

spectrum was a more important consideration than the error at a single point.

In the study of hydrolyzed polynucleotides it is difficult to obtain enough of the pure component nucleotides to weigh and thus measure the spectra at known concentrations. The effect of concentration can be eliminated with normalization by dividing each point by the vector length, the area under the curve or the absorbance at a fixed wavelength (e.g. 2600). The solution of the normalized mixture vector is then obtained in fractional parts.

This linear programming method which minimizes the small, nonsystematic, experimental errors leads to a much improved numerical solution of the chemically known polynucleotides over the classical least squares methods. The advantages appear to lie in disallowing negative solutions and in the choosing of significant points on which to base the solution while allowing the possibility of small positive or negative errors to be reflected as slack.

ACKNOWLEDGMENT

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Algorithms

J. H. WEGSTEIN, Editor

ALGORITHM 150 SYMINV2

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procedure *syminv2*(*a*,*n*) **result:** (*a*) **exit:** (*fail*); **value** *n*; **integer** *n*; **array** *a*; **label** *fail*;

comment *syminv2* obtains inverse of a symmetric matrix *a* of order *n* by a method which is similar to that given by Busing and Levy [*Comm. ACM* 5 (1962), 446] but requires no interchanges of rows and columns nor storage space for an additional matrix *Q*, yet is numerically equivalent. The procedure requires the upper triangular part of *a* to be given and overwrites it by the upper triangular part of the inverse which is again denoted by *a*. All pivots are chosen on the diagonal, and if all further diagonal elements which are eligible as pivots vanish (this is impossible for a positive definite matrix *a*) then exit through *fail* occurs;

begin

real *bigajj*;

integer *i*, *j*, *k*;

real array *p*, *q*[1:*n*];

Boolean array *r*[1:*n*];

for *i* := 1 **step** 1 **until** *n* **do** *r*[*i*] := **true**;

grand loop:

for *i* := 1 **step** 1 **until** *n* **do**

begin

search for pivot:

bigajj := 0;

for *j* := 1 **step** 1 **until** *n* **do**

begin

if *r*[*j*] \wedge *abs*(*a*[*j*,*j*]) > *bigajj* **then**

begin

bigajj := *abs*(*a*[*j*,*j*]);

k := *j*

end;

end;

if *bigajj* = 0 **then go to** *fail*;

preparation of elimination step i:

r[*k*] := **false**;

q[*k*] := 1/*a*[*k*,*k*];

p[*k*] := 1;

a[*k*,*k*] := 0;

for *j* := 1 **step** 1 **until** *k*-1 **do**

begin

p[*j*] := *a*[*j*,*k*];

q[*j*] := (**if** *r*[*j*] **then** -*a*[*j*,*k*] **else** *a*[*j*,*k*]) \times *q*[*k*];

a[*j*,*k*] := 0

end;

for *j* := *k*+1 **step** 1 **until** *n* **do**

begin

p[*j*] := **if** *r*[*j*] **then** *a*[*k*,*j*] **else** -*a*[*k*,*j*];

q[*j*] := -*a*[*k*,*j*] \times *q*[*k*];

a[*k*,*j*] := 0

end;

elimination proper:

for *j* := 1 **step** 1 **until** *n* **do**

```

    for  $k := j$  step 1 until  $n$  do
       $a[j,k] := a[j,k] + p[j] \times q[k]$ 
    end grand loop
end syminv2

```

ALGORITHM 151 LOCATION OF A VECTOR IN A LEXICO- GRAPHICALLY ORDERED LIST

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integer procedure LOCATE (*min, n, c, v, combinatorial*);

value *v*; **integer** *min, n, c*; **integer array** *v*;

integer procedure combinatorial;

comment This procedure locates the position, LOCATE, of a given vector in a list of vectors without searching the list. The list consists of all the combinations of n consecutive digits taken d at a time. *Min* is the smallest of the n integers. Each vector (combination) is written in ascending order from left to right, as, for example, 378 and the vectors are listed lexicographically, by which is meant, that, considered as d digit numbers, the vectors are listed in ascending order. For example, with $min = 1$, $d = 3$, and $n = 6$, the vectors in order are 123, 124, 125, 126, 134, 135, ..., 456. Given the vector, $v = 356$, the procedure locates this vector as the 19th in the list;

begin integer *i, r, max, part, whole*;

$r := 1$; $v[0] := min - 1$; $max := min - 1 + n$;

for $i := 0$ step 1 until $c - 1$ do

begin *part* := $c - i - 1$;

ask: **if** $v[i+1] - v[i] > 1$ **then**

begin *whole* := $max - v[i] - 1$;

$r := r + combinatorial(whole, part)$;

$v[i] := v[i] + 1$;

go to *ask*

end;

end;

locate := r

end;

ALGORITHM 152

NEXCOM

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procedure nexcom (*char, n, setcomplete, nullvector*);

array *char*; **integer** *n*;

label *setcomplete, nullvector*;

comment *char* is a column vector containing n elements each of which is either 1 or 0. Nexcom transforms *char* into another vector containing the same number of 1's and 0's, but in a different sequence. Starting with *char* in the state of having 1 in each of the element positions 1, ..., r and zeros elsewhere then repeated application of nexcom generates all nC_r patterns of *char*. The procedure terminates if the presented vector *char* has 1 in each of the positions $n, n-1, \dots, n-r+1$ and zeros elsewhere. Termination is indicated by exit through the formal label 'setcomplete'. If *char* is the null vector then procedure exists through the formal label 'nullvector';

begin integer *n, p, m*;

comment find the first 1 in *char*;

for $n := 1$ step 1 until N do **if**

$char[n] = 1$ **then go to** *A*;

go to *nullvector*;

comment how many adjacent 1's;

A: $p := 0$;

for $m := n + 1$ step 1 until N do

if $char[m] = 1$ **then** $p := p + 1$ **else go to** *B*;

comment Have all combinations been generated;

B: **if** $p + n = N$ **then go to** *setcomplete*;

comment Set up next combination; $char[n+p+1] := 1$;

for $m := n + p$ step - 1 until n do $char[m] := 0$;

for $m := 1$ step 1 until p do $char[m] := 1$;

end nexcom;

ALGORITHM 153

GOMORY

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procedure Gomory (*a, m, n*) result: (*a*) exit: (*no solution*);

value *m, n*;

integer *m, n*;

integer array *a*;

label *no solution*;

comment Gomory algorithm for all-integer programming. The objective of this procedure is to determine the integer solution of a linear programming problem with integer coefficients only. The tableau-matrix *a* consists of $m + 1$ rows and n columns. The top row of *a* is the objective row, the last column represents the right-hand sides. The tableau-columns, with the exception of the last column, have to be lexicographically positive. The algorithm is finished if all entries in the last column, except the top most entry, are nonnegative. Then the top most entry of the last column represents the value of the objective function. The other entries of the last column define the coordinates of the optimal solution. There are always the same variables connected with the same rows. The exit *no solution* is used if a row is found which has a negative entry in the last column, but otherwise only nonnegative entries;

begin integer *i, k, j, l, r*;

real *lambda*;

integer array $t[1:n-1], c[1:n]$;

1: **for** $i := 1$ step 1 until m do **if** $a[i,n] < 0$ **then**

begin $r := i$; **go to** 2 **end**;

go to *end*;

2: **for** $k := 1$ step 1 until $n-1$ do **if** $a[r,k] < 0$ **then**

go to 4;

go to *no solution*;

4: $l := k$;

for $j := k+1$ step 1 until $n-1$ do **if** $a[r,j] < 0$ **then**

begin $i := 0$;

3: **if** $a[i,j] < a[i,l]$ **then** $l := j$ **else**

if $a[i,j] = a[i,l]$ **then**

begin $i := i+1$; **go to** 3 **end**

end;

for $j := 1$ step 1 until $n-1$ do **if** $a[r,j] < 0$ **then**

begin **if** $a[0,l] \neq 0$ **then** $t[j] := entier(a[0,j]/a[0,l])$

else $t[j] := 1$

end;

$lambda := abs(a[r,1]/t[1])$;

for $j := 2$ step 1 until $n-1$ do **if** $a[r,j] < 0$ **then**

begin **if** $abs(a[r,j]/t[j]) > lambda$ **then**

$lambda := abs(a[r,j]/t[j])$ **end**;

for $j := 1$ step 1 until n do **if** $j \neq l$ **then**

begin $c[j] := entier(a[r,j]/lambda)$;

if $c[j] \neq 0$ **then**

for $i := 0$ step 1 until m do $a[i,j] := a[i,j] + c[j] \times a[i,l]$

end;

go to 1;

end: **end**;

CERTIFICATION OF ALGORITHM 32
 MULTINT [R. Don Freeman, *Comm. ACM*, Feb. 1961]
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* Work supported by the U. S. Atomic Energy Commission.

The procedure was transcribed into the ACT-III language for the LGP-30 computer, and was tested on the integrals:

$$(1) \int_0^1 \int_0^1 \int_0^1 \int_0^1 k[\cos u - 7u \sin u - 6u^2 \cos u + u^3 \sin u] dw dx dy dz = \sin k$$

where $u = kwx yz$, and

$$(2) \int_0^1 \int_0^{\sqrt{1-x^2}} \int_0^{\sqrt{1-x^2-y^2}} \frac{dz dy dx}{x^2 + y^2 + (z-k)^2} = \pi \left(2 + \frac{1}{2} \left(\frac{1}{k} - k \right) \log \left| \frac{1+k}{1-k} \right| \right).$$

The ALGOL procedures for the second integral are:

```

real procedure Low (j,x);
Low := 0;
real procedure Upp(j,x); comment z ≡ x[3], y ≡ x[2], x ≡
x[1];
begin
integer i; real temp;
temp := 1.0;
for i := j-1 step - 1 until 1 do
temp := temp - x[j] × x[j];
Upp := sqrt(temp)
end;
real procedure Funev(j,x);
comment The real parameter k is global;
Funev := if j < 3 then 1.0 else 1/(x[1]×x[1]+x[2]×x[2]+(x[3]-k)
↑ 2);
  
```

The first integral was tested only with $s[j] = 1$, and with various Gaussian formulas for integrals over the interval $(-1, +1)$. Results were as follows:

k	$\pi/2$	π	$3\pi/2$	2π
true	1.0000000	0.0000000	-1.0000000	0.0000000
p = 2	0.993704	-0.0333603	+0.020166	6.881490
p = 3	1.000032	0.0000848	-1.061651	-0.597419
p = 4	0.999999	0.0000001	-0.998407	+0.0027035
p = 5	1.000000	-0.0000002	-1.000028	-0.0007857

For the second integral, two values of $s = s[1] = s[2] = s[3]$ were used, and two values of p . Results were as follows:

k	1/2		2	
	1	2	1	2
true	11.46027376		1.10609687	
p = 2	5.454460	11.838651	1.0368770	1.1184305
p = 3	9.361666	12.408984	1.1343551	1.1094278

The effect of the pole at $(0,0,k)$ is obvious.

For the algorithm to run in any compiler, the semicolon following $x[T]$; in the fourth line above the end of the comment must be deleted. The array bounds on the arrays r and d must be increased to $[1 : T+1]$.

For a system which permits variable array bounds, the introduction of the integer T appears superfluous. For such a system, T may be replaced by n throughout with a probable gain in efficiency. For most translators, the presence of undefined elements in an array will not cause difficulties, provided these elements do not appear in an expression before they are assigned a value.

The statement "for $j := 1$ step 1 until T do $x[j] := 0.0$;" is thus superfluous. The semicolon before the **end** which precedes the label "sum" also appears unnecessary.

In spite of these minor corrections, the algorithm appears to be extremely convenient for multiple quadratures over arbitrary regions using the Cartesian product of any explicit one-dimensional formula (and not merely a Gaussian formula) for integrating over the range $[-1,1]$. If endpoints are used in the formula, it will, of course, repeat the calculation for each section of the range.

CERTIFICATION OF ALGORITHM 73
 INCOMPLETE ELLIPTIC INTEGRALS [David K.
 Jefferson, *Comm. ACM* 4, Dec. 1961]
 NOELLE A. MEYER
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Ellint was hand-coded in FORTRAN for the IBM 7070. The following corrections were made:

The statement

$$E := (2 \times n - 1) / (2 \times N);$$

should be

$$E := (2 \times n - 1) / (2 \times n);$$

The statement

$$F := \text{abs}(k) \times \text{sqrt}(1 - \text{sinphi} \uparrow 2) \times (1 - k \uparrow 2 \times \text{sinphi} \uparrow 2) \uparrow \frac{1}{(2 \times n - 1) / (2 \times n)};$$

should be

$$F := (\text{abs}(k) \times \text{sqrt}(1 - \text{sinphi} \uparrow 2) \times (1 - k \uparrow 2 \times \text{sinphi} \uparrow 2) \uparrow (n - .5)) / (2 \times n)$$

The statement

$$L[2] := L[1] + 1 / (n \times 2 \times n - 1);$$

should be

$$L[2] := L[1] + 1 / (n \times (2 \times n - 1));$$

In order to accommodate negative ϕ the following changes were made:

The statement

$$\text{if } \text{abs}((\text{sigma}[1] + \text{del}[1]) - \text{sigma}[1]) > 0 \wedge \text{phi} \times \text{sinphi} \uparrow (2 \times n) \geq A[2] \text{ then go to step 1};$$

was changed to

$$\text{if } \text{abs}((\text{sigma}[1] + \text{del}[1]) - \text{sigma}[1]) > 0 \wedge \text{abs}(\text{phi} \times \text{sinphi} \uparrow (2 \times n)) \geq \text{abs}(A[2]) \text{ then go to step 1};$$

Also the following was inserted before the last statement (*stop*: **end**)

```

if phi < 0 then go to wait else go to stop;
wait: F := -F;
      E := -E;
  
```

The revised algorithm yielded satisfactory answers when compared with the DiDonato and Hershey tables. Differences occurred in the eighth significant digit as shown in the following difference tables.

DIFFERENCE TABLES

F-TABLE

θ (in degrees)

(in degrees)	0	30	60	90
0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-3×10^{-8}
60	1×10^{-8}	1×10^{-8}	2×10^{-8}	-3×10^{-8}
90	0.	2×10^{-8}	6×10^{-8}	0.

E-TABLE

(in degrees)	0	30	60	90
0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}
60	1×10^{-8}	1×10^{-8}	-7×10^{-8}	3×10^{-8}
90	0.	0.	1×10^{-8}	0.