

THE N -STEP ITERATION PROCEDURES

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This paper presents a few of the results obtained by the author while writing a doctoral thesis at the Massachusetts Institute of Technology. In addition to presenting what is believed to be a new N -step procedure for the solution of simultaneous linear equations, the author attempts to show the close relationship between several of these procedures.

One considers the task of finding the solution to a set of N simultaneous linear equations. It is desired to guess the N numbers which represent the solution, and to correct this trial answer until the correct answer is obtained.

Thus, in matrix notation, the problem is

$$Ax = y,$$

where A is the matrix of coefficients of the N unknowns x , and y is the column matrix of the constants.

One begins by choosing x_0 , a set of N numbers, as an initial trial solution. One can now substitute these numbers in the equations to see if they constitute a good approximation to the true answers. Since the first trial is rarely good, one wishes to correct this by altering the vector x_0 by some specified amount so that the new approximation is nearer the answer x . More generally, one wishes to establish a sequence of vectors x_0, x_1, x_2, \dots which converge toward the solution x . Thus, if x_k is the k^{th} such trial, one wishes to consider those procedures which obtain the next trial using the relationship

$$x_{k+1} = x_k - m_k p_k.$$

p_k will be one of a set of vectors chosen according to some rule which is specified in such a way that the sequence of x_k 's converges toward x . The m_k is one of a set of scalars, the significance of which will be made clearer below.

N -Step Procedures. Starting with an arbitrary guess to the solution of a set of N simultaneous linear equations, the exact answer can be obtained in N steps, or with N corrections. The N -step procedures have been devised principally by Fox, Huskey, and Wilkinson¹, Lanczos², Hestenes^{3, 5}, Stiefel^{4, 5}, and the author⁶. In that which follows, an entirely general attack will be made, which will encompass the work of all those above.

The reader is asked to envision the answers to the set of N equations as the N co-ordinates of a point in N dimensional space. Further, the reader is asked to envision the N numbers which constitute the initial trial answer as the co-ordinates of another point in this space.

Let us call the directed line joining x to x_0 the vector $e_0 = x_0 - x$. Thus finding x may be restated as the task of reducing e_0 to zero. One proceeds in the following manner.

Choose N vectors, p_0, p_1, \dots, p_{N-1} such that they constitute an independent set, i.e., they span the N dimensional space. Therefore

$$e_0 = m_0 p_0 + m_1 p_1 + \dots + m_{N-1} p_{N-1} \quad (1)$$

states that the vector e_0 can be made up of a linear combination of these vectors p_k . The m_k are constants so chosen that the equality holds.

Evidently the problem is solved if one can evaluate the numbers m_k . This is quite simple if the N vectors p_k are mutually B -orthogonal, i.e. if

$$p_j * B p_k = 0, \quad j \neq k. \quad (2)$$

The asterisk indicates the transposed matrix (or conjugate transposed if complex).

Premultiplying (1) by $p_j * B$:

$$p_j * B e_0 = m_0 p_j * B p_0 + m_1 p_j * B p_1 + \dots + m_j p_j * B p_j + \dots + m_{N-1} p_j * B p_{N-1} \quad (3)$$

All terms on the right side vanish because of (2) except the coefficient of m_j , hence

$$m_j = \frac{p_j * B e_0}{p_j * B p_j}. \quad (4)$$

Evidently some restrictions must be placed upon B . In general it is necessary for B to be symmetric (or hermitian if complex). Should B be positive definite, it is clear that the denominator of (4) cannot vanish, but the definiteness of B is not necessary. The procedures hereinafter described will converge if for *no* k

$$p_k * B p_k = 0.$$

However, it is practically more expedient, due to computational errors to require B to be positive definite.

It is now convenient to define

$$e_k = e_{k-1} - m_{k-1} p_{k-1} = x_k - x. \quad (5)$$

Thus one imagines that the sequence e_1, e_2, \dots is obtained from (1) by evaluating m_0, m_1, \dots in succession, and subtracting $m_0 p_0, m_1 p_1, \dots$ from the right hand side of (1). There are two ways in which such a procedure can be visualized geometrically:

(a) e_0 can be thought of as being a linear combination of the N independent vectors $B p_k$, $k = 0, 1, 2, \dots, N-1$. By hypothesis p_j is orthogonal to all the $B p_k$, except $B p_j$. Hence, subtracting *any* amount of p_j from e_j will not alter the projection of the resultant vector on the vectors $B p_k$, $k \neq j$. Hence m_j is chosen such that all of e_j 's projection on $B p_j$ is reduced to zero, i.e.

$$(B p_j) * (e_j - m_j p_j) = 0$$

or

$$m_j = \frac{p_j * B e_j}{p_j * B p_j} \quad \text{as before.}$$

(b) using the relation

$$e_{j+1} = e_j - m_j p_j$$

one can formulate the quadratic form $e_{j+1}^* B e_{j+1}$ as a function of m_j , and can then choose m_j such that this quadratic form is stationary. Again this yields

$$m_j = \frac{p_j^* B e_j}{p_j^* B p_j}.$$

It might be pointed out that if B is positive definite, the quadratic form is minimized as a function of m_j . Again, this is not necessary theoretically, but practically expedient.

While all these relationships are nice, several questions arise at this point. First, how can one evaluate these constants when the e_j are unknown? (It will be recalled that $e_j = x_j - x$, and since x is the solution for which one is looking, e_j is unknown.) Secondly, how does one find a set of vectors p_k which are B -orthogonal? Thirdly, what is B ?

Eliminating e_0 . Since $e_k = x_k - x$, then $A e_k = A x_k - A x$. But $A x = y$, hence the quantity, $r_k = A e_k = A x_k - y$ can be evaluated, and is usually called the k^{th} residual, i.e., that which remains when x_k is tried as a solution of the problem $A x - y = 0$.

If A is symmetric, then it can be written in equation (4) for B :

$$m_j = \frac{p_j^* A e_j}{p_j^* A p_j} = \frac{p_j^* r_j}{p_j^* A p_j}, \quad (6)$$

where the more general e_j is used for e_0 .

Another possibility, in the event A is not symmetric, is to use $A^* A$ for B . Hence, substitution in (4) above yields:

$$m_j = \frac{p_j^* A^* A e_j}{p_j^* A^* A p_j} = \frac{(A p_j)^* r_j}{(A p_j)^* (A p_j)}. \quad (7)$$

These are the procedures of Stiefel and Hestenes. The author has one more to submit. His procedure is derived from (4) above by defining a new set of vectors b_j which are related to the p_j by $p_j = A^* b_j$. Substituting this in (4), and letting $B = I$, the unit matrix:

$$m_j = \frac{p_j^* e_j}{p_j^* p_j} = \frac{(A^* b_j)^* e_j}{(A^* b_j)^* (A^* b_j)} = \frac{b_j^* A e_j}{(A^* b_j)^* (A^* b_j)} = \frac{b_j^* r_j}{(A^* b_j)^* (A^* b_j)}. \quad (8)$$

As in equation (7), the matrix A may be any non-singular matrix.

Hence since,

$$x_k = e_k + x \quad (9)$$

$$e_{k+1} = e_k - m_k p_k \quad (10)$$

then
$$x_{k+1} = x_k - m_k p_k . \quad (11)$$

Premultiplying (10) by A , and noting that $Ae_k = r_k$:

$$r_{k+1} = r_k - m_k A p_k . \quad (12)$$

With these relations, one can now write down the three procedures.

Procedure I. A symmetric, and non-singular.

$$x_{k+1} = x_k - m_k p_k, \quad r_k = A x_k - y, \quad m_k = p_k^* r_k / p_k^* A p_k$$

and

$$p_j^* A p_k = 0, \quad j \neq k.$$

Procedure II. A non-symmetric or symmetric, non-singular.

$$x_{k+1} = x_k - m_k p_k, \quad r_k = A x_k - y, \quad m_k = (A p_k)^* r_k / (A p_k)^* (A p_k)$$

and

$$p_j^* A^* A p_k = 0, \quad j \neq k.$$

Procedure III. A non-symmetric or symmetric, non-singular.

$$x_{k+1} = x_k - m_k A^* b_k, \quad r_k = A x_k - y, \quad m_k = b_k^* r_k / (A^* b_k)^* (A^* b_k)$$

and

$$b_j^* A A^* b_k = 0, \quad j \neq k.$$

Obtaining the B -Orthogonal Set. One still needs a simple way of obtaining the B -orthogonal vectors p_k . A method for showing this is given here, but it asks the reader to accept a result first demonstrated by Lanczos². A less general form is proved in references 2 and 6. The present general form is stated by Forsythe, Hestenes, and Rosser³, and is stated here as

Lanczos' Theorem. Given the vector sequence, p_k , generated from an arbitrary vector p_0 by

$$p_0 \quad (i)$$

$$c_1 p_1 = B p_0 - \alpha_0 p_0 \quad (ii)$$

$$c_2 p_2 = B p_1 - \alpha_1 p_1 - \beta_0 p_0 \quad (iii)$$

$$c_3 p_3 = B p_2 - \alpha_2 p_2 - \beta_1 p_1 \quad (iv)$$

$$\text{and in general} \quad c_k p_k = B p_{k-1} - \alpha_{k-1} p_{k-1} - \beta_{k-2} p_{k-2} \quad (v)$$

with

$$\alpha_{k-1} = \frac{p_{k-1}^* C B p_{k-1}}{p_{k-1}^* C p_{k-1}} \quad (vi)$$

and

$$\beta_{k-2} = \frac{p_{k-2}^* C B p_{k-1}}{p_{k-2}^* C p_{k-2}}. \quad (\text{vii})$$

Then for any non-zero constants c_k , and for B and C symmetric matrices such that $BC = CB$,

$$p_j^* C p_k = 0 \quad j \neq k,$$

that is, the vectors of the sequence are C -orthogonal.

The proof of this is omitted, but an outline of the proof is given below. It will be shown that p_3 is C -orthogonal to p_0 . α_2 and β_1 are chosen so that p_3 is C -orthogonal to p_2 and p_1 . The other α 's and β 's are chosen so that all other combinations of p_0 , and p_1 , and p_2 are C -orthogonal. Thus, from equation (iv), if one premultiplies by $p_0^* C$:

$$c_3 p_0^* C p_3 = p_0^* C B p_2 - \alpha_2 p_0^* C p_2 - \beta_1 p_0^* C p_1$$

$$c_3 p_0^* C p_3 = p_0^* C B p_2.$$

Since the right hand side of the last equation is a scalar,

$$c_3 p_0^* C p_3 = p_2^* B C p_0 \quad \text{since } B \text{ and } C \text{ are both symmetric.} \quad (\text{viii})$$

If equation (ii) is premultiplied by $p_2^* C$:

$$c_1 p_2^* C p_1 = p_2^* C B p_0 - \alpha_0 p_2^* C p_0.$$

But the coefficients of c_1 and α_0 are zero, hence

$$p_2^* C B p_0 = 0. \quad (\text{ix})$$

Now if C and B are such that $BC = CB$, then substituting (ix) in (viii) yields

$$p_0^* C p_3 = 0.$$

In an entirely similar way, by using methods of induction, one can complete the proof.

One now proceeds to show that for each of the previous procedures one may set up a recursion formula for the p_k such that Lanczos' Theorem is satisfied. In each procedure one has the relation

$$r_k = r_{k-1} - m_{k-1} A p_{k-1}. \quad (12)$$

Procedure I. The p_k will form an A -orthogonal set if

$$p_k = r_k + \epsilon_{k-1} p_{k-1} \quad (13)$$

$$\epsilon_{k-1} = r_k^* r_k / r_{k-1}^* r_{k-1}, \quad p_0 = r_0.$$

For a proof of this see reference 5.

Procedure II. The p_k will form an A^*A -orthogonal set if

$$p_k = A^*r_k + \epsilon_{k-1}p_{k-1} \quad (14)$$

$$\epsilon_{k-1} = (A^*r_k)^*(A^*r_k)/(A^*r_{k-1})^*(A^*r_{k-1}), \quad p_0 = A^*r_0.$$

For a proof of this see reference 5.

Procedure III. The b_k will form an AA^* -orthogonal set if

$$b_k = r_k + \epsilon_{k-1}b_{k-1} \quad (15)$$

$$\epsilon_{k-1} = r_k^*r_k/r_{k-1}^*r_{k-1}, \quad b_0 = r_0. \quad (16)$$

It is desired to demonstrate that Procedure III satisfies Lanczos' Theorem, and hence that the A^*b_k form a mutually orthogonal set.

Rewriting equations (12) and (15) for convenience:

$$r_k = r_{k-1} - m_{k-1}AA^*b_{k-1} \quad (12)$$

and

$$b_k = r_k + \epsilon_{k-1}b_{k-1} \quad (15)$$

where the relationship $A^*b_k = p_k$ has been used in (12).

If equation (12) is substituted in (15),

$$b_k = r_{k-1} - m_{k-1}AA^*b_{k-1} + \epsilon_{k-1}b_{k-1}. \quad (17)$$

Replacing k by $k - 1$ in equation (15), solving for r_{k-1} , and substituting in (17) one obtains

$$-(1/m_{k-1})b_k = AA^*b_{k-1} - \frac{(1 + \epsilon_{k-1})}{m_{k-1}} b_{k-1} + \frac{\epsilon_{k-2}}{m_{k-1}} b_{k-2}. \quad (18)$$

Thus if $C = AA^* = B$, $c_k = -(1/m_{k-1})$, $\alpha_{k-1} = (1 + \epsilon_{k-1})/m_{k-1}$, and $\beta_{k-2} = -\epsilon_{k-2}/m_{k-1}$, equation (18) is identical to Lanczos' formula. Actually one does not use this similarity to compute the constants, though it is possible. Since it is known that only two constants are necessary to ensure an orthogonal set, they can be obtained in any way one desires.

Let us assume that

$$m_{k-1} = \frac{b_{k-1}^*r_{k-1}}{b_{k-1}^*AA^*b_{k-1}} \quad (19)$$

and choose ϵ_{k-1} such that

$$b_k^*AA^*b_{k-1} = 0.$$

This last can be done by premultiplying equation (15) by $b_{k-1}^*AA^*$ remembering that $p_k = A^*b_k$:

$$b_{k-1}^*AA^*b_k = 0 = b_{k-1}^*AA^*r_k + \epsilon_{k-1}b_{k-1}^*AA^*b_{k-1}$$

or

$$\epsilon_{k-1} = \frac{-b_{k-1} * AA * r_k}{b_{k-1} * AA * b_{k-1}}. \quad (20)$$

It is now necessary to show that with (19), (20), (12), and (15) that

$$\frac{1 + \epsilon_{k-1}}{m_{k-1}} = \alpha_{k-1} = \frac{b_{k-1} * AA * AA * b_{k-1}}{b_{k-1} * AA * b_{k-1}} \quad (21)$$

and

$$\frac{-\epsilon_{k-2}}{m_{k-1}} = \beta_{k-2} = \frac{b_{k-2} * AA * AA * b_{k-1}}{b_{k-2} * AA * b_{k-2}} \quad (22)$$

where $C = B = AA*$ has been used.

Equation (21) is quite simple to demonstrate. Premultiplying equation (18) by $b_{k-1} * AA*$, yields

$$\begin{aligned} & -(1/m_{k-1})b_{k-1} * AA * b_k \\ &= b_{k-1} * AA * AA * b_{k-1} - \frac{(1 + \epsilon_{k-1})}{m_{k-1}} b_{k-1} * AA * b_{k-1} + \frac{\epsilon_{k-2}}{m_{k-1}} b_{k-1} * AA * b_{k-2}. \end{aligned}$$

The left side of the equation vanishes by choice of ϵ_{k-1} , and the last term on the right by choice of ϵ_{k-2} , and so

$$\frac{(1 + \epsilon_{k-1})}{m_{k-1}} = \frac{b_{k-1} * AA * AA * b_{k-1}}{b_{k-1} * AA * b_{k-1}} \quad \text{Q.E.D.}$$

Premultiplying equation (12) by $b_{k-1}*$, and using the definition (19),

$$b_{k-1} * r_k = 0. \quad (23)$$

Premultiplying (12) by $b_{k-2}*$

$$b_{k-2} * r_k = b_{k-2} * r_{k-1} - m_{k-1} b_{k-2} * AA * b_{k-1}.$$

The first term on the right is zero by (23), and the second is zero by choice of ϵ_{k-2} , hence

$$b_{k-2} * r_k = 0. \quad (24)$$

From (15) $r_{k-1} = b_{k-1} - \epsilon_{k-2} b_{k-2}$, so premultiplying both sides by r_k* and using (23) and (24):

$$r_k * r_{k-1} = 0. \quad (25)$$

Premultiplying (12) by r_k* , and using (25),

$$r_k * r_k = -m_{k-1} r_k * AA * b_{k-1}. \quad (26)$$

Substituting this in (20) one obtains

$$\epsilon_{k-1} = \frac{r_k * r_k}{m_{k-1} b_{k-1} * AA * b_{k-1}} = \frac{r_k * r_k}{b_{k-1} * r_{k-1}}. \quad (27)$$

The last step was performed by using equation (19).

Before continuing, it will be useful to show that $r_k * r_{k-2} = 0$.

Proof: (by induction)

From (12) $r_2 = r_1 - m_1 AA * b_1$ so $r_2 * r_0 = r_1 * r_0 - m_1 b_1 * AA * r_0$. But $r_1 * r_0 = 0$ by equation (25), and since $b_0 = r_0$, the second term on the right is zero by choice of ϵ_0 , hence $r_2 * r_0 = 0$. The hypothesis is true for $k = 2$. Assume that it is true for $k \leq q$. Thus $r_k * r_{k-2} = 0$ for $k \leq q$. Replacing k by $k - 1$ in equation (12), and premultiplying by $r_k *$:

$$r_k * r_{k-1} = r_k * r_{k-2} - m_{k-2} r_k * AA * b_{k-2}.$$

The left side vanishes by equation (25), the first term on the right by hypothesis, so $r_k * AA * b_{k-2} = 0$ for $k \leq q$. Since from (15) $r_k = b_k - \epsilon_{k-1} b_{k-1}$, substitution in the last equation yields

$$0 = b_k * AA * b_{k-2} - \epsilon_{k-1} b_{k-1} * AA * b_{k-2}.$$

The second term on the right is zero by choice of ϵ_{k-2} so $b_k * AA * b_{k-2} = 0$ for $k \leq q$. But from (15) $b_{k-2} = (1/\epsilon_{k-2})(b_{k-1} - r_{k-1})$. Substituting this in the last equation

$$b_k * AA * b_{k-2} = 0 = b_k * AA * b_{k-1} - b_k * AA * r_{k-1}.$$

The first term vanishes by choice of ϵ_{k-1} , and so

$$b_k * AA * r_{k-1} = 0 \quad \text{for } k \leq q.$$

Replacing k by $k + 1$ in equation (12), and postmultiplying its transpose by r_{k-1}

$$r_{k+1} * r_{k-1} = r_k * r_{k-1} - m_k b_k * AA * r_{k-1}.$$

The first term on the right vanishes by equation (25), and the last by the previous equation, hence

$$r_{k+1} * r_{k-1} = 0 \quad \text{for } k \leq q, \quad (28)$$

hence for all k .

From equation (12) one gets the two relations

$$r_k - r_{k-1} = -m_{k-1} AA * b_{k-1}, \quad r_{k-1} - r_{k-2} = -m_{k-2} AA * b_{k-2}.$$

Multiplying the right and left sides together gives

$$r_k * r_{k-1} - r_k * r_{k-2} - r_{k-1} * r_{k-1} + r_{k-1} * r_{k-2} = m_{k-1} m_{k-2} b_{k-1} * AA * AA * b_{k-2}.$$

The first and fourth terms on the left vanish by (25), and the second by (28), so

$$r_{k-1} * r_{k-1} = -m_{k-1} m_{k-2} b_{k-1} * AA * AA * b_{k-2}.$$

Substitution of this relation in (27), after replacing k in that equation by $k - 1$:

$$\epsilon_{k-2} = - \frac{m_{k-1} m_{k-2} b_{k-1} * AA * AA * b_{k-2}}{b_{k-2} * r_{k-2}}.$$

Dividing both sides by m_{k-1} , and multiplying through by -1 , and using (19) for m_{k-2} one obtains

$$-\frac{\epsilon_{k-2}}{m_{k-1}} = \frac{b_{k-1} * AA * AA * b_{k-2}}{b_{k-2} * AA * b_{k-2}}. \quad (29)$$

But this is equation (22) which was to be proved.

Thus, it has been demonstrated that the vectors b_k do form an AA^* -orthogonal set, and are the same vectors one would obtain by using Lanczos' scheme, if one starts with $b_0 = r_0$. A similar proof can be written for the two procedures of Stiefel and Hestenes. It can be further demonstrated that the residuals thus obtained form an orthogonal set.

It is possible to simplify the expressions for m_k and ϵ_k . Premultiply equation (15) by r_k^* :

$$r_k^* b_k = r_k^* r_k + \epsilon_{k-1} r_k^* b_{k-1}.$$

The last term on the right is zero by equation (23), so

$$r_k^* b_k = r_k^* r_k \quad (30)$$

Using (30) in equations (19) and (27) gives the formulae

$$m_k = \frac{r_k^* r_k}{b_k^* AA^* b_k} \quad (31)$$

and

$$\epsilon_{k-1} = \frac{r_k^* r_k}{r_{k-1}^* r_{k-1}}. \quad (32)$$

Putting the author's procedure all together in compact form one has

$$\begin{aligned} x_{k+1} &= x_k - m_k A^* b_k & m_k &= |r_k|^2 / |A^* b_k|^2 \\ b_k &= r_k + \epsilon_{k-1} b_{k-1} \\ b_0 &= r_0 & \epsilon_{k-1} &= |r_k|^2 / |r_{k-1}|^2 \\ r_k &= Ax_k - y \end{aligned}$$

Variations on the Author's Procedure. As indicated in the last section, an additional result of this procedure is the fact that the residuals form an orthogonal set. It is possible to use Lanczos' Theorem to put this procedure in an entirely different form.

In the Theorem, let us let $C = I$, and $B = AA^*$. Let us choose r_k as the vectors, instead of p_k , hence

$$c_k r_k = AA^* r_{k-1} - \alpha_{k-1} r_{k-1} - \beta_{k-2} r_{k-2}.$$

Premultiplying by A^{-1} , and noting that $A^{-1} r_j = e_j$, the error vector

$$c_k e_k = A^* r_{k-1} - \alpha_{k-1} e_{k-1} - \beta_{k-2} e_{k-2}.$$

Since $e_j = x_j - x$, this reads

$$c_k x_k - c_k x = A^* r_{k-1} - \alpha_{k-1} x_{k-1} + \alpha_{k-1} x - \beta_{k-2} x_{k-2} + \beta_{k-2} x.$$

Since x is unknown, it can be eliminated by letting $c_k = -(\alpha_{k-1} + \beta_{k-2})$. This yields the result that

$$-(\alpha_{k-1} + \beta_{k-2}) x_k = A^* r_{k-1} - \alpha_{k-1} x_{k-1} - \beta_{k-2} x_{k-2}.$$

It can be shown that, with a little algebra, and with the values of α_{k-1} and β_{k-2} given by the Theorem, if one defines

$$m_k = r_k * r_k / r_k * A A * r_k \quad \text{and} \quad n_{k-1} = m_k r_k * A A * r_{k-1} / r_{k-1} * r_{k-1}$$

that the recursion formula

$$x_{k+1} = [1/(1 + n_{k-1})] (x_k + n_{k-1}x_{k-1} - m_{k-1}A * r_{k-1})$$

gives the same iteration procedure as that of the previous section. The difference seems to be one of computation, and it remains to be seen which is the better insofar as roundoff error is concerned.

Conclusion. It has been the author's intention to demonstrate (1) that these N -step procedures involve, at each step, a computation of two arbitrary constants, (2) that these procedures are really special applications of Lanczos' Theorem.

It can be shown (ref. 6) that only in the event the matrix A is skew symmetric do these procedures reduce to the evaluation of but one constant at each step. Premature convergence (i.e. less than N steps) of these procedures is possible if more than one characteristic number are equal, or if the initial guess is such that the error vector e_0 is deficient in some of the characteristic vectors of the matrix used, i.e. A , $A * A$, and $A A *$ in Procedures I, II, and III respectively.

When these procedures are used with automatic computing machines the results obtained are good providing the number of digits the machine carries is in excess of the number of digits in the square root of the ratio of the largest to smallest characteristic numbers of the matrix $A * A$. Good results can be obtained when this condition is not met, but only as a result of a happy initial trial.

The life of these procedures lies in an adequate analysis of errors due to the rounding of products *before* a problem is attempted.

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