# **Householder Reduction of Linear Equations**

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This tutorial discusses Householder reduction of n linear equations to a triangular form which can be solved by back substitution. The main strength of the method is its unconditional numerical stability. We explain how Householder reduction can be derived from elementary-matrix algebra. The method is illustrated by a numerical example and a Pascal procedure. We assume that the reader has a general knowledge of vector and matrix algebra but is less familiar with linear transformation of a vector space.

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Additional Key Words and Phrases: Householder reduction

#### INTRODUCTION

The solution of *linear equations* is important in many areas of science and engineering [Kreyszig 1988]. This tutorial discusses Householder reduction of n linear equations to a triangular form that can be solved by back substitution [Householder 1958; Press et al. 1989]. The main strength of the method is its unconditional numerical stability. Text books on numerical analysis often produce Householder reduction like a rabbit from a magician's top hat. We will explain how the method can be derived from elementary matrix algebra. The method is illustrated by a numerical example and a Pascal procedure.

We assume that the reader has a general knowledge of vector and matrix algebra but is less familiar with linear transformation of a vector space.

We begin by looking at Gaussian elimination.

### 1. GAUSSIAN ELIMINATION

The classical method for solving a system of linear equations is *Gaussian elimination*. Suppose we have three linear equations with three unknowns  $x_1, x_2, x_3$ :

$$2x_1 + 2x_2 + 4x_3 = 18$$
  
 $x_1 + 3x_2 - 2x_3 = 1$   
 $3x_1 + x_2 + 3x_3 = 14$ .

First, we eliminate  $x_1$  from the second equation by subtracting  $\frac{1}{2}$  of the first equation from the second one. Then, we eliminate  $x_1$  from the third equation by subtracting  $\frac{3}{2}$  of the first equation from the third one. Now, we have three equations in which  $x_1$  occurs in the first equation only:

$$2x_1 + 2x_2 + 4x_3 = 18$$
  
 $2x_2 - 4x_3 = -8$   
 $-2x_2 - 3x_3 = -13$ .

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Finally, we eliminate  $x_2$  from the third equation by adding the second equation to the third one. The equations have now been reduced to a triangular form that has the same solution as the original equations but is easier to solve:

$$2x_1 + 2x_2 + 4x_3 = 18$$

$$2x_2 - 4x_3 = -8$$

$$-7x_3 = -21.$$

The triangular equations are solved by back substitution. From the third equation we immediately have  $x_3 = 3$ . By substituting this value in the second equation, we find  $x_2 = 2$ . Substituting these two values in the first equation we obtain  $x_1 = 1$ .

In general we have n linear equations with n unknowns

The a's and b's are known real numbers. The x's are the unknowns we must find.

The equation system (1) can be expressed as a vector equation

$$Ax = b \tag{2}$$

where A is an  $n \times n$  matrix,

$$A = egin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \ a_{21} & a_{22} & \cdots & a_{2n} \ \cdot & \cdot & \cdots & \cdot \ \cdot & \cdot & \cdots & \cdot \ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

while x and b are n-dimensional column vectors

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$\begin{bmatrix} b_1 \\ \vdots \end{bmatrix}$$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

The equation system has a unique solution only if the matrix A is nonsingular as defined in the Appendix.

Gaussian elimination reduces Eq. (2) to an equivalent form

$$Ux = c$$

where U is an  $n \times n$  upper triangular matrix

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

with all zeros below the main diagonal. The elimination process replaces the original righthand side b by another n-dimensional column vector c.

The scaling of equations is a source of numerical errors in Gaussian elimination. To eliminate the first unknown  $x_1$  from, say, the second equation, we subtract the first equation multiplied by  $a_{21}/a_{11}$  from the second equation. However, if the *pivot element*  $a_{11}$  is very small, the scaling factor  $a_{21}/a_{11}$  becomes very large, and we may end up subtracting very large reals from very small ones. This makes the results highly inaccurate.

The numerical instability of Gaussian elimination can be reduced by a process called *pivoting*: By changing the order in which the equations are written, we can make the pivot element as large as possible. We examine the first coefficient of every equation, that is

$$a_{11}, a_{21}, \ldots, a_{n1}.$$

If the largest of these coefficients is, say,  $a_{51}$ , then we exchange Equations 1 and 5. After this rearrangement, we subtract multiples of the (new) first equation from the remaining ones. The pivoting process is repeated for each submatrix during the Gaussian elimination.

Pivoting rearranges both the rows of the matrix and the elements of the righthand side. The algorithm must keep track of this permutation in an additional vector. Although pivoting does not guarantee numerical stability, numerical analysts believe that it works in practice [Golub and Van Loan 1989; Press et al. 1989].

In the following, we describe an alternative method that is numerically stable and does not require pivoting. This method has been used in a parallel algorithm [Brinch Hansen 1990a, 1990b].

# 2. SCALAR PRODUCTS

Householder's method requires the computation of scalar products and vector reflections. The following is a brief explanation of these basic operations. The Appendix defines the elementary laws of vector and matrix algebra, which we will take for granted.

Let a and b be two n-dimensional column vectors

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

The transpose of a and b are the row vectors

$$a^{T} = \begin{bmatrix} a_1 a_2 & \cdots & a_n \end{bmatrix}$$
$$b^{T} = \begin{bmatrix} b_1 b_2 & \cdots & b_n \end{bmatrix}.$$

The scalar product of a and b is

$$a^Tb = a_1b_1 + a_2b_2 + \dots + a_nb_n.$$
 (3)

A scalar product is obviously symmetric

$$a^T b = b^T a. (4)$$

The Euclidean norm

$$||a|| = \sqrt{a_1^2 + a_2^2 + \dots + a_n^2}$$
 (5)

is the length of an n-dimensional vector a.

From Eqs. (3) and (5) we obtain an equivalent definition of the norm

$$||a||^2 = a^T a. (6)$$

#### 3. REFLECTION

Householder reduction of an  $n \times n$  real matrix has a simple geometric interpretation: The matrix columns are regarded as vectors in an n-dimensional space. Each vector is replaced by its mirror image on the other side of a particular plane. This plane reflects the first column onto the first axis of the coordinate system to produce a new column with all zeros after the first element.

Let us first look at reflection in threedimensional space. The reflection plane P includes the origin O and is perpendicular to a given vector v. For an arbitrary vector a, we wish to find another vector b, which is the reflection of aon the other side of the plane P. Figure 1 shows a plane that includes the vectors v, a, and b. The dotted line represents the reflection plane P, which is perpendicular to v.

The concept of *reflection* is defined by three equations. The reflection plane P is determined by the vector v. To simplify the algebra, we assume that v is of length 1.

$$||v|| = 1. \tag{7}$$

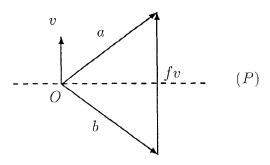


Figure 1. Reflection.

Reflection preserves the norm of a vector:

$$||a|| = ||b||. (8)$$

The difference between a vector a and its reflection b is a vector fv, which is a multiple of v:

$$fv = a - b. (9)$$

The (unknown) scalar f is the distance between the vector and its reflection.

We must find the reflection of an arbitrary vector a through a plane P defined by a given unit vector v. We have

$$||a||^{2} = ||b||^{2} by (8)$$

$$= (a - fv)^{T} (a - fv)$$

$$by (6), (9)$$

$$= a^{T}a - fa^{T}v - fv^{T}a + f^{2}v^{T}v$$

$$= ||a||^{2} - 2fv^{T}a + f^{2}$$

$$by (4), (6), (7).$$

This equality determines the distance f between vector a and its image b:

$$f = 2v^T a. (10)$$

The reflection of b into a displaces b by the same distance f in the opposite direction. So we can also express the distance as

$$f = -2v^T b. (11)$$

Finally we define b in terms of a and v:

$$b = a - vf by (9)$$

$$= Ia - v(2v^{T}a) by (10)$$

$$= (I - 2vv^{T})a$$

where I is the  $n \times n$  identity matrix defined in the Appendix.

In other words, the reflection of a vector a is the vector

$$b = Ha \tag{12}$$

obtained by multiplying a by the  $n \times n$  reflection matrix

$$H = I - 2vv^T. (13)$$

*H* is also called a *Householder matrix*. This is the "rabbit" that is often pulled out of the hat without any explanation of why it has this particular form.

Figure 1 is a geometric definition of reflection in three-dimensional space. However, the algebraic equations derived from this figure make no assumptions about the dimension of space. In the following, we will simply say that Eqs. (12) and (13) define a transformation of an n-dimensional vector. By analogy, we will call this transformation a "reflection" through an (n-1)-dimensional plane. The essential property is that reflection of an n-dimensional vector preserves the norm:

$$||Ha|| = ||a||.$$

This follows from Eqs. (8) and (12).

If we reflect a vector twice through the same plane, we get the same vector again:

$$H(Ha) = a$$
.

In other words, two reflections are equivalent to an identity transformation:

$$HH = I$$
.

Consequently, H is a nonsingular matrix that is its own inverse:

$$H^{-1} = H$$

(see the Appendix).

#### 4. HOUSEHOLDER REDUCTION

We are looking for an algorithm that reduces an  $n \times n$  real matrix A to triangular form without increasing the magnitude of the elements significantly.

An element of a column can never exceed the total length of the column vector. That is

$$|a_{i,j}| \le ||a_i||$$
 for  $i, j = 1, 2, ..., n$ .

In other words, the norm of a column vector is an upper bound on the magnitude of its elements.

A method that changes the elements of a matrix A without changing the norms of its columns will obviously limit the magnitude of the matrix elements. This can be achieved by multiplying A by a Householder matrix H.

If we multiply a system of linear equations

$$Ax = b$$

by a nonsingular matrix H, we obtain an equation

$$(HA)x = Hb$$

that has the same solution as the original system.

The first step in Householder reduction produces a matrix *HA* that has all zeros below the first element of the first column.

The reflection must transform column

$$a_1 = [a_{11} \ a_{21} \ \cdots \ a_{n1}]^T$$
 (14)

into a column of the form

$$Ha_1 = [d_{11} \ 0 \ \cdots \ 0]^T$$
 (15)

where the diagonal element is

$$d_{11} = \pm ||a_1||. \tag{16}$$

The choice of sign will be made later.

Equations (14)–(16) define the computation of the first column of the matrix *HA*.

The difference between column  $a_1$  and its reflection  $Ha_1$  is the column vector

$$f_1 v = a_1 - b_1$$
 by (9)  
=  $a_1 - Ha_1$  by (12).

Combining this with Eqs. (14) and (15) we find

$$f_1 v = [w_{11} \ a_{21} \ \cdots \ a_{n1}]^T \quad (17)$$

where the first element is

$$w_{11} = a_{11} - d_{11}. (18)$$

The distance between  $a_1$  and its image  $Ha_1$  is  $f_1$  where

$$f_1^2 = f_1(-2v^T H a_1) \qquad \text{by (11), (12)}$$

$$= -2(f_1 v)^T H a_1$$

$$= -2w_{11}d_{11} \qquad \text{by (3), (15), (17).}$$

In short,

$$f_1 = \sqrt{-2w_{11}d_{11}} \,. \tag{19}$$

The unit vector v that determines the appropriate Householder matrix is

$$v = f_1 v / f_1$$

or by Eq. (17):

$$v = [w_{11} \ a_{21} \ \cdots \ a_{n1}]^T / f_1.$$
 (20)

After the transformation of the first column  $a_1$ , each remaining column  $a_i$  is also replaced by its reflection through the same plane defined by Eqs. (9), (10), and (12).

$$Ha_i = a_i - f_i v \tag{21}$$

$$f_i = 2v^T a_i \tag{22}$$

The reflection of a column is obtained by subtracting a multiple of the unit vector v.

# 5. NUMERICAL STABILITY

We still need to decide which sign to use for the diagonal element  $d_{11}$  in Eq. (16).

If  $d_{11} = a_{11}$ , the scalars  $w_{11}$  and  $f_1$  are zero by Eqs. (18) and (19), and the division by  $f_1$  in Eq. (20) causes overflow. We can avoid this problem by selecting the sign that makes  $d_{11} \neq a_{11}$ .

The overflow problem occurs when  $a_1$ is a multiple of the unit vector

$$e_1 = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}^T.$$

For  $a_1 = a_{11}e_1$  there are four cases to

$$a_{11}>0\colon d_{11}=+\|a_1\|=\quad a_{11} \end{tabular}$$
 (overflow) 
$$d_{11}=-\|a_1\|=-a_{11} \end{tabular}$$
 (no overflow) 
$$a_{11}<0\colon d_{11}=+\|a_1\|=-a_{11} \end{tabular}$$
 (no overflow) 
$$d_{11}=-\|a_1\|=\quad a_{11} \end{tabular}$$
 (overflow)

If  $a_1$  is close to a multiple of  $e_1$ , serious rounding errors may occur if  $f_1$  is very

This insight leads to the following rule:

$$d_{11} = \text{if } a_{11} > 0$$
 
$$\text{then } -\|a_1\| \text{ else } \|a_1\|. \ \ (23)$$

#### 6. COMPUTATIONAL RULES

We are now ready to summarize the rules for computing the matrix HA as defined by Eqs. (3), (6), (15), and (18)–(23):

$$\begin{split} \|a_1\| &= \sqrt{a_1^T a_1} \\ d_{11} &= \text{if } a_{11} > 0 \text{ then } -\|a_1\| \text{ else } \|a_1\| \\ w_{11} &= a_{11} - d_{11} \\ f_1 &= \sqrt{-2w_{11}d_{11}} \\ Ha_1 &= [d_{11} \ 0 \ \cdots \ 0]^T \\ v &= [w_{11} \ a_{21} \ \cdots \ a_{n1}]^T / f_1 \\ f_i &= 2v^T a_i \text{ for } 1 < i \le n \\ Ha_i &= a_i - f_i v \end{split}$$
 (24)

Householder's algorithm reduces a system of linear equations to upper triangular form in n-1 steps.

The first step reduces A to a matrix HA with all zeros below the diagonal element in the first column. At the same time, b is transformed into a vector Hb. This computation, defined by Eq. (24), is called a Householder transformation.

HA

The second step reduces the (n-1) × (n-1) submatrix of HA shown above by Householder transformation. Now, we obtain a matrix with zeros below the diagonal elements in the first two columns. The same transformation is applied to the  $(n-1) \times 1$  subvector of  $H\bar{b}$  shown above.

By a series of Householder transformations, applied to smaller and smaller submatrices and subvectors, the equation system is reduced, one column at a time, to upper triangular form.

### 7. A NUMERICAL EXAMPLE

We now return to the previous example of three equations with three unknowns. For convenience, we combine the matrix A and the vector b into a single  $3 \times 4$ matrix

$$A0 = \begin{bmatrix} 2 & 2 & 4 & 18 \\ 1 & 3 & -2 & 1 \\ 3 & 1 & 3 & 14 \end{bmatrix}.$$

First, we reduce A0 to a matrix A1 with all zeros below the diagonal element in the first column. This is done column by column using Eq. (24). The numbers shown below were produced by a computer using 64-bit real arithmetic and rounded to four decimal places in the printing.

First column:

$$a_1 = \begin{bmatrix} 2 & 1 & 3 \end{bmatrix}^T$$
 $v = \begin{bmatrix} 0.8759 & 0.1526 & 0.4577 \end{bmatrix}^T$ 
 $f_1 = 6.5549$ 
 $Ha_1 = \begin{bmatrix} -3.7417 & 0 & 0 \end{bmatrix}^T$ .

Second column:

$$a_2 = [2 \ 3 \ 1]^T$$
 $f_2 = 5.3344$ 

$$Ha_2 = [-2.6726 \ 2.1862 \ -1.4414]^T.$$

Third column:

$$a_3 = \begin{bmatrix} 4 & -2 & 3 \end{bmatrix}^T$$

$$f_3 = 9.1433$$

$$Ha_3 = [-4.0089 -3.3949 -1.1846]^T$$
.

Fourth column:

$$a_4 = [18 \ 1 \ 14]^T$$

$$f_4 = 44.6536$$

$$Ha_4 = [-21.1136 -5.8123 -6.4368]^T.$$

We now have the matrix

$$A1 = \begin{bmatrix} -3.7417 & -2.6726 & -4.0089 & -21.1136 \\ 0 & 2.1862 & -3.3949 & -5.8123 \\ 0 & -1.4414 & -1.1846 & -6.4368 \end{bmatrix}.$$

The next step of the algorithm reduces the  $2 \times 2$  submatrix

$$A1' = \begin{bmatrix} 2.1862 & -3.3949 & -5.8123 \\ -1.4414 & -1.1846 & -6.4368 \end{bmatrix}$$

to

$$A2' = \begin{bmatrix} -2.6186 & 2.1822 & 1.3093 \\ 0 & -2.8577 & -8.5732 \end{bmatrix}.$$

The final triangular matrix

$$A2 = \begin{bmatrix} -3.7417 & -2.6726 & -4.0089 & -21.1136 \\ 0 & -2.6186 & 2.1822 & 1.3093 \\ 0 & 0 & -2.8577 & -8.5732 \end{bmatrix}$$

consists of the first row and column of A1 and the submatrix A2'.

The triangular equation system is solved by back substitution to obtain

$$x = [1.0000 \ 2.0000 \ 3.0000]^T.$$

# 8. PASCAL PROCEDURE

The following Pascal procedure assumes that the matrix A is stored by columns, that is, a[i] denotes the ith column of A. For each submatrix of A, the eliminate operation is applied to the first column, and the transform operation is applied to each remaining column (including b).

```
column = array [1..n] of real;
  matrix = array [1..n] of column;
procedure reduce (var a: matrix;
  var b: column);
var vi: column; i, j: integer;
  function product(i: integer;
    var a, b: column) real;
  { the scalar product of
    elements i..n of a and b }
  var ab: real; k: integer;
  begin
     ab = 0.0
    for k := 1 to n do
       ab := ab + a[k]*b[k],
    product = ab
  end:
  procedure eliminate(i: integer;
    var ai, vi: column);
  var anorm, dii, fi, wii: real;
    k: integer;
  begin
    anorm :=
       sqrt(product(i, ai, ai));
    if ai[i] > 00
       then dn := -anorm
       else dii := anorm,
    wii = ai[i] - dii;
    fi = sqrt(-2.0*wii*dii);
    v_1[i] := w_{ii}/f_i;
    a_1[1] := d_{1i}
    for k := 1 + 1 to n do
    begin
       vi[k] := ai[k]/fi;
       ai[k] := 0.0
    end
  end:
  procedure transform(i: integer;
    var aj, vi: column);
  var fi: real; k: integer;
  begin
    fi := 2.0*product(i, vi, aj);
    for k := i to n do
       aj[k] = aj[k] - fi^k vi[k]
  end;
begin
  for i := 1 to n - 1 do
  begin
    eliminate (i, a[i], v1);
    for i := i + 1 to n do
       transform(i, a[j], vi);
    transform(i, b, vi);
  end
end
```

For  $n \gg 1$ , the *execution time* of the algorithm is dominated by the transform procedure, which uses one addition, one subtraction, and two multiplications per array element. The ith submatrix requires n-i+1 transform operations, each involving 4(n-i+1) arithmetic operations. So the total number of numerical operations is approximately

$$\sum_{i=1}^{n-1} 4(n-i+1)^2 = \sum_{k=2}^{n} 4k^2 \approx 4n^3/3.$$

A similar analysis shows that Gaussian elimination requires  $2n^3/3$  arithmetic operations only.

### **SUMMARY**

We have explained Householder's method for reducing a matrix to triangular form. The main advantage of the method is its unconditional numerical stability. We have illustrated the computation by a numerical example and a Pascal procedure.

Gaussian elimination and Householder reduction of an  $n \times n$  matrix both have  $O(n^3)$  complexity. However, Householder reduction requires twice as many numerical operations. For that reason, Householder reduction is seldom used to solve linear equations on a sequential computer.

Why then should we be interested in Householder reduction?

(1) For some matrices, Gaussian elimination with pivoting is highly inaccurate. Numerical analysts believe that ill-conditioned matrices are so rare that pivoting is stable "in practice." However, we have not found a theoretical or statistical justification of this claim in the literature. Householder's method is unconditionally stable, both in theory and in practice. An engineer usually prefers a stable method with reasonable speed to a faster, but potentially unstable, technique.

(2) When a *multicomputer* with *p* processors solves *n* linear equations in parallel, the solution time has the form

$$T_p = an^3/p + bn^2$$

where a and b are system-dependent constants of matrix transformation and processor communication. The transformation time is reduced by the number of processors. The communication time is proportional to the number of matrix elements. Parallelism reduces the transformation time, but not the communication time. Since Gaussian elimination and Householder reduction require the same amount of communication, a multicomputer reduces the time difference between these methods. On a Computing Surface with 45 transputers, we used both methods to solve 1000 equations. The parallel solution times differed by 50% only [Brinch Hansen 1990b, 1992]. For parallel solution of linear equations. Householder reduction is an attractive compromise between unconditional numerical stability and computing speed.

(3) Finally, it should be mentioned that Householder reduction is used for least squares and eigenvalue computations in the Linpack procedures developed at Argonne National Laboratory [Dongarra et al. 1979].

Householder reduction is an interesting example of a fundamental computation with a subtle theory and a short algorithm. The reader who is interested in further details and alternative methods will find them in the books by Golub and Van Horn [1989] and Press et al. [1989].

#### APPENDIX: MATRIX ALGEBRA

In the algebraic laws, A, B, and C denote matrices, while k is a scalar.

The identity matrix is

$$I = egin{bmatrix} 1 & 0 & \cdots & 0 & 0 \ 0 & 1 & \cdots & 0 & 0 \ & & \cdots & & & \ 0 & 0 & \cdots & 1 & 0 \ 0 & 0 & \cdots & 0 & 1 \ \end{pmatrix}.$$

The transpose  $A^T$  is the matrix obtained by exchanging the rows and columns of the matrix A.

The inverse of a matrix A is a matrix  $A^{-1}$  such that

$$AA^{-1}=I$$
.

If  $A^{-1}$  exists then A is called a nonsingular matrix.

The laws apply also to vectors since they are  $n \times 1$  (or  $1 \times n$ ) matrices.

Identity Law:

$$IA = AI = A$$

Symmetry Law:

$$A + B = B + A$$

Associative Laws:

$$A \pm (B \pm C) = (A \pm B) \pm C$$
$$A(BC) = (AB)C$$

Distributive Laws:

$$A(B \pm C) = AB \pm AC$$
$$(A \pm B)C = AC \pm BC$$

Transposition Laws:

$$I^{T} = I$$
 $(A^{T})^{T} = A$ 
 $(A \pm B)^{T} = A^{T} \pm B^{T}$ 
 $(AB)^{T} = B^{T}A^{T}$ 

Scaling Laws:

$$kA = Ak$$

$$k(AB) = (kA)B = A(kB)$$

$$kA^{T} = (kA)^{T}$$

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