# APPENDIX A

## The Variable-Size Simplex Rules and Worksheet

### The Variable-Size Simplex Rules [129]

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 better than or equal to". And the combination of symbols "≦" should be read, "is worse than or equal to".

**Table A-1** Rules 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 $\mathbf{N} \leqq \mathbf{R} \leqq \mathbf{B}$, use simplex **B..NR**, and go to 3.
   - B. If $\mathbf{R} > \mathbf{B}$, calculate and evaluate **E:**
     - i. If $\mathbf{E} \geqq \mathbf{B}$, use simplex **B..NE**, and go to 3.
     - ii. If $\mathbf{E} < \mathbf{B}$, use simplex **B..NR**, and go to 3.
   - C. If $\mathbf{R} < \mathbf{N}$:
     - i. If $\mathbf{R} \geqq \mathbf{W}$, calculate and evaluate $\mathbf{C_R}$, use simplex **B..NC**$_R$, and go to 3.
     - ii. If $\mathbf{R} < \mathbf{W}$, calculate and evaluate $\mathbf{C_W}$, use simplex **B..NC**$_W$, 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 [129]

Figure A-1 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 simplex numbers is a heading labeled "Factor", and under this heading are four columns 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 next-to-the-worst response; and **W**, normally the vertex giving the worst response, the vertex "in the worksheet", 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 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 Vertexes.** At the left side of the worksheet is the heading, "Coordinates of Retained Vertexes". The rows in this section simply contain information about the retained vertexes. All of these vertexes 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 $X_1$ values for the best through the next-to-the-worst vertexes. The second space on 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.

$\overline{P} = \Sigma/k$. 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 $C_w$ contraction.

**$C_r = \overline{P} - (\overline{P} - W)$ /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**.

| Simplex No.--- → --- | Factor | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $X_1$ | $X_2$ | $X_3$ | $X_4$ | Response | Rank | Vertex Number | Times Retained |
| Coordinates of retained vertexes | | | | | | B | | |
| | | | | | | | | |
| | | | | | | | | |
| | | | | | | N | | |
| $\Sigma$ | | | | | | | | |
| $\overline{P} = \Sigma/k$ | | | | | | | | |
| 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 | | |

**Figure A-1** Worksheet for four-factor variable-size simplex calculations

# APPENDIX B

## Worksheets of Simplex Optimization for FIA Spectrophotometric Determination of Copper (section 3.1.4)

| Simplex No. 1 → 2 | Factor | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $X_1$ | $X_2$ | $X_3$ | $X_4$ | Response | Rank | Vertex Number | Times Retained |
| **Coordinates of retained vertexes** | 0.04 | 30 | 3.2 | 20 | 11.5 | B | 1 | 1 |
| | 0.03 | 30 | 2.6 | 20 | 11.0 | | 2 | 1 |
| | 0.04 | 40 | 3.8 | 25 | 10.5 | | 4 | 1 |
| | 0.03 | 20 | 3.2 | 20 | 10.0 | N | 3 | 1 |
| $\Sigma$ | 0.14 | 120 | 12.8 | 85 | | | | |
| $\bar{P} = \Sigma/k$ | 0.05 | 30 | 3.2 | 21.25 | | | | |
| **W** | 0.05 | 40 | 3.8 | 25 | 9.5 | W | 5 | 1 |
| $(\bar{P} - W)$ | -0.02 | -10 | -1 | -3.75 | | | | |
| $R = \bar{P} + (\bar{P} - W)$ | 0.02 | 20 | 2.6 | 18 | 9.7 | R | 6 | 0 |
| $(\bar{P} - W)/2$ | | | | | | | | |
| $C_w = \bar{P} - (\bar{P} - W)/2$ | | | | | | $C_w$ | | |
| $C_r = \bar{P} - (\bar{P} - W)/2$ | 0.03 | 25 | 3.2 | 19 | 11.2 | $C_r$ | 7 | 0 |
| $E = R + (\bar{P} - W)$ | | | | | | E | | |

**Figure B-1** Worksheet showing the next simplex moved "Simplex No. 1→ 2".

| Simplex No. 2 → 3 | Factor | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $X_1$ | $X_2$ | $X_3$ | $X_4$ | Response | Rank | Vertex Number | Times Retained |
| **Coordinates of retained vertexes** | 0.04 | 30 | 3.2 | 20 | 11.5 | B | 1 | 2 |
| | 0.03 | 25 | 3.2 | 19 | 11.2 | | 7 | 1 |
| | 0.03 | 30 | 2.6 | 20 | 11.0 | | 2 | 2 |
| | 0.04 | 40 | 3.8 | 25 | 10.5 | N | 4 | 2 |
| $\Sigma$ | 0.14 | 125 | 12.8 | 84 | | | | |
| $\overline{P} = \Sigma/k$ | 0.035 | 31.25 | 3.2 | 21 | | | | |
| **W** | 0.03 | 20 | 3.2 | 20 | 10.0 | W | 3 | 2 |
| $(\overline{P} - W)$ | 0.005 | 11.25 | 0 | 1 | | | | |
| $R = \overline{P} + (\overline{P} - W)$ | 0.04 | 43 | 3.2 | 22 | 10.3 | R | 8 | 0 |
| $(\overline{P} - W)/2$ | 0.025 | 5.62 | 0 | 0.5 | | | | |
| $C_w = \overline{P} - (\overline{P} - W)/2$ | | | | | | $C_w$ | | |
| $C_r = \overline{P} - (\overline{P} - W)/2$ | 0.04 | 37 | 3.2 | 22 | 10.7 | $C_r$ | 9 | 0 |
| $E = R + (\overline{P} - W)$ | | | | | | E | | |

**Figure B-2** Worksheet showing the next simplex moved "Simplex No. 2→ 3".

| Simplex No. 3 → 4 | Factor | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $X_1$ | $X_2$ | $X_3$ | $X_4$ | Response | Rank | Vertex Number | Times Retained |
| **Coordinates of retained vertexes** | 0.04 | 30 | 3.2 | 20 | 11.5 | B | 1 | 3 |
| | 0.03 | 25 | 3.2 | 19 | 11.2 | | 7 | 2 |
| | 0.03 | 30 | 2.6 | 20 | 11.0 | | 2 | 3 |
| | 0.04 | 37 | 3.2 | 22 | 10.7 | N | 9 | 1 |
| $\Sigma$ | 0.14 | 122 | 12.4 | 81 | | | | |
| $\bar{P} = \Sigma/k$ | 0.035 | 30.5 | 3.2 | 20.25 | | | | |
| **W** | 0.04 | 40 | 3.8 | 25 | 10.5 | W | 4 | 3 |
| $(\bar{P} - W)$ | | | | | | | | |
| $R = \bar{P} + (\bar{P} - W)$ | 0.03 | 21 | 2.6 | 16 | 10.5 | R | 10 | 0 |
| $(\bar{P} - W)/2$ | | | | | | | | |
| $C_w = \bar{P} - (\bar{P} - W)/2$ | | | | | | $C_w$ | | |
| $C_r = \bar{P} - (\bar{P} - W)/2$ | | | | | | $C_r$ | | |
| $E = R + (\bar{P} - W)$ | | | | | | E | | |

**Figure B-3** Worksheet showing the next simplex moved "Simplex No. 3→ 4".

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*National Conferences*

1. B. Purachat and P. Purachat, "Using of Simplex Method for the Selection of Parameter for the Spectrophotometric Determination of Sulphate in water", 24th Congress on Science and Technology of Thailand, Bangkok, 1998.
2. B. Purachat, S. Liawruangrath, S. Rattanaphani, D. Buddhasukh and P. Sooksamiti, "Determination of Copper by Flow Injection Spectrophotometry Using Nitroso-R Salt as Complexing Agent", 26th Congress on Science and Technology of Thailand, Bangkok, 2000.
3. B. Purachat, S. Liawruangrath, S. Rattanaphani, D. Buddhasukh and P. Sooksamiti, "Study of Copper Adsorption on Perlites and Synthetic zeolites from Perlites", 27th Congress on Science and Technology of Thailand, Songkla, 2001.