113.1
W9	297.4	21.8	85.0	-118.1	178.2	190.2
W10	199.5	9.5	66.0	-97.6	147.8	196.9
W11	239.2	0.6	71.8	-91.8	152.0	206.6
W12	330.5	1.8	93.5	-90.0	195.9	202.8
W13	202.6	3.5	83.3	-95.4	141.9	197.2
W14	263.0	-30	66.4	-73.4	162.1	190.3
W15	179.1	1.0	88.0	-76.2	142.9	188.8
W16	216.6	12.2	57.4	-78.0	149.6	194.4
W17	292.9	13.0	64.4	-74.1	178.3	196.8
W18	176.8	6.1	90.0	-87.2	146.9	196.6
W19	200.0	10.3	115.8	-85.2	149.3	170.0
W20	185.9	14.2	96.9	-77.6	149.9	170.2

Software:

Custom Developed Software for Real-time data acquisition and CBR processing. This software was developed in Java for Sun JRE 1.2 or compatible. This fact enable it to run the application over any platform and Operative System (Windows, UNIX, Linux, …).