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Non-Euclidean Simplex Optimization

Gary L. Silver

August 15, 1977

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Abstract

Geometric optimization techniques useful for studying chemical equilibrium traditionally rely upon principles of euclidean geometry, but such algorithms may also be based upon principles of a non-euclidean geometry. The sequential simplex method is adapted to the hyperbolic plane, and application of optimization to problems such as the potentiometric titration of plutonium is suggested.

Introduction

The method of proportional equations, $\sum |A| = 0$, where $|A|$ represents the absolute value of a reaction isotherm from which the multiplicative factor (RT) has been removed, is a novel method of characterizing chemical equilibrium [1]. This technique uses an empirical method of mathematical optimization, such as the sequential simplex method. But, for one reason or another, empirical optimization methods sometimes do not function satisfactorily. In circumstances where it is not practical to select another optimization technique, it is desirable to modify either the problem, or the optimization routine, or both, so that the probability of satisfactory convergence is increased. This report offers several suggestions for modifying chemical equilibrium problems as well as methods for modifying the sequential simplex method itself. The conclusions are that optimization techniques need not be based on traditional, euclidean geometry, and that the adaptation of non-euclidean geometry to optimization schemes adds flexibility to the practice of mathematical optimization. A method of studying optimum conditions for potentiometric titrations is illustrated for the case of plutonium.

Sequential Simplex Optimization

Recently, minimization of the reaction isotherm absolute value by the sequential simplex technique has been suggested as a method of characterizing chemical equilibrium [1]. But the sequential simplex method is only one optimization method suitable for minimization of the reaction isotherm absolute value [2]. While the sequential simplex technique has the advantage of not being difficult to understand or to computerize, it has several disadvantages when used to minimize the sum of several reaction isotherm absolute values. One of these disadvantages is convergence to a false optimum, i.e., convergence to a numerical value which is not zero, or which is not satisfactorily close to zero, even though it is within the capacity of the computer to approach zero. These false optima may occur through use of insufficient numerical precision, for example.

When convergence to a false optimum is a problem, several possible remedies may be applied. Perhaps the simplest of these remedies is to choose a completely new set

of starting points in the hope that convergence to zero, or to a value satisfactorily close to zero, will result from simplex movements beginning at the new initial points. Alternatively, the coordinates of the objective function at the point of false convergence may be used as one of the new starting points together with a new set of remaining initial points. These new points may include some of the original initial points, but should not be simple multiples of one another. It may also be helpful to increase the precision of the computations. Increased precision is often useful when it is desired to minimize the sum of three or more reaction isotherm absolute values, when reaction isotherms contain very large or very small equilibrium constants, or when the equilibrium concentration of a species is represented as a small difference between two comparatively large numbers.

Modifying the Simplex

Reviewed below are a few sequential simplex strategies useful in the process of optimization. The five strategies listed below are an integral part of the traditional variable-sized simplex routine, and are described in References 3-6:

- Reflection, R
- Expansion, E
- Contraction, C_r
- Contraction, C_w
- Rejection of next-to-worst vertex

Less commonly used strategies, but occasionally useful additions to the simplex routine include the following operations:

- Shrinkage of the simplex [7]
- Rotation of the simplex [7]
- Unlimited expansion of the simplex, or translation of the simplex [7, 8]
- Change of scale factors for the operations of reflection, expansion, or contraction of the simplex [7]
- Halved expansion of the simplex (i.e., the addition of the option of expansion by half, or by some other fraction, between the traditional reflection and expansion points.)
- Skewed reflection in the simplex (i.e., reflection through a point which is not the centroid of one simplex face, but some other point, perhaps halfway between the centroid and the vertex with the best response of the objective function.)

Changes may be made in the priorities of a simplex routine. In the traditional, sequential simplex technique it is customary to make certain decisions and movements in regard to the vertex with the next-to-worst response of the objective function. (This next-to-worst vertex is usually denoted by the letter N.) But such decisions and movements can also be made if the point N is redefined as the next-to-best point in three-dimensional problems, or as some intermediate point in higher dimensional simplex routines for higher dimensional problems. This change is useful partly because it is so simple to implement in computer programs representing the simplex algorithm. The possibility of this change has been noted in Table 6 of Reference 9. P dimensional optimization problems may be tried in simplex routines designed for P+1 dimensional problems, or even in simplex routines designed for higher dimensional problems. This suggestion has also

been made in Table 6 of Reference 9. These simple modifications or adaptations of the sequential simplex algorithms may occasionally be useful for hastening convergence, or for avoiding the problem of false convergence.

Modifying the Objective Function

Another useful strategy for problems amenable to simplex solution involves modification of the objective function. This strategy deserves consideration because it can take such a wide variety of forms, and because it is often easy to implement. It is sometimes possible to replace one objective function with a second objective function, equivalent to the first, for the purpose of problem solving by optimization. Many chemical equilibrium problems may be formulated in more than one manner. That is, P reaction isotherms may be necessary to define an equilibrium problem, but there may be many possible reaction isotherms from which to select P isotherms. False convergence or slow convergence with one set of isotherms does not necessarily mean false convergence or slow convergence with another set.

The variables in an objective function may be replaced with other variables by simple algebraic changes. These are easy substitutions which can be quite useful. Suppose that an objective function is given in terms of the variables, P and Q . Then there will always be two numbers, U and V , such that $P = U + V$ and $Q = U - V$, and the function may be rewritten in terms of the new variables, U and V . Suppose again that a function is given in terms of the three variables, P , Q , and R . Then

numbers, A and B , may always be found such that $P = (A)(Q)$ and $R = (B)(Q)$, or $P = Q/A$ and $R = Q/B$. The objective function may thus be rewritten in terms of the new variables, Q , A , and B .

A chemical equilibrium problem can sometimes be restated in such a manner that an ill-behaved objective function is replaced by a well-behaved objective function. One of the problems with the method of proportional equations is that occasionally the concentration of a particular species appears as the small difference between two comparatively large numbers. Actual subtraction of such numbers may yield a difference with so much round-off error that it is a very poor representation of the actual concentration of the species. In this circumstance it is sometimes possible to rewrite the problem in such a manner that the offending difference no longer occurs. This may be done by shifting the operation of subtraction elsewhere by the use of substitution variables as described above. Alternatively, the problem may be rewritten in such a manner that the operation of subtraction is no longer necessary.

An Example

In the case of the disproportionation of tetravalent plutonium, for example, Reference 1 shows the species PuO_2^+ appearing as the difference, $P-Q$. In this particular representation of the disproportionation reaction, the total concentration of plutonium, T , was assigned a fixed value. But the assignment of a fixed value may be made elsewhere, so that the total concentration becomes a variable. For example, let $\text{PuO}_2^+ = 1$. Then the concentration of hexavalent plutonium may be taken as the variable, M , and, by virtue of charge conservation, the concentration of trivalent

plutonium is $(1 + 2M)$. Trivalent, hexavalent, and pentavalent plutonium are now described in terms of one variable (M) and a fixed constant (unity). The unknown concentration of tetravalent plutonium may be assigned another variable, for example, X . Reaction isotherms representing the disproportionation of tetravalent plutonium may thus be written in terms of the two variables, X and M . X and M may be of any value; however, the total concentration of plutonium is always the sum of its constituent parts. This sum may be used to divide the concentration of any oxidation state to find the fraction of plutonium present as that oxidation state. Hence, the complete valence state distribution of plutonium at equilibrium may be found without employing the operation of subtraction.

The manipulations above may be explained as follows. Suppose that PuO_2^+ were assigned a variable, such as Y . Then, in the operation of finding fractional valence state distributions, the variable Y disappears by cancellation, so that its actual numerical value is immaterial, and may be conveniently replaced by a constant. For this cancellation, the concentration of hexavalent plutonium may be visualized as the product of M and Y , and the concentration of tetravalent plutonium, as the product of X and Y .

An alternate method of determining valence state distributions is outlined in the Supplement, p. 26.

Transformations

Transformations interposed between the variables in an objective function and the

variables in the simplex algorithms are often useful because they are easily implemented and because they may yield convergence paths quite distinct from the path of convergence which might have been taken by the simplex in the absence of the transformations. Simple transformations interposed between the objective function variables and the variables in the simplex algorithm may, therefore, be useful in avoiding false convergence. Suppose that an objective function and a simplex algorithm are written in terms of the two variables, J and K . If the objective function is rewritten in terms of other variables, A and B , several interesting possibilities arise.

If $A = J$ and $B = K$, the path of convergence is the same as would be obtained without transformation. But suppose $A = (C)\log(J)$ and $B = (C)\log(K)$, where (C) is a constant, not necessarily the same in the two cases. With this transformation, A and B change more slowly in the objective function than J and K in the simplex algorithm. The simplex often has a tendency to contract as it moves through function space, so that more slowly changing variables in the objective function may provide greater opportunity for the expansion option to be exercised. Either common or natural logarithms may be used, but negative arguments of the logarithms must be avoided. All variables may be transformed, or only some of them.

Again, suppose that $A = (C)\exp(J)$ and $B = (C)\exp(K)$. The function variables now change more rapidly than the program variables. The exponentiation operation may be to base "e" or base 10. Again, suppose that $A = C-C/(1+J)$ and $B = C-C/(1+K)$. Here the constant is some number which is certain to exceed the optimum value of the variables, A and B . As J tends to zero,

A also tends to zero; whereas when J tends to infinity, A tends to C. In summary, there are a very large number of simple transformations which may be useful in hastening convergence, or in avoiding the problem of false convergence, such as $A = (C)(J^3)$ or $B = C/K^3$. The constants may be positive or negative.

Computer Statements for Optimization

Just as there are a variety of operations and transformations which may be incorporated into a sequential simplex routine, likewise, computer programs for optimization may exhibit differences even when the number and type of operations are the same. The possibility of substantial improvement in a computerized optimization routine by small program changes should, therefore, never be overlooked. Simple computer programs for minimizing functions of two and three variables have been illustrated in Tables 5 and 6, respectively, of Reference 9. (For functions which are to be maximized instead of minimized, Tables 5 and 6 of Reference 9 may be used if the objective function is multiplied by minus one.)

Table 1 herein illustrates an improvement in Table 5 of Reference 9 (the two-variable sequential simplex routine) as well as an improvement in Table 6 of Reference 9 (the three-variable sequential simplex routine). Paragraphs 11 and 9, respectively, of Table 1 herein may be substituted for paragraphs 11 and 9 of these two- and three-variable minimization routines. Additionally, the two-variable simplex routine given in Reference 9 may be modified, with

potential for improvement, by adding lines 9.28, 9.30, 9.32, and 9.34 of Table 4 (see page 19). (Paragraph 9 in Table 1 herein may also be modified by insertion of the statement "GOTO 5.02" at steps 9.36 or 9.46.)

Non-euclidean Optimization

Many mathematical schemes have been developed for computer-assisted optimization [6]. Many of these schemes are amenable to geometric interpretation, which is often useful for the purpose of visualizing the mechanics of an optimization technique. Such interpretations always seem to be formulated in terms of euclidean geometry, perhaps because this is the familiar geometry in everyday use. But there are other geometries based on assumptions different from those of euclidean geometry, and it is the purpose of this section to suggest that one of these geometries may be more useful for some optimization schemes than ordinary euclidean geometry.

To illustrate this, a two-variable simplex routine has been adapted to geometry on a hyperbolic plane, although no arguments present this geometry as more suitable for purposes of optimization than euclidean geometry, or some other geometry. Similarly, there seems to be no reason to believe that the sequential simplex method is the best optimization method for adaptation to some non-euclidean geometry, although the simplicity of the sequential simplex method may allow it to be more easily converted than some other, more complicated optimization technique.

Hyperbolic geometry and euclidean geometry share the property that lines are infinite

Table 1 - MODIFICATIONS OF THE TWO- AND THREE-VARIABLE SEQUENTIAL SIMPLEX
ROUTINES GIVEN IN REFERENCE 9

Two-Variable Routine:

```

11.02 S PJ=(WJ+BJ)/2; S PK=(WK+BK)/2
11.04 S RJ=PJ+(PJ-NJ); S RK=PK+(PK-NK)
11.06 S J(1)=BJ; S K(1)=BK; S J(2)=WJ; S K(2)=WK
11.08 S J(3)=RJ; S K(3)=RK; GOTO 5.02

```

Three-Variable Routine:

```

09.04 I (RG-NG)5.02,9.06,9.06
09.06 I (RG-WG)9.10,9.20,9.20
09.10 S CJ=PJ+(PJ-WJ)/2; S CK=PK+(PK-WK)/2; S CL=PL+(PL-WL)/2
09.12 S J(1)=CJ; S K(1)=CK; S L(1)=CL
09.14 S A=1; D 2; S CG=G(1)
09.16 I (CG-WG)5.02,9.20,9.20
09.20 S QJ=PJ-(PJ-WJ)/2; S QK=PK-(PK-WK)/2; S QL=PL-(PL-WL)/2
09.22 S J(1)=QJ; S K(1)=QK; S L(1)=QL
09.24 S A=1; D 2
09.26 S QG=G(1); I (QG-WG)5.02,9.30,9.30
09.30 S PJ=(BJ+NJ+WJ)/3; S PK=(BK+NK+WK)/3; S PL=(BL+NL+WL)/3
09.32 S YJ=PJ+(PJ-VJ); S YK=PK+(PK-VK); S YL=PL+(PL-VL)
09.34 S J(1)=YJ; S K(1)=YK; S L(1)=YL
09.36 S A=1; D 2
09.38 S YG=G(1); I (YG-WG)5.02,9.40,9.40
09.40 S PJ=(BJ+VJ+WJ)/3; S PK=(BK+VK+WK)/3; S PL=(BL+VL+WL)/3
09.42 S ZJ=PJ+(PJ-NJ); S ZK=PK+(BK-NK); S ZL=PL+(BL-NL)
09.44 S J(1)=ZJ; S K(1)=ZK; S L(1)=ZL
09.46 S A=1; D 2
09.48 S ZG=G(1); I (ZG-WG)5.02,9.50,9.50
09.50 S J(1)=RK; S K(1)=RL; S L(1)=RJ
09.52 S J(2)=BJ; S K(2)=BK; S L(2)=BL
09.54 S J(3)=QK; S K(3)=QL; S L(3)=QJ
09.56 S J(4)=PL; S K(4)=PJ; S L(4)=PK; GOTO 5.02

```

in extent. This similarity is an advantage, since the variables in an objective function may be arbitrarily large or small, positive or negative. In both of these geometries, then, a simplex may progress infinitely far in any direction, whereas in geometries which have lines of finite length, this may not be possible. For this reason, hyperbolic space may appear more suitable for optimization problems than other non-euclidean spaces, such as one of the elliptic spaces. Certain easily adjusted parameters of a model of hyperbolic space also make this geometry appealing.

There are at least three computational models of hyperbolic space which may be useful for elementary applications of the sequential simplex technique: the Klein cross ratio model [10], the Poincare cross ratio model [11], and the Wylie hyperbolic cosine model [12]. All three models visualize two-dimensional space as the interior of a circle, and three-dimensional space as the interior of a sphere. The Klein and Wylie models will be of interest here. In the Klein model, distance measurements are made by the "cross ratio" technique, whereas in the Wylie model, an inverse hyperbolic cosine function is used for distance evaluations.

Euclidean Simplex; Euclidean Function Evaluation

In the adaptation of an optimization scheme to a geometry such as hyperbolic geometry, four possibilities arise. The first of these possibilities is that the simplex algorithm may operate according to the rules of euclidean geometry in the

usual manner, and that the numerical values of the objective function may be evaluated from the values of the euclidean coordinates of the simplex vertices. This is the traditional sequential simplex routine: both simplex movements and objective function response values are determined by euclidean geometry. Symbolically, this possibility may be denoted by the letter pair (E,E), where the first E denotes simplex movements by the rules of euclidean geometry, and the second E denotes objective function evaluation by the euclidean coordinates of the simplex vertices. The other cases are then denoted as (E,H), (H,H), and (H,E), and are discussed below.

Euclidean Simplex; Hyperbolic Function Evaluation

A simplex may be located with euclidean coordinates (Beltrami coordinates when the radius of the circle is unity) in the interior of a circle or sphere. Likewise, the simplex may be moved about this interior region in the customary manner using the rules of euclidean geometry, and it may also be constrained to this interior by rules based upon euclidean geometry. For purposes of objective function evaluation, however, the coordinates of the simplex vertices may be given hyperbolic interpretations, so that the parameters of the objective function are interpreted in a non-euclidean sense. For example, a simplex may be located within the circle of center $(x,y) = (0,0)$, with a radius (R) of one unit, such that one simplex vertex is at the euclidean point $(0.99,0)$, i.e., very close to the circle perimeter. While the euclidean x-coordinate (also Beltrami x-coordinate, since $R = 1$) of this vertex

may be 0.99, the hyperbolic x-coordinate may be some larger number whose numerical value depends upon the value of the metric constant of the hyperbolic space. The objective function may be interpreted according to this larger number. This manner of operation may be denoted as sequential simplex in the (E,H) form.

Table 2 contains two methods of converting euclidean numbers representing the coordinates of a simplex vertex into their hyperbolic counterparts. The first entry in Table 2 is suitable for a two-variable simplex routine, while the second entry in Table 2 is suitable for a three-variable simplex routine. Both entries use the cross ratio method (Klein model) for determining hyperbolic distances. The hyperbolic distances which are computed are those distances from a point to the coordinate axes along lines from the point to each of the coordinate axes. These lines are perpendicular to the coordinate axes in both euclidean and hyperbolic senses. Thus, the euclidean x-coordinate of a point is converted to the hyperbolic x-coordinate by using the cross ratio method applied to a chord intersecting the point and perpendicular to the y-axis of the circle or sphere. See Figure 1. This computation assigns to each point in the circle or sphere a set of numbers taken to be the hyperbolic coordinates of the point. Each point within the circle or sphere has a unique set of euclidean coordinates, and the numbers taken as hyperbolic coordinates of the point are thus uniquely determined. This coordinate system for the hyperbolic plane is apparently new.*

*C. R. Wylie, Furman University, to G. L. Silver, private communication.

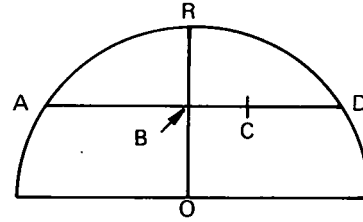


FIGURE 1 - Cross-ratio method of measuring hyperbolic distance. In the semi-circle, chord AD is perpendicular to the radius at point B in both euclidean and hyperbolic senses. The hyperbolic length of segment BC is the metric constant times the natural logarithm of the euclidean ratio $(BD \cdot CA)/(CD \cdot BA)$. This length is the hyperbolic x-coordinate of point C.

The first and second entries in Table 2 may be taken as the second paragraph in the two- and three-variable simplex routines, respectively, as illustrated in Reference 9. Table 3 presents similar hyperbolic coordinate evaluation schemes according to the Wylie hyperbolic cosine model of computing hyperbolic distance measurements. The two entries in Table 3 may similarly be taken as second paragraphs in sequential simplex routines for two and three variables, respectively, such as illustrated in Tables 5 and 6 of Reference 9.

Each entry in Tables 2 and 3 requires specification of the square of the radius, R, of the circle or sphere, representing two- or three-dimensional hyperbolic space, respectively. The square of this radius is denoted by the letters RR. Each entry also requires specification of the metric constant of the hyperbolic space, denoted by the letters MC. The metric constant defines the unit of measure in hyperbolic space, i.e., the number of distance units between two arbitrarily selected points. [12]. The hyperbolic distance between the center and the periphery of the circle

Table 2 - CROSS RATIO METHOD FOR CONVERTING EUCLIDEAN COORDINATES J(A)
INTO HYPERBOLIC COORDINATES HJ(A)

Two-Variable Conversion:

```

02.02 S DS=RR-J(A)^2-K(A)^2; I (DS)2.30,2.30,2.04
02.04 S XP=RR-K(A)^2; S YP=RR-J(A)^2
02.06 S X1=FSQT(XP); S X2=-X1; S Y1=FSQT(YP); S Y2=-Y1
02.08 S ZJ=(X2-J(A))*X1/(X2*(X1-J(A)))
02.10 S ZK=(Y2-K(A))*Y1/(Y2*(Y1-K(A)))
02.12 S HJ(A)=MC*FLOG(ZJ); S HK(A)=MC*FLOG(ZK)
02.14 S G(A)=-50+HJ(A)^2-24*HJ(A)+HK(A)^2-36*HK(A)
02.16 R
02.30 S G(A)=1E+12
-

```

Three-Variable Conversion:

```

02.02 S DS=RR-J(A)^2-K(A)^2-L(A)^2; I (DS)2.50,2.50,2.04
02.04 S XP=RR-K(A)^2-L(A)^2; S YP=RR-J(A)^2-L(A)^2
02.06 S ZP=RR-J(A)^2-K(A)^2; S X1=FSQT(XP); S X2=-X1
02.08 S Y1=FSQT(YP); S Y2=-Y1; S Z1=FSQT(ZP); S Z2=-Z1
02.10 S ZJ=(X2-J(A))*X1/(X2*(X1-J(A)))
02.12 S ZK=(Y2-K(A))*Y1/(Y2*(Y1-K(A)))
02.14 S ZL=(Z2-L(A))*Z1/(Z2*(Z1-L(A)))
02.16 S HJ(A)=MC*FLOG(ZJ); S HK(A)=MC*FLOG(ZK); S HL(A)=MC*FLOG(ZL)
02.20 S G(A)=-50+HJ(A)^2-24*HJ(A)+HK(A)^2-36*HK(A)+HL(A)^2-18*HL(A)
02.22 R
02.50 S G(A)=1E+12
-

```


Table 3 - WYLIE MODEL FOR CONVERTING EUCLIDEAN COORDINATES J(A)
INTO HYPERBOLIC COORDINATES HJ(A)

Two-Variable Conversion:

```

02.02 S DS=RR-J(A)^2-K(A)^2; I (DS)2.50,2.50,2.04
02.04 S XX=RR-K(A)^2; S AA=XX*(XX-J(A)^2); I (AA)2.50,2.50,2.06
02.06 S YY=RR-J(A)^2; S BB=YY*(YY-K(A)^2); I (BB)2.50,2.50,2.08
02.08 S XN=(FSQT(XX^2-AA)+XX)/FSQT(AA)
02.10 S YN=(FSQT(YY^2-BB)+YY)/FSQT(BB)
02.12 S HJ(A)=MC*FLOG(XN); S HK(A)=MC*FLOG(YN)
02.14 I (J(A))2.16,2.16,2.18
02.16 S HJ(A)=-HJ(A)
02.18 I (K(A))2.20,2.20,2.22
02.20 S HK(A)=-HK(A)
02.22 S G(A)=-50+HJ(A)^2-24*HJ(A)+HK(A)^2-36*HK(A)
02.24 R
02.50 S G(A)=1E+12

```

Three-Variable Conversion:

```

02.02 S DS=RR-J(A)^2-K(A)^2-L(A)^2; I (DS)2.50,2.50,2.04
02.04 S XP=RR-K(A)^2-L(A)^2; S AA=XP*(XP-J(A)^2); I (AA)2.50,2.50,2.06
02.06 S YP=RR-J(A)^2-L(A)^2; S BB=YP*(YP-K(A)^2); I (BB)2.50,2.50,2.08
02.08 S ZP=RR-J(A)^2-K(A)^2; S CC=ZP*(ZP-L(A)^2); I (CC)2.50,2.50,2.10
02.10 S XN=(FSQT(XP^2-AA)+XP)/FSQT(AA)
02.12 S YN=(FSQT(YP^2-BB)+YP)/FSQT(BB)
02.14 S ZN=(FSQT(ZP^2-CC)+ZP)/FSQT(CC)
02.16 S HJ(A)=MC*FLOG(XN); S HK(A)=MC*FLOG(YN); S HL(A)=MC*FLOG(ZN)
02.18 I (J(A))3.20,2.20,2.22
02.20 S HJ(A)=-HJ(A)
02.22 I (K(A))2.24,2.24,2.26
02.24 S KH(A)=-KH(A)
02.26 I (L(A))2.28,2.28,2.30
02.28 S HL(A)=-HL(A)
02.30 S G(A)=-50+HJ(A)^2-24*HJ(A)+HK(A)^2-36*HK(A)+HL(A)^2-18*HL(A)
02.32 R
02.50 S G(A)=1E+12

```

or sphere, representing all two- or three-dimensional hyperbolic space, respectively, is infinite, however, regardless of the value of the metric constant. (The euclidean distance between these centers and peripheries is the square root of RR .) As a point within the circle or sphere moves closer, in the euclidean sense, to the periphery of the circle or sphere, the hyperbolic distance from the center of the circle or sphere increases rapidly. Thus an ordinary reflection operation of the euclidean simplex in hyperbolic space may appear as an expansion, even an enormous expansion, to the hyperbolic observer. To the euclidean observer the simplex in the circle or sphere may move in a predictable and regular manner, but these same movements may appear unpredictable and irregular to an observer in hyperbolic space. It is this apparent irregularity which lends the element of interest to the euclidean simplex in hyperbolic space.

When the sequential simplex method is operated in the (E,H) mode, occasionally a reflection or expansion operation will project a simplex vertex outside the circle or sphere used to represent two- and three-dimensional hyperbolic spaces. To the hyperbolic observer this movement is without meaning, since the projected vertex lies "beyond infinity," and such a movement destroys the simplex. When this happens, the objective function is given the arbitrarily large value $1E+12$. To avoid this circumstance, the value of the metric constant can be increased. Since both the radius of the model of hyperbolic space as well as the metric constant of the model may be quickly and easily changed by the user, a great many possible convergence paths are immediately available, and some of these paths may

avoid the problem of false convergence. The entries in Tables 2 and 3 set the objective function equal to $1E+12$ in the event that one of the initial points of the starting simplex lies outside or on the periphery of the euclidean model of the hyperbolic space.

The entries in Tables 2 and 3 yield response values of the test function which differ because of a factor of 2 intrinsic to the method of computation. Thus, the first entry in Table 2 with $R=50$ and $MC=3$ yields the same parameter response values (within round-off error) as the first entry in Table 3 with $R=50$ and $MC=6$. (The sample test function is denoted by the symbol $G(A)$ and is a simple polynomial.) Where optimum values of the parameters in some objective function are small, e.g., unity or less, it is sometimes helpful to select large values of R , the radius of the model of the hyperbolic space, together with small values of the metric constant, MC . The meanings of the adjectives "small" and "large" depend upon the particular circumstances, but might represent such values as 1-50 for R , and 0.5-5 for MC . Larger values of MC may be more appropriate for larger optimum parameter values. The important point, however, is that simply changing the values of R and MC causes considerable flexibility in the (E,H) simplex routine. Note that the optimum values of the objective function parameters are the hyperbolic values (preceded by the letter H in Tables 2 and 3), and not the corresponding euclidean values used to direct the simplex movements.

The number of significant digits carried by the computer may affect the usefulness of the mixed geometry model of the simplex algorithm. With six-digit precision, for example, the smallest relative difference

in the parameters of the objective function is $\pm 10^{-6}$. This may have the effect of placing limits on the sizes of the numbers available to the simplex routine. Since logarithms are used in the models illustrated herein, these limits may be rather restricted. For example, the distance between the center of the circle and the periphery of the circle representing two-dimensional hyperbolic space is infinite in the hyperbolic sense. But with six-digit precision, the closest approach to infinity in the hyperbolic sense is the euclidean number 0.999999R, and the optimum value of a parameter in the objective function may be some hyperbolic number lying between the euclidean numbers 0.999999R and R. If a problem arises because of this granularity of the the number system in the computer, it may sometimes be overcome by increasing the value of the metric constant.

Several other problems may also arise. The circle or sphere may not be the best euclidean model of hyperbolic space; an ellipse or an ellipsoid may instead be more appropriate for some problems, such as cases where the magnitudes of the optimum parameter values are considerably different. The equations of circles and spheres may be changed to the equations of ellipses and ellipsoids by division of the squared, coordinate terms in Tables 2 and 3 by unequal constants. Use of an ellipse or an ellipsoid as the model for hyperbolic space introduces the possibility of anisotropic spaces for optimization problems. Also, increasing the value of R, the radius of the model of hyperbolic space, will progressively reduce computational precision. If R were selected as 1000, for example, then RR would be 1,000,000, and a computer

carrying six-digit precision might not be able to find precise, fractional values of the parameters in an objective function.

Precision is lost when small numbers are subtracted from large numbers such as one million; the Klein and Wylie models illustrated herein depend upon the operation of subtraction. Precision is also lost because both of these computational models depend upon the use of logarithms. As the simplex contracts in the neighborhood of an optimum, the distance between two simplex vertices decreases. Precision is lost, and error may be introduced, since the computer may not be able to differentiate between the logarithms of closely spaced numbers. Since geometry about a point is euclidean, any advantage which non-euclidean optimization may offer would appear to be progressively diminished as the simplex progressively contracts about an optimum.

Hyperbolic Simplex; Hyperbolic Function Evaluation

The development of a sequential simplex routine in which the operations of reflection, expansion, and contraction are taken in hyperbolic context may follow from the Klein cross ratio method or from the Wylie hyperbolic cosine method. Let the latter method be arbitrarily selected [12]. In this model, k represents the metric constant denoted earlier in this report as MC. According to this model, the distance between the two points B and N is given by

$$P_B P_N = (k) \cosh^{-1} \frac{f(P_B P_N)}{\sqrt{f(P_B P_B) f(P_N P_N)}} \quad (1)$$

The point C is equidistant from points B and N when $P_B P_C = P_N P_C$ or

$$\frac{f(P_B P_C)}{\sqrt{f(P_C P_C) f(P_B P_B)}} = \frac{f(P_N P_C)}{\sqrt{f(P_N P_N) f(P_C P_C)}} \quad (2)$$

where a term such as $f(P_B P_B)$ is defined as $RR - X_B^2 - Y_B^2$ and a term such as $f(P_B P_C)$ is defined as $RR - X_B X_C - Y_B Y_C$, X_B and Y_B representing the euclidean x- and y- coordinates of point B. Note that, in this statement of distance equivalence, the metric constant (k) disappears. Squaring both sides of Equation 2 yields

$$\frac{f^2(P_B P_C)}{f(P_C P_C) f(P_B P_B)} = \frac{f^2(P_N P_C)}{f(P_N P_N) f(P_C P_C)} \quad (3)$$

or

$$\frac{f^2(P_B P_C)}{f^2(P_N P_C)} = \frac{f(P_B P_B)}{f(P_N P_N)} = DQ^2 \quad (4)$$

where DQ is a number which may be evaluated from Equation 4.

Equation 4 may be reduced to a linear equation in X_C and Y_C , the euclidean x- and y- coordinates of the point C equidistant from points B and N:

$$RR(1-DQ) = X_C(X_B - X_N DQ) + Y_C(Y_B - Y_N DQ) \quad (5)$$

But the points B and N determine both a euclidean and a hyperbolic line. Since point C is on this line, the equation of the euclidean line through points B and N may take the form

$$BB = -(MM)(X_C) + Y_C \quad (6)$$

where the terms BB and MM represent the numbers customarily associated with the equation of a straight line. Equations 5 and 6 may be solved together by determinants and Cramer's rule to give explicit numerical definition to the points X_C and

Y_C , the euclidean x- and y- coordinates of point C, the point equidistant from points B and N. Hence, point C is a point of the line connecting B and N (Equation 6), and is equidistant (in the hyperbolic sense only) from points B and N (Equation 4).

If the letters B, N, and W represent the vertices of a simplex with the best, next-to-worst, and worst responses of an objective function, respectively, then the points W and C (the hyperbolic centroid of the line connecting points B and N) also determine a straight line. This line may contain the reflection point, R, the expansion point, E, and the two contraction points, C_R and C_W . Point R lies on this line, which may take the same form as Equation 6:

$$Y_R = (MM)X_R + BB \quad (7)$$

But point C is equidistant from points R and W so that

$$\frac{f(P_R P_C)}{\sqrt{f(P_R P_R) f(P_C P_C)}} = \frac{f(P_C P_W)}{\sqrt{f(P_C P_C) f(P_W P_W)}} \quad (8)$$

Squaring both sides of Equation 8 yields

$$\frac{f^2(P_R P_C)}{f(P_R P_R) f(P_C P_C)} = \frac{f^2(P_C P_W)}{f(P_C P_C) f(P_W P_W)} = QR \quad (9)$$

or

$$\frac{(RR - X_C X_R - Y_C Y_R)^2}{RR - X_R^2 - Y_R^2} = QR \quad (10)$$

where QR is a number that can be evaluated from Equation 9.

Equation 7 may be substituted into Equation 10 to yield an equation which is quadratic in X_R . This equation has two

solutions for X_R , say X_1 and X_2 . Both lie along the line defined by Equation 7, and both are equidistant from C. Two points satisfy these criteria: the desired hyperbolic reflection point, and point W. The desired value of the x-coordinate of the reflection point (X_R) may be determined by a small test. The value $|X_1| - |X_W|$ should be nonzero if the solved value of X_1 is the x-coordinate of the reflection point, and zero if the solved value of X_1 is the x-coordinate of point W. Due to round-off error in the computer, the value of the difference $|X_1| - |X_W|$ may not always be exactly zero when calculated X_1 is the coordinate of the W point. However, when X_1 is the coordinate of the point W the difference $|X_1| - |X_W|$ will be smaller than the similar difference when X_1 is the coordinate of the reflection point. In other words, if the difference $||X_1| - |X_W|| - ||X_2| - |X_W||$ is negative, then X_2 is the x-coordinate of the reflection point; whereas if this difference is positive, the x-coordinate of the reflection point is X_1 . These calculations are summarized in paragraphs 4 and 12 of Table 4.

Table 4 is a statement of a two-variable, sequential simplex routine in the (H,H) form, i.e., hyperbolic movements of the simplex and hyperbolic interpretation of the euclidean coordinates of the simplex vertices. This is the sequential simplex method as the observer in the hyperbolic space might use it. Paragraph 3 of Table 4 finds the euclidean coordinates of the centroid of the line connecting points B and N. As the simplex approaches the periphery of the circle, round-off error may occasionally project one of the simplex vertices outside the circle. In

this event, a "violation" message is printed and the program terminates. An increase in the value of the metric constant may prevent this problem.

Paragraphs 4 and 12 find the euclidean coordinates of the reflection point. Paragraphs 6 and 12 find the euclidean coordinates of the expansion point; paragraph 8, the euclidean coordinates of the C_R point; while paragraph 10 finds the euclidean coordinates of the C_W point. Paragraph 11 is for rejection of point N. With the exception of paragraph 2 and the above mentioned paragraphs, the remaining paragraphs represent a suggested form of the traditional sequential simplex routine. Paragraph 2 gives hyperbolic interpretation to the euclidean (x,y) coordinates of the hyperbolic points C, R, E, C_R and C_W . Paragraph 2 uses the cross ratio technique for this calculation, whereas the remainder of the program uses the hyperbolic cosine technique. Table 4 is thus a hybrid program containing both the Klein and Wylie techniques for hyperbolic distance evaluations. There is no specific reason for using the Klein technique in paragraph 2 of Table 4; it has been inserted only as a matter of curiosity, and because it is somewhat shorter than the similar Wylie form. If desired, the Wylie method of evaluating hyperbolic coordinates from euclidean coordinates may be inserted in paragraph 2. Merely take the first entry in Table 3 and insert it as paragraph 2 in Table 4. (Table 4 presently contains the first entry in Table 2.) Table 4 thus presents the possibility of two hyperbolic sequential simplex schemes in the (H,H) form. Either of these schemes may be useful for optimization.

Table 4 - HYPERBOLIC TWO-DIMENSIONAL SEQUENTIAL SIMPLEX ROUTINE

C-FOCAL, 5/8K-71 F

```

01.10 T "HYPERBOLIC SIMPLEX, HYPERBOLIC INTERPRETATION", !
01.12 T "FOR TEST FUNCTION MINIMIZATION", !
01.20 A "J(1)= ", J(1), " K(1)= ", K(1), !
01.22 A "J(2)= ", J(2), " K(2)= ", K(2), !
01.24 A "J(3)= ", J(3), " K(3)= ", K(3), !
01.26 A "GIVE CIRCLE RADIUS ", R, !; S RR=R*R; S A=0
01.28 A "GIVE METRIC CONSTANT ", MC, !; GOTO 5.02

02.02 S DS=RR-J(A)^2-K(A)^2; I (DS)2.30,2.30,2.04
02.04 S XP=RR-K(A)^2; S YP=RR-J(A)^2
02.06 S X1=FSQT(XP); S X2=-X1; S Y1=FSQT(YP); S Y2=-Y1
02.07 I (X1-J(A))2.08,2.30,2.08
02.08 S ZJ=(X2-J(A))*X1/(X2*(X1-J(A)))
02.09 I (Y1-K(A))2.10,2.30,2.10
02.10 S ZK=(Y2-K(A))*Y1/(Y2*(Y1-K(A)))
02.12 S HJ(A)=MC*FLOG(ZJ); S HK(A)=MC*FLOG(ZK)
02.14 S G(A)=-50+HJ(A)^2-24*HJ(A)+HK(A)^2-36*HK(A)
02.16 R
02.30 S G(A)=1E+12

03.06 S DB=RR-BJ^2-BK^2; I (DB)3.50,3.50,3.08
03.08 S DN=RR-NJ^2-NK^2; I (DN)3.50,3.50,3.10
03.10 S DW=RR-WJ^2-WK^2; I (DW)3.50,3.50,3.12
03.12 S DQ=FSQT(DB/DN); S T1=RR*(1-DQ); S T2=NJ*BK-BJ*NK
03.14 S C1=BJ-NJ*DQ; S C2=BK-NK; S B1=BK-NK*DQ; S B2=NJ-BJ
03.18 S XC=(T1*B2-T2*B1)/(C1*B2-C2*B1); S YC=(C1*T2-C2*T1)/(C1*B2-C2*B1)
03.22 S QR=(RR-WJ*XC-WK*YC)^2/(RR-WJ^2-WK^2);
03.24 S SX=XC; S SY=YC; GOTO 4.06
03.50 T "VIOLATION"; Q

04.06 S BB=(WJ*YC-WK*XC)/(WJ-XC); S MM=(WK-YC)/(WJ-XC)
04.08 S Q1=RR-YC*BB; S Q2=XC+YC*MM; S Q3=RR-BB^2; S Q4=2*BB*MM
04.10 S Q5=1+MM^2; S Q6=QR*Q5+Q2^2; S Q7=QR*Q4-2*Q1*Q2
04.12 S Q8=Q1^2-QR*Q3; D 12; S A3=FABS(WJ)
04.16 S DD=FABS(X1-A3)-FABS(X2-A3); I (DD)4.18,4.20,4.20
04.18 S RJ=XR(2); GOTO 4.22
04.20 S RJ=XR(1)
04.22 S RK=BB+MM*RJ

05.02 F A=1,1,3;D 2
05.04 I (G(1)-G(2))5.06,5.24,5.24
05.06 I (G(2)-G(3))5.08,5.30,5.30
05.08 I (G(1)-G(2))5.10,5.36,5.36
05.10 S BG=G(1); S NG=G(2); S WG=G(3)
05.12 S BJ=J(1); S NJ=J(2); S WJ=J(3)
05.14 S BK=K(1); S NK=K(2); S WK=K(3)
05.16 T BG, !
05.22 GOTO 7.02
05.24 S TG=G(1); S G(1)=G(2); S G(2)=TG
05.26 S TJ=J(1); S J(1)=J(2); S J(2)=TJ
05.28 S TK=K(1); S K(1)=K(2); S K(2)=TK; GOTO 5.06
05.30 S TG=G(2); S G(2)=G(3); S G(3)=TG
05.32 S TJ=J(2); S J(2)=J(3); S J(3)=TJ
05.34 S TK=K(2); S K(2)=K(3); S K(3)=TK; GOTO 5.08
05.36 S TG=G(1); S G(1)=G(2); S G(2)=TG
05.38 S TJ=J(1); S J(1)=J(2); S J(2)=TJ
05.40 S TK=K(1); S K(1)=K(2); S K(2)=TK; GOTO 5.10

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Table 4 - HYPERBOLIC TWO-DIMENSIONAL SEQUENTIAL SIMPLEX ROUTINE
(CONTINUED)

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06.06 S QE=(RR-SX*RJ-SY*RK)^2/(RR-SX^2-SY^2); S Q1=RR-RK*BB
06.08 S Q2=RJ+RK*MM; S Q3=RR-BB^2; S Q4=2*MM*BB; S Q5=1+MM^2
06.10 S Q6=QE*Q5+Q2^2; S Q7=Q4*QE-2*Q1*Q2; S Q8=Q1^2-QE*Q3
06.12 D 12; S AC=FABS(SX); S DD=FABS(X1-AC)-FABS(X2-AC)
06.14 I (DD)6.16,6.18,6.18
06.16 S EJ=XR(2); GOTO 6.20
06.18 S EJ=XR(1)
06.20 S EK=BB+MM*EJ

07.02 D 3; D 4; S J(1)=RJ; S K(1)=RK; S J(2)=BJ; S K(2)=BK
07.04 S J(3)=NJ; S K(3)=NK; F A=1,1,3;D 2; S RG=G(1)
07.06 I (RG-BG)7.08,9.04,9.04
07.08 D 6; S J(1)=EJ; S K(1)=EK; F A=1,1,3;D 2; S EG=G(1)
07.10 I (EG-BG)7.16,7.12,7.12
07.12 S J(1)=BJ; S K(1)=BK; S J(2)=RJ; S K(2)=RK
07.14 S J(3)=NJ; S K(3)=NK; GOTO 5.02
07.16 S J(1)=EJ; S K(1)=EK; S J(2)=BJ; S K(2)=BK
07.18 S J(3)=NJ; S K(3)=NK; GOTO 5.02

08.04 S DC=RR-SX^2-SY^2; S DR=RR-RJ^2-RK^2; I (DC)3.50,8.06,8.06
08.06 I (DR)3.50,3.50,8.08
08.08 S DQ=FSQT(DC/DR)
08.10 S CJ=(BB*(SY-RK*DQ)-RR*(1-DQ))/(-MM*(SY-RK*DQ)-(SX-RJ*DQ))
08.12 S CK=(-MM*RR*(1-DQ)-BB*(SX-RJ*DQ))/(-MM*(SY-RK*DQ)-(SX-RJ*DQ))

09.04 I (RG-NG)7.12,9.20,9.20
09.20 I (RG-WG)9.22,9.40,9.40
09.22 D 8; S J(1)=CJ; S K(1)=CK; S J(2)=BJ; S K(2)=BK
09.28 S J(3)=NJ; S K(3)=NK; F A=1,1,3;D 2; S CG=G(1)
09.30 I (CG-WG)9.32,9.40,9.40
09.32 S J(1)=BJ; S K(1)=BK; S J(2)=NJ; S K(2)=NK
09.34 S J(3)=CJ; S K(3)=CK; GOTO 5.02
09.40 D 10; S J(1)=BJ; S K(1)=BK; S J(2)=NJ; S K(2)=NK
09.42 S J(3)=QJ; S K(3)=QK; F A=1,1,3;D 2; S QG=G(3)
09.50 I (QG-WG)9.52,11.02,11.02
09.52 S J(1)=BJ; S K(1)=BK; S J(2)=NJ; S K(2)=NK
09.56 S J(3)=QJ; S K(3)=QK; GOTO 5.02

10.02 S DW=RR-WJ^2-WK^2; S DC=RR-SX^2-SY^2; I (DC)3.50,3.50,10.04
10.04 I (DW)3.50,10.06,10.06
10.06 S DQ=FSQT(DW/DC); S T1=RR*(1-DQ)
10.08 S QJ=(T1-BB*(WK-SY*DQ))/(WJ-DQ*SX+MM*(WK-SY*DQ))
10.10 S QK=(BB*(WJ-DQ*SX)+MM*T1)/(WJ-DQ*SX+MM*(WK-SY*DQ))

11.02 S DW=RR-WJ^2-WK^2; S DB=RR-BJ^2-BK^2; S DQ=FSQT(DW/DB)
11.04 S T1=RR*(1-DQ); S T2=WJ*BK-BJ*WK; S C1=WJ-DQ*BJ
11.06 S C2=BK-WK; S B1=WK-DQ*BK; S B2=WJ-BJ; D 3.18
11.08 S WJ=NJ; S WK=NK; D 3.22; D 4; S J(1)=BJ; S K(1)=BK
11.10 S J(2)=WJ; S K(2)=WK; S J(3)=RJ; S K(3)=RK
11.12 GOTO 5.02

12.02 S RD=Q7^2-4*Q6*Q8; I (RD)12.04,12.06,12.06
12.04 S RD=0
12.06 S XR(1)=(FABS(Q7)+FSQT(RD))*FSQN(-Q7)/(2*Q6)
12.08 I (XR(1))12.14,12.10,12.14
12.10 S XR(1)=(-Q7-FSQT(RD))/(2*Q6)
12.12 S XR(2)=(-Q7+FSQT(RD))/(2*Q6)
12.14 S XR(2)=Q8/(XR(1)*Q6); S X1=FABS(XR(1)); S X2=FABS(XR(2))

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Note: The euclidean counterparts (XE, YE) to any set of hyperbolic coordinates (XH, YH) may be found by use of a short program such as is illustrated below. In a circle of radius 1 unit and metric constant 3, the point with euclidean coordinates (0.306, 0.306) has hyperbolic coordinates (1, 1), and a simplex started at these hyperbolic coordinates should be started

in the Table 4 program at the point $J(1)=0.306$, $K(1)=0.306$. Since these euclidean coordinates have been calculated with the hyperbolic cosine model, the metric constant 3 is changed to 1.5 when these coordinates are entered into the program in Table 4. (Coordinate signs are determined by the quadrant into which point falls.)

Table 4 - APPENDIX

C-PS/8 FOCAL, 1971

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01.02 T "CONVERSION OF HYPERBOLIC TO EUCLIDEAN COORDINATES (WYLIE)", !
01.03 T "ABSOLUTE VALUES ONLY", !!
01.04 A "CIRCLE RADIUS= ", R, " METRIC CONSTANT= ", MC, !
01.06 A "HX= ", HX, " HY= ", HY, !
01.08 S HX=HX/MC; S HY=HY/MC; S RR=R*R
01.10 S A=(FEXP(HX)+FEXP(-HX))/2; S B=(FEXP(HY)+FEXP(-HY))/2
01.12 S C=A^2+B^2-1
01.14 S X2=RR*(A^2-1)/C; S Y2=RR*(B^2-1)/C
01.16 S XE=FSQT(X2); S YE=FSQT(Y2)
01.18 T "XE= ", XE, " YE= ", YE, !!
01.20 GOTO 1.06

```

*
G
CONVERSION OF HYPERBOLIC TO EUCLIDEAN COORDINATES (WYLIE)
ABSOLUTE VALUES ONLY

CIRCLE RADIUS= 1, METRIC CONSTANT= 3,
HX= 1, HY= 1,
XE= 0.3060818637E+00 YE= 0.3060818637E+00

HX=

Hyperbolic Simplex; Euclidean Function Evaluation

Table 4 may be converted to a sequential simplex routine in the (H,E) form merely by replacing paragraph 2 with a simple statement of the objective function, as shown in Table 5 of Reference 9. When used in the (H,E) form, care must be taken that the radius of the circle is larger than the absolute value of the largest parameter in the function to be optimized. The metric constant is not used in the (H,E) form.

Figure 2 illustrates hyperbolic movements of an arbitrary simplex BNW. The euclidean coordinates of points B, N, and W are

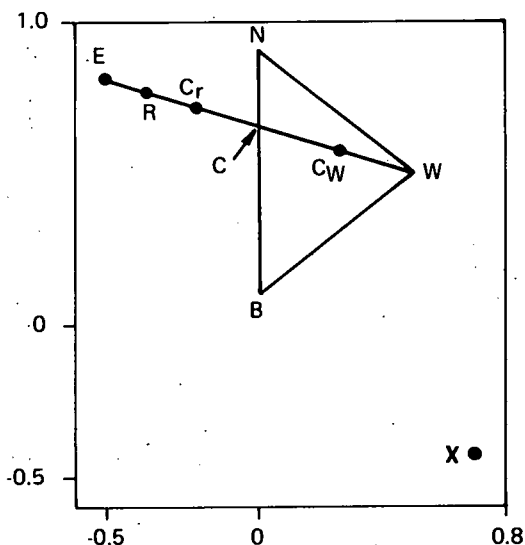


FIGURE 2 - Movements of an arbitrary hyperbolic simplex. The simplex has euclidean (x,y) coordinates B(0, 0.1), N(0, 0.9), and W(0.5, 0.5). It may move to E(-0.506, 0.814), R(-0.368, 0.771), C_r(-0.218, 0.724), and C_w(0.258, 0.576) through centroid C(0, 0.656). It may also move to point X(0.686, -0.429). Radius of circle is one unit.

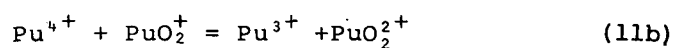
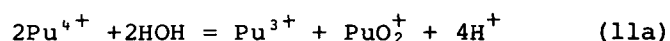
(0, 0.1), (0, 0.9), and (0.5, 0.5), respectively. The simplex has been placed in a circle with a radius of unity, and this circle represents all two-dimensional hyperbolic space. The hyperbolic distances between points E and R, between points R and C (the centroid of line BN), between points C and W, and between points C_r and C_w are all equal, and are equal to twice the hyperbolic distance between points W and C_w, C_w and C, and C_r and C. Point X in Figure 2 is the point formed by reflection of point N through the centroid of the line BW, this reflection and centroid being taken in the hyperbolic senses. The euclidean coordinates of points E, R, C, C_r, and C_w are, respectively, (-0.506, 0.814), (-0.368, 0.771), (0.0, 0.656), (-0.218, 0.724) and (0.258, 0.576).

A computer program for hyperbolic sequential simplex may also be based on some of the distance formulas conveniently listed by Martin [13]. Although not strictly non-euclidean in the traditional sense, interesting optimization algorithms may be developed by applying a distance measurement such as the cross ratio technique to the interior of any closed, convex curve such as, for example, $x^4 + y^4 = \text{constant}$.

Non-euclidean simplex optimization may be used in the laboratory as well as in the computer. Changing the value of the metric constant in the (H,H) algorithm changes the path of a simplex even when started at the same initial points. This situation occurs because hyperbolic planes with differing metric constants are only "almost isomorphic".

The Nonequilibrium Titration of Plutonium

Optimization problems arise not only in mathematical expressions, but also in such matters as determining the optimum conditions for nonequilibrium titrations. As an aid to the understanding of potentiometric titrations of plutonium in dilute acid, for example, the potential and potential derivatives of plutonium valence state distributions might be examined [9]. It has also been suggested that the inflection point and the stoichiometric end point of plutonium potentiometric titrations may not always correspond, and this lack of correspondence has to be further explored [14]. It might be possible to simulate a nonequilibrium potentiometric titration of plutonium if values were known for the actual concentration quotients, Q_1 , and Q_2 , for reactions 11a and 11b, respectively.



In 10M acid, where $Q_1 = K_1 = 6.97\text{E}-04$ and $Q_2 = K_2 = 13.2$ at equilibrium, the inflection point slightly precedes the stoichiometric end point [9]. In 1M acid, on the other hand, an inflection point in the neighborhood of the stoichiometric end point is not easy to discern under equilibrium conditions [9].

As a nonequilibrium potentiometric titration of trivalent plutonium nears the stoichiometric end point in dilute acid, it seems likely that the actual concentration of tetravalent plutonium will exceed its equilibrium concentration, while the nonequilibrium concentrations of other

plutonium species are likely to be less than their equilibrium values. Hence, the value of Q_1 is likely to be less than K_1 , the equilibrium constant for Equation 11a. Likewise, the value of Q_2 may also be less than K_2 , the equilibrium constant for Equation 11b. Hence, for purposes of simulating nonequilibrium titrations in dilute acid, values of Q_1 and Q_2 which are less than the values of K_1 and K_2 may be used in the plutonium (N,H) characteristic equation. The problems which then arise are: how much less than K_1 and K_2 should be the values of Q_1 and Q_2 , respectively; and what value should be given the ratio Q_2/Q_1 . In nonequilibrium circumstances it seems unlikely that the ratio Q_2/Q_1 would be some constant multiple of the ratio K_2/K_1 . As an illustration, however, assume that $Q_2/Q_1 = K_2/K_1$ as the values of Q_2 and Q_1 are decreased. For example, when $Q_1 = 6.97\text{E}-07$ and $Q_2 = 13.2\text{E}-03$, an inflection point is observed near a plutonium average oxidation number of about 3.998. (The average oxidation number at the stoichiometric end point is 4.000.) As the values of Q_1 and Q_2 are decreased still farther, the point of potential inflection and the stoichiometric end point correspond more and more closely; this suggests that the optimum circumstances for potentiometric titration in 1M acid devoid of complexing agents are circumstances far from the equilibrium distribution of plutonium valence states.

The simulation described above may be criticized for a variety of reasons, among them the arbitrary assignment of the value of Q_2/Q_1 as equal to that of the ratio K_2/K_1 . For the sake of diversity, therefore, let this ratio have some other arbitrary value, such as the ratio of the specific rate constants [15] for reactions 1 and 2. Thus, $Q_2/Q_1 = 37.1/2.56\text{E}-05$.

Again it is found that, as the absolute values of Q_1 and Q_2 are diminished, the inflection point and the stoichiometric end point of the titration correspond more and more closely. As an example of lack of correspondence of these parameters, however, it may be noted that when $Q_2 = 37.1E-02$ and $Q_1 = 2.56E-07$, the inflection point occurs near the plutonium average oxidation number of 3.994.

This simulation procedure may also be criticized because it assumes that the potential of the potential-sensing electrode corresponds to the nonequilibrium $\text{PuO}_2^{2+}/\text{PuO}_2^+$ ratio, or to the nonequilibrium $\text{Pu}^{4+}/\text{Pu}^{3+}$ ratio. That the potential-sensing electrode accurately reflects the ratios of these nonequilibrium redox pairs has not been demonstrated. Yet the electrode response is in some manner surely due to some redox couple, even though, as assumptions suggest, an inflection in the response of an electrode may not necessarily correspond to a stoichiometric end point. In other words, in a plutonium solution which is undergoing volumetric or electrometric titration, the plutonium ion alpha coefficients and the solution acidity may be taken as constants to a first approximation. For such a titration, nonequilibrium circumstances may occur such that the numerical values of Q_1 and Q_2 lead to a plutonium (N,H) characteristic equation for which the potentiometric inflection point and stoichiometric end point fail to correspond. Thus, arbitrary assignment of the potential inflection point as the stoichiometric end point of a titration may not be justified.

That a potential inflection point may occur apart from the stoichiometric end point may be further illustrated by

consideration of the coulometric titration of plutonium in sulfuric acid solution [16]. This procedure is commonly used for the accurate assay of plutonium and involves coulometric titration of the plutonium from the trivalent to the tetravalent state in half molar sulfuric acid. In the constant potential version of this titration, the oxidation potential is taken as +0.67 volt vs. S.C.E., i. e., about +0.91 volt vs. N.H.E. In order for this titration to give accurate, reliable, and reproducible results, the initial oxidation number of the plutonium should be close to 3.0, and the final oxidation number of the plutonium, near 4.0. If the plutonium initial and final oxidation numbers are exactly 3.0 and 4.0, respectively, then accurate measurement of the coulombs which have passed through the titration cell, corrected for background currents, may yield an accurate measurement of the plutonium present in the solution. Otherwise, chemical calibration of the titration, as with accurately assayed specimens of plutonium, is desirable.

It has generally been assumed that the coulometric titration of plutonium does proceed from $N=3.0$ to $N=4.0$ within a small error which may be assayed by a calculation from the formal potentials of plutonium in sulfuric acid. Such formal potentials pertain to equilibrium, however, and this circumstance may not be well approximated in actual titration circumstances. That a potential of 0.91 volt leads to a plutonium oxidation number which is close to 4.0, and which is reproducible from one titration to the next, may still await demonstration.

Often, in the sulfuric acid titration of plutonium by constant potential coulometry, a small correction factor is desirable in

order that the coulombs accumulated in the instrument will closely correspond to the plutonium in the beaker. In some circumstances, this correction factor is about 0.1% of the plutonium being titrated, i.e., the instrument accumulates about 0.1% too much current.* During the course of the titration, the values of Q_1 and Q_2 are difficult to assay with accuracy. There are several reasons for this, among them the inaccurately known alpha coefficients for plutonium, the extent to which the plutonium has been perturbed from its equilibrium distribution, and the rate at which disproportionation reactions attempt to correct this imbalance. Owing to these circumstances, however, the values of Q_1 and Q_2 are likely to be considerably less than K_1 and K_2 , respectively. Some selected values of Q_1 and Q_2 with an acidity of 1M and a potential of 0.91 volt may, therefore, be combined in the plutonium (E,H) characteristic equation, in order to examine valence state distributions accompanying nonequilibrium circumstances.

When a valence state distribution has thus been assayed, the average oxidation number of the plutonium in the titration vessel may be ascertained by a simple calculation.

As an example of this approach, it is found that where $Q_1 = (6.97)(10^{-10})$ and $Q_2 = (13.2)(10^{-7})$, then the average oxidation number for uncomplexed plutonium at an imposed potential of 0.91 volt vs N.H.E. is about 4.001, i.e., about 0.1% more oxidation has occurred than suspected. Other values of Q_1 and Q_2 similarly yield plutonium valence state distributions

which do not correspond exactly to $N=4.0$. For example, when $Q_1 = 10^{-7}$ and $Q_2 = 10^{-4}$, oxidation of the plutonium is about 0.1% greater than may have been predicted. Since the values of Q_1 and Q_2 in a real titration depend upon a variety of factors, a titration carried out at some preselected oxidation potential may not correspond to a plutonium average oxidation number of exactly 4.0 at the end of the titration. Either too much or too little oxidation of the plutonium may occur, so chemical and electrical calibration of a coulometer should not be assumed to yield an exact 1:1 correspondence. Hence, chemical calibration of a plutonium titration may always be desirable. Complexation effects do not change the essence of the foregoing arguments. For example, when the alpha coefficients AW, AX, AY, AZ, for the tri-, tetra-, penta-, and hexa-valent states of plutonium are taken as 100, 10,000, 1, and 10, respectively, then at a potential of +0.91 V the average oxidation number of the plutonium is about 4.001 for $Q_1 = 10^{-6}$ and $Q_2 = 10^{-6}$.

The location of the inflection point in a potentiometric titration of plutonium depends upon the alpha coefficients of the various plutonium ions, as illustrated elsewhere [9]. An alpha coefficient of considerable interest is the one which derives from the first hydrolysis reaction of the tetravalent plutonium cation. Many years ago, an attempt was made to determine the value of this alpha coefficient by direct potentiometry [17]. (The term $H/(H+KH)$ measured in Reference 17 is the reciprocal of the alpha coefficient $1+(KH/H)$; KH is the first Pu(IV) hydrolysis constant.) In this determination, the potentials of solutions containing initially prescribed values of the

*R. J. Seiler, Mound Laboratory, to G. L. Silver, private communication.

Pu(IV)/Pu(III) ratio were measured as a function of the solution acidity. Depending upon the initial, fixed value of this ratio, such solutions will be increasingly distant from equilibrium as the acidity of the solutions decreases or increases, since, for a given acidity, there is only one equilibrium value of the Pu(IV)/Pu(III) ratio.* Hence, if potential measurements are made soon after the preparation of such solutions, some of the measurements may pertain to solutions not at equilibrium. Since a chemical reaction may occur at the surface of an electrode placed in a solution which is not at equilibrium, and since the values of the Pu(IV)/Pu(III) and Pu(VI)/Pu(V) ratios are not their equilibrium values in such a solution, any potential recorded from an electrode in this circumstance may

*The establishment of fixed initial quantities of Pu(III) and Pu(IV) establishes the value of the plutonium average oxidation number in the solution. For any prescribed average oxidation number, the equilibrium value of the Pu(IV)/Pu(III) ratio is uniquely established by the equilibrium acid concentration of the solution.

be a mixed potential. But mixed potentials are often difficult to interpret unambiguously, and may bear no simple relation to potentials predicted by the Nernst equation [18]. Such potentials may, therefore, be insufficiently reliable to ascertain the first hydrolysis constant of tetravalent plutonium (KH) beyond question, and this unreliability may explain in part the discrepancies observed in various experimental determinations of the value of KH [19]. Similar arguments may be extended to experimental determinations of the formal potentials of the various plutonium couples [20]. Changes in observed potentials in plutonium solutions of fixed plutonium average oxidation number may derive from more than one cause: hydrolysis may be one cause, but the progressive rearrangement of plutonium oxidation states may also be a cause. Thus, the mixed potentials observed under nonequilibrium circumstances may not be sufficiently reliable for accurate endpoint determinations in plutonium titrations or for equilibrium constant evaluations in aqueous plutonium solutions.

Supplement

Algorithms suitable for solving the plutonium (N,H) equation include the bisection method and the modified Regula Falsi method [21]. Other methods are also available, however; among them is solution by infinite series. While a series may be easier to adapt to popular "pocket" calculators than one of the iterative techniques, a series solution of equations is not without drawbacks, such as failure of the series to converge, failure of the series to converge sufficiently rapidly, or convergence to the wrong root. In the last case, the correct root may be obtained from the knowledge that the characteristic equation has but one positive root, that this positive root is the desired root, and that, given any root of the equation, the other roots may be obtained by a simple calculation involving the coefficients of the cubic equation.

The purpose of this section is to examine one particular series for the root of a cubic equation, and to remark that other series solutions for cubic equations are also available [22]. The method illustrated here depends upon the now obscure theorem of Lagrange [23, 24].

To apply the theorem of Lagrange, it is first desirable to take the general cubic equation

$$AX^3 + BX^2 + CX + D = 0 \quad (12)$$

and divide all coefficients by A, the coefficients of the cubed term:

$$X^3 + pX^2 + qX + r = 0 \quad (13)$$

Equation 13 may be reduced to Equation 14 or Equation 15

$$Y^3 - aY + b = 0 \quad (14)$$

$$Y = (b/a) + (Y^3/a) \quad (15)$$

by means of the substitution

$$X = Y - p/3 \quad (16)$$

$$\text{where } a = p^2/3 - q \quad (17)$$

$$\text{and } b = r - (pq)/3 + 2p^3/27 \quad (18)$$

The theorem of Lagrange states that the desired expansion $f(z)$ is $f(z) =$

$$f(y) + \sum_{N=1}^{\infty} \frac{\partial^{N-1}}{\partial y^{N-1}} \left[(\phi(y))^{N-1} f^1(y) \right] \frac{X^N}{N!} \quad (19)$$

which, when applied to Equation 15 yields

$$Y = (b/a) + (b/a)^3 (1/a) + (6/2!) (b/a)^5 (1/a)^2 + (9)(8/3!) (b/a)^7 (1/a)^3 + (12)(11)(10/4!) (b/a)^9 (1/a)^4 + (15)(14)(13)(12/5!) (b/a)^{11} (1/a)^5 + (18)(17)(16)(15)(14/6!) (b/a)^{13} (1/a)^6 + \dots \quad (20)$$

where terms beyond the third (b/a counted as the 0th term) may be computed from the recursion relation

$$A(N+1) = \frac{3(3N+2)(3N+1)}{(2N+3)(2N+2)} (b/a)^2 (1/a) (A(N)) \quad (21)$$

Example: By means of Lagrange's theorem, evaluate the root of the plutonium (N,H) polynomial which represents the equilibrium valence distribution of plutonium of average oxidation number 5.0 in one molar acid. Neglect hydrolysis and complexation effects. The polynomial whose root is to be evaluated is

$$M^3 - (1.9)(10^4)M - (5)(10^5) = 0 \quad (22)$$

and this is the form of Equation 14 without further modification. Application of

Lagrange's theorem for a cubic equation (Equation 20 above) yields $M = -27.398$. Since M is negative, this is not the desired root. However, the sum of all the roots is zero

$$-27.398 + R_1 + R_2 = 0 \quad (23)$$

whereas the product of all the roots is $(5)(10^5)$

$$(5)(10^5) = (-27.398)(R_1)(R_2) \quad (24)$$

and the desired root is thus found to be $M = 149.28$.

Bromwich lists other series for the cubic equation in its various forms [25].

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