APPENDIX

The Variable-Size Simplex Rules and Worksheet

The Variable-Size Simplex Rules and Worksheet

The two modifications allow the simplex to expand in directions that are favorable and to contract in directions that are unfavorable. Because the modified algorithm allows the simplex to change its size, it is often referred to as the "variable-size simplex".

Table A-1 gives the written rules for the variable-size simplex algorithm. In the table the symbol ">" should be read, "is better than". The symbol "<" should be read, "is worse than". Similarly, the combination of symbols "≧" should be read, "is batter than or equal to". And the combination of symbols "≦" should be read, "is wose than or equal to".

Table A-1 Rule for the Variable-Size simplex

1. Rank the vertexes of the first simplex on a worksheet in decreasing order of response from best to worst. Put the worst vertex into the row labeled W.
2. Calculate and evaluate R:
   A. If **N ≦ R ≦ B**, use sinplex **B..NR**, and go to 3.
   B. If **R > B**, calculate and evaluate **E**:
      i. If **E ≧ B**, use simplex **B..NE**, and go to 3.
      ii. If **E < B**, use simplex **B..NR**, and go to 3.

C. If **R<N**:

i. If **R ≧ W**, calculate and evaluate $\mathbf{C_R}$, use simplex $\mathbf{B..NC_R}$ and go to 3.

ii. If R < W, calculate and evaluate Cw, use simplex B..NCw, and go to 3.

3. *Never* transfer the current row labeled **W** to the next worksheet. *Always* transfer the current row labeled **N** to the row labeled **W** on the next work sheet. Rang the remaining retained vertexes in order of decreasing response on the new worksheet, and go to 2.

The Variable-Size Worksheet

Table A-2 is a blank variable-size worksheet. The various parts of the worksheet deserve some comment before we use it for further calculations.

Simplex No. In the upper left corner of the worksheet are two spaces to list simplex numbers. Because worksheets are used to go from one simplex to another, it is useful to fill these spaces with the number of the current simplex, followed by a right arrow, followed by the number of the next simplex.

Factor. To the right of the simple numbers is a heading labeled "Factor", and under this heading are four column labeled "X_1", "X_2", "X_3" and "X_4". These columns contain the X_1, X_2, X_3 and X_4 coordinates of the vertex involved in the four-factor simplex.

Response. To the right of the factors is a column labeled "Response". The responses are listed here. Not every row is provided with a space for recording the response. Responses are listed only for the rows that correspond to simplex vertexes, not for rows containing intermediate calculations.

Rank. To the right of the responses is a column labeled “Rank”. The letters in this column are B, the vertex giving the best response: N, normally the vertex giving the worst response, the vertex “in the worlsheet”. The vertex that will be discarded.

Vertex Number. The column to the right of the rank is labeled “Vertex Number”. This column provided a place to record each vertex’s unchanging identity.

Time retained. The column to the right of the vertex number is labeled “Times Retained”. This column to the right of the vertex number is labeled

is a bookkeeping tool. When a vertex is transferred to the next worksheet, the corresponding value in the times retained column will be incremented by one.

Coordinates of retained vertexs. At the left side of the worksheet id the heading, “coordinates of retained vetexes”. The rows in this section simply contain information about the retained vertexes. All of these vertexed will eventually be transferred to the next worksheet.

Σ. This row is used to sum the values above it. The first space on this row will contain the sum of the X_i values for the best through the next-to-the-worst vertexes. Thw second space of this row will contain the sum of the X_2 values for the best through the next-to-the-worst vertexes. And so on, if there are more factors and therefore more columns.

$\overline{P}$=Σ/k. The next row is labeled **P** followed by the formula for calculating the centroid, the summation divided by the number of factors k.

W. The next row is provided for listing the coordinates of the rejected vertex, **W.**

($\overline{P}$-W). This row has been found more descriptive to simply call it “p-bar minus w”. This calculation is emphasized in the worksheet.

R= $\overline{P}$ +($\overline{P}$-W). A row labeled **R** for the reflection vertex is listed and a formula for calculating is also given.

($\overline{P}$ – W)/2. The fourth row from the bottom is for calculation of the quantity ½

($\overline{P}$ - W). A quantity that is used when either contraction is carried out. Unless a contraction is to be carried out, this row should not be used.

C_w= $\overline{P}$ – ($\overline{P}$ - W) /2. This row is used for calculating the coordinates of a **C_r** contraction.

E = R + ($\overline{P}$ - W). This row is used for calculating the coordinates of an expansion vertex **R**.

Table A-2 Worksheet for four- factor variable-size simplex calculations

Simplex No. ---→---	Factor							
	X_1	X_2	X_3	X_4	Response	Rank	Vertex Number	Times Retained
Coordinate of retained vertexes						B		
						N		
Σ								
$\overline{P}$ = Σ /k								
W						W		
($\overline{P}$ - W)								
R=$\overline{P}$+($\overline{P}$-W)						R		
($\overline{P}$-W)/2								
C_w=$\overline{P}$-($\overline{P}$-W)/2							C_w	
C_r=$\overline{P}$-($\overline{P}$-W)/2						C_r		
E=R-($\overline{P}$-W)						E		

CURRICULUM VITAE

Name: Mr. Wish Thanasarakhan

Date of Birth: April 5, 1978

Academic status:

- B.Sc. 2nd honor (Chemistry), Chiang Mai University, 2002
- Ph.D. student in analytical chemistry, Chiang Mai University, 2005-2010.

Awards/Scholarships:

- The Royal Golden Jubilee Ph.D. Research Program (RGJ)
- The "Postgraduate Education and Research Program in Chemistry (PERCH)"

List of Publications:

1. Wish Thanasarakhan, Saisunee Liawruangrath, Sunanta Wangkarn and Boonsom Liawruangrath, "Sequential injection spectrophotometric determination of zinc(II) in pharmaceuticals based on zinc(II)-PAN in non-ionic surfactant medium", *Talanta*, **71**(2007) 1849-1855.
2. Senee Kruanetr, Wish Thanasarakhan, Urai Tengjarornkul, Boonsom Liawruangrath and Saisunee Liawruangrath, "A simple flow injection spectrophotometric determination of iron using Nitroso_R salt as complexing agent", *J. Flow Injection Anal.*, **24**(2007) 114-118.

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3. Wish Thanasarakhan, Richard R. Deming and Saisunee Liawruangrath, "Determination of active ingredients in cough-cold pharmaceutical by Micellar liquid chromatography", The Postgraduate Education and Research Program in Chemistry (PERCH) Congress IV, Jomtien Palm Beach Resort Pattaya, Chonburi, Thailand, 8-12 May 2005, p.p103.