

INF1004 L4 Matrices

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- 2 The Inverse and Determinant of a Matrix
- 3 Matrix transpose
- 4 Orthogonal matrices
- 5 Householder transformation
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Given a matrix A of shape (n, d) and a matrix B of shape (d, f) , their multiplication AB is defined as a matrix of shape (n, f) and its component $(AB)_{i,k}$ at row i and column k is given as

$$(AB)_{i,k} = A_{(i,:)} \cdot B_{(:,k)} = \sum_{r=1}^d A_{i,r} B_{rk}$$

as an inner product between the i -th row of the left matrix and the k -th column of the right matrix.

Important: the number or dimensions in the second axis of A must be equal to the number or dimensions in the first axis of B . Otherwise matrix multiplication is not possible.

Therefore a matrix- matrix multiplication is a matrix consisting of inner products:

$$AB = \begin{bmatrix} A_{(0,:)} \cdot B_{(:,0)} & A_{(0,:)} \cdot B_{(:,1)} & A_{(0,:)} \cdot B_{(:,2)} & \dots & A_{(0,:)} \cdot B_{(:,f-1)} \\ A_{(1,:)} \cdot B_{(:,0)} & A_{(1,:)} \cdot B_{(:,1)} & A_{(1,:)} \cdot B_{(:,2)} & \dots & A_{(1,:)} \cdot B_{(:,f-1)} \\ A_{(2,:)} \cdot B_{(:,0)} & A_{(2,:)} \cdot B_{(:,1)} & A_{(2,:)} \cdot B_{(:,2)} & \dots & A_{(2,:)} \cdot B_{(:,f-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{(n-1,:)} \cdot B_{(:,0)} & A_{(n-1,:)} \cdot B_{(:,1)} & A_{(n-1,:)} \cdot B_{(:,2)} & \dots & A_{(n-1,:)} \cdot B_{(:,f-1)} \end{bmatrix}$$

Memorizing

- Matrix-Matrix multiplication results in a matrix, if shapes are permissible:
 $(n, d)(d, f) \rightarrow (n, f)$.
- The component $(AB)_{i,k}$ at row i and column k is given as the inner product between row i of the left matrix and column k of the right matrix.
That also tells you which axes must match in dimensionality: left matrix - the number of columns = the dimensionality of the second axis. right matrix - the number of rows = the dimensionality of the first axis.

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & -1 \\ -1 & 0 & 6 \end{bmatrix} \begin{bmatrix} 5 & -1 & -2 \\ 3 & 9 & -3 \\ -2 & 1 & 2 \end{bmatrix} = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

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- The inverse of a matrix
- Determinant of a matrix
- Matrix transpose
- Symmetric and Orthogonal matrices
- Householder transformation

Definition of a Linear mapping

A function $f : V \rightarrow Y$ which takes a vector $v \in V$ and outputs a vector $f(v) \in Y$ is a linear mapping if

$$\begin{aligned}f(cv) &= cf(v) \\ f(v + w) &= f(v) + f(w)\end{aligned}$$

holds

Intuition of a Linear mapping

- you can swap linear mappings with multiplication with a constant

$$f(cv) = cf(v)$$

Linear mapping of a multiplication = multiplication of the linear mapping

- you can swap linear mappings with addition of two inputs

$$f(v + w) = f(v) + f(w)$$

Linear mapping of a sum = sum of linear mappings

Inner products can be used to define linear mappings:

$$f_z(v) = z \cdot v$$

is a linear mapping in the vector argument v .

Reason:

$$f_z(cv) = z \cdot (cv) = \sum_i z_i cv_i = cz \cdot v = cf_z(v)$$

$$f_z(v_0 + v_1) = z \cdot (v_0 + v_1) = \sum_i z_i(v_{0,i} + v_{1,i}) = \sum_i z_i v_{0,i} + \sum_i z_i v_{1,i} = f_z(v_0) + f_z(v_1)$$

Way 1:

$$g_A(v) = Av$$

is a linear mapping in the vector argument v .

Way 2:

$$h_v(A) = Av$$

is a linear mapping in the matrix argument A .

Reason:

$$g_A(v_0 + v_1) = A(v_0 + v_1) = Av_0 + Av_1 = g_A(v_0) + g_A(v_1)$$

$$h_v(A_0 + A_1) = (A_0 + A_1)v = A_0v + A_1v = h_v(A_0) + h_v(A_1)$$

the same also works when we check for constants $g_a(cv) = \dots, h_v(cA) = \dots$

$$d_A(B) = AB$$

is a linear mapping in the matrix argument B .

$$e_B(A) = AB$$

is a linear mapping in the matrix argument A .

Matrix-Matrix and Matrix-vector multiplications define linear mappings

$$g_A(v) = Av$$

linear in argument v

$$h_v(A) = Av$$

linear in argument A

$$d_A(B) = AB$$

linear in argument B

$$e_B(A) = AB$$

linear in argument A

Learning goals

- be able to use the matrix inverse and transpose on products of matrices
- be able to compute the determinant of a matrix
- be able to check if a matrix is orthogonal or symmetric
- be able to explain the property preserved in vectors when multiplied with an orthogonal matrix
- be able to define a Householder rotation from one vector to another unit vector, and to apply it to a matrix

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Identity matrix

Definition: The identity matrix $I(n)$ is a matrix of shape (n, n) such that all entries are zero except the entries on the main diagonal, which are 1.

$$I(n)_{a,b} = 0 \text{ if } a \neq b$$

$$I(n)_{a,a} = 1$$

The identity matrix has the property that its multiplication leaves any vector unchanged:

$$Ix = x = xI$$

Examples:

$$I_1 = \begin{bmatrix} 1 \end{bmatrix}$$

$$I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$I_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Definition: The inverse of a matrix

Definition: A square matrix A of shape (n, n) is invertible if another matrix A^{-1} exists such that

$$AA^{-1} = I_n = A^{-1}A$$

A^{-1} is defined as the matrix inverse of A .

Intuition behind Invertibility:

If a matrix A is invertible, then its operation on any vector x can be undone, no matter from what side it is applied:

$$y = Ax \Rightarrow A^{-1}y = A^{-1}Ax = Ix = x$$

$$y = xA \Rightarrow yA^{-1}xAA^{-1} = xI = x$$

The same holds if we replace the vector x by a matrix X . So invertible matrices define all undoable matrix multiplication operations.

Note: The matrix inverse requires a square matrix, that is, a matrix of shape (d, d) .

uniqueness of the matrix inverse

If the matrix inverse A^{-1} of a matrix A exists, then it is unique.

Proof: Let A be invertible, and B and C be two matrices which behave like an Inverse of A :

$$AB = I = AC \Rightarrow A^{-1}AB = I = A^{-1}AC \Rightarrow B = C$$

You do not need to memorize the normalizer for this, except it is required by the probability part of this lecture.

- used in the multivariate normal distribution

$$p(x|\mu, \Sigma) = \frac{1}{(2\pi)^{d/2} \det(\Sigma)^{1/2}} \exp \left(-\frac{1}{2} (x - \mu)^\top \Sigma^{-1} (x - \mu) \right)$$

You do not need to memorize the density for this.

- ⊙ used in the multivariate Student distribution (a high-dimensional analogue of the 1-d cauchy distribution)

$$p(x|\nu, \mu, \Sigma) = \frac{\Gamma(\frac{\nu+p}{2})}{\Gamma(\frac{\nu}{2})(\nu\pi)^{p/2}\det(\Sigma)^{1/2}} \left(1 + \frac{1}{\nu}(x - \mu)^\top \Sigma^{-1}(x - \mu)\right)^{-\frac{\nu+p}{2}}$$

You do not need to memorize the derivation for this.

- ⊙ used in the explicit solution of the ridge regression problem

$$f_{w^*}(x) = w^* \cdot x$$

find a linear mapping which

$$w^* = \operatorname{argmin}_w \sum_{i=1}^n (f_w(x^{\{i\}}) - y^{\{i\}})^2 + \frac{\lambda}{2} \|w\|_2^2 \quad \text{minimizes a square loss on data} + \text{regularizer}$$

$$w^* = \operatorname{argmin}_w \sum_{i=1}^n (w \cdot x^{\{i\}} - y^{\{i\}})^2 + \frac{\lambda}{2} \|w\|_2^2$$

This can be written in matrix form

$$\begin{aligned} w^* &= \operatorname{argmin}_w \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|_2^2 \\ &= \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|_2^2 \\ &= (Xw - y)^\top (Xw - y) + \frac{\lambda}{2} w^\top I w \end{aligned}$$

and solved as:

$$\begin{aligned} & \nabla((Xw - y)^T(Xw - y) + \frac{\lambda}{2}w^T I w) \\ &= X^T 2(Xw - y) + 2\lambda w \end{aligned}$$

$$\begin{aligned} & \nabla(\dots) = 0 \\ & \Rightarrow X^T(Xw - y) + \lambda w = 0 \\ & \Rightarrow X^T X w + \lambda I w = X^T y \\ & \Rightarrow (X^T X + \lambda I)w = X^T y \end{aligned}$$

Therefore:

$$w^* = (X^T X + \lambda I)^{-1} X^T y$$

Therefore:

$$w^* = (X^\top X + \lambda I)^{-1} X^\top y$$

where

$$y = \begin{bmatrix} y^{\{0\}} \\ y^{\{1\}} \\ \dots \\ y^{\{n-1\}} \end{bmatrix} \quad y.shape = (n, 1)$$
$$X = \begin{bmatrix} x^{\{0\}} \\ x^{\{1\}} \\ \dots \\ x^{\{n-1\}} \end{bmatrix}, \quad X.shape = (n, d)$$

A sufficient condition for non-invertibility

- If a matrix A has a zero row or a zero column, then no inverse for it exists.
- if for a non-zero vector $v \neq 0$ we have

$$Av = 0$$

then no inverse for A exists. For this also, the other direction holds: if A is not invertible, then a $v \neq 0$ must exist, such that $Av = 0$.

Proof:

- Assume the i -th row of A is all zero ($A_{i,:} = 0$), and there exists a matrix B such that $AB = I$
- then consider the matrix multiplication of the i -th row of A with the i -th column of B :

$$\begin{aligned} AB = I &\Rightarrow AB_{ij} = I_{ij} = 1 \\ &\Rightarrow A_{i,:} \cdot B_{:,i} = 1 \\ &\Rightarrow A_{i,:} \cdot B_{:,i} = 0 \cdot B_{:,i} = 0 \end{aligned}$$

which is not possible

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Proof:

If we assume that the i -th column of A is all zero, then we do the same with a matrix B multiplied from the left.

$$BA = I \Rightarrow 1 = I_{ii} = (BA)_{ii} = B_{i,:} \cdot A_{:,i} = 0$$

A sufficient condition for non-invertibility

- If a matrix A has a zero row or a zero column, then no inverse for it exists.
- if for a non-zero vector $v \neq 0$ we have

$$Av = 0$$

then no inverse for A exists. For this also, the other direction holds: if A is not invertible, then a $v \neq 0$ must exist, such that $Av = 0$.

Proof:

if $v \neq 0$ and we have $Av = 0$, and we assume that an inverse A^{-1} exists, then

$$A^{-1}Av = Iv = v$$

$$A^{-1}Av = A^{-1}0 = 0$$

$$\Rightarrow v = 0$$

which is a contradiction. So $Av = 0$ for $v \neq 0$ rules out the existence of an inverse.

One more condition for non-invertibility

- If a matrix A has linearly dependent rows or columns, that is if its rank is less than its number of rows/columns, then no inverse for A exists.

For this also, the other direction holds. If A is not invertible, then its rank must be less than the number of rows and columns.

Proof: If a matrix A has linearly dependent rows or columns, then we can find a vector space of solutions other than only the zero vector $v = 0$ when solving $Av = 0$.

You got to remember this one:

Properties of the inverse

$$(A^{-1})^{-1} = A$$

$$(AB)^{-1} = B^{-1}A^{-1}$$

Proof of the second property:

$$B^{-1}A^{-1}(AB) = I = (AB)B^{-1}A^{-1} \text{ due to uniqueness this must be the inverse}$$

No need to remember the next one, which gives an idea how matrix inverse behaves under addition:

- Sherman-Morrison-Woodbury formula

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} - VA^{-1}U)^{-1}VA^{-1}$$

- useful sometimes as a special case when A is the identity matrix I :

$$(I + UCV)^{-1} = I - U(C^{-1} - VA^{-1}U)^{-1}V$$

This one you should remember!

$$\begin{bmatrix} a_0 & 0 & 0 & \cdots & 0 \\ 0 & a_1 & 0 & \cdots & 0 \\ 0 & 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{d-1} \end{bmatrix}^{-1} = \begin{bmatrix} a_0^{-1} & 0 & 0 & \cdots & 0 \\ 0 & a_1^{-1} & 0 & \cdots & 0 \\ 0 & 0 & a_2^{-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{d-1}^{-1} \end{bmatrix}$$

Obviously, a diagonal matrix is not invertible, if one of the $a_i = 0$

This will be useful for computing matrix inverses of smaller matrices. Also reused for computing eigenvalues one lecture later.

Definition: Determinant of a Matrix

Let M be an (n, n) -shaped matrix. Define $M_{-i, -k}$ the $(n - 1, n - 1)$ matrix, which one obtains when deleting the i -th row and k -th column from M .

Then the determinant can be recursively defined as (by going through columns of the k -th row):

$$\det(M) = \sum_{k=0}^{n-1} (-1)^{i+k} M_{i,k} \det(M_{-i, -k}) \text{ for any } i$$

$$\det([a]) = a, \text{ one possible end of the recursion}$$

or (by going through rows of the k -th column) as:

$$\det(M) = \sum_{i=0}^{n-1} (-1)^{i+k} M_{i,k} \det(M_{-i, -k}) \text{ for any } k$$

FYI, this formula is called Laplace-Expansion of the Determinant.

Determinant of a (2 2)-Matrix

$$\det\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) = ad - bc$$

Proof: apply the above recursive computation.

Remembering the determinant for a (3,3)-matrix:

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{matrix} a & b \\ d & e \\ g & h \end{matrix}$$

$$\det() = +aei + bfg + cdh - gec - hfa - idb$$

in principle you write the matrix twice (last column omitted as it is not needed)

Determinant of a (33)-Matrix

$$\det \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = +aei + bfg + cdh - gec - hfa - idb$$

see the graphic to memorize

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{\det(A)} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

Obviously, a (2,2)-matrix is not invertible, if $\det(A) = ad - bc = 0$.

Can one memorize this ?

- for the (2,2)-case you always put in place $M_{-i,-k}$ times a sign $-1, +1$. The sign is given as $(-1)^{i+k}$
- then it gets transposed

You can see a structure in this formula if you check how it looks like for (3,3)-shape matrices

$$\begin{aligned}
 \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}^{-1} &= \\
 &= \frac{1}{\det(A)} \begin{bmatrix} (-1)^{0+0} \det(A_{-0,-0}) & (-1)^{0+1} \det(A_{-0,-1}) & (-1)^{0+2} \det(A_{-0,-2}) \\ (-1)^{1+0} \det(A_{-1,-0}) & (-1)^{1+1} \det(A_{-1,-1}) & (-1)^{1+2} \det(A_{-1,-2}) \\ (-1)^{2+0} \det(A_{-2,-0}) & (-1)^{2+1} \det(A_{-2,-1}) & (-1)^{2+2} \det(A_{-2,-2}) \end{bmatrix}^T \\
 &= \frac{1}{\det(A)} \begin{bmatrix} \det(A_{-0,-0}) & (-1) \det(A_{-1,-0}) & \det(A_{-2,-0}) \\ (-1) \det(A_{-0,-1}) & \det(A_{-1,-1}) & (-1) \det(A_{-2,-1}) \\ \det(A_{-0,-2}) & (-1) \det(A_{-1,-2}) & \det(A_{-2,-2}) \end{bmatrix}
 \end{aligned}$$

The matrix is not invertible, if $\det(A) = 0$.

You do not need to remember the formula for inverting a (3, 3) matrix. If needed, it will be given to you.

The matrix M involved in the determinant and its version C multiplied with signs have names:

$$M_{ij} = \det(A_{-i,-j})$$

$$M = (M_{ij})_{i=1\dots n, j=1\dots n} \text{ minor matrix of } A$$

$$C_{ij} = (-1)^{i+j} M_{ij}$$

$$C = (C_{ij})_{i=1\dots n, j=1\dots n}, \text{ cofactor matrix of } A$$

$$C^T \text{ adjoint matrix of } A$$

A condition for non-invertibility

- If a matrix A has a zero determinant, it is not invertible, and vice versa.

What to remember about the Inverse:

- uniqueness of the inverse
- the inverse and matrix multiplication
- the inverse of the inverse is the original matrix
- two conditions for non-invertibility
- the inverse of a diagonal matrix
- the determinant of a matrix in general, and for $(2,2)$ and $(3,3)$ matrices
- the inverse of a $(2,2)$ matrix

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Matrix transpose

the matrix transpose A^T of a matrix A is defined as:

$$(A^T)_{i,k} = A_{k,i}$$

Graphically all entries get mirrored along the main diagonal.

$$A = \begin{bmatrix} 1 & 0 & 2 \\ -2 & 8 & 9 \\ 3 & 7 & 5 \end{bmatrix},$$

$$B = \begin{bmatrix} 1 & 0 \\ -2 & 8 \\ 3 & 7 \end{bmatrix},$$

$$A^T = \begin{bmatrix} 1 & -2 & 3 \\ 0 & 8 & 7 \\ 2 & 9 & 5 \end{bmatrix}$$

$$B^T = \begin{bmatrix} 1 & -2 & 3 \\ 0 & 8 & 7 \end{bmatrix}$$

Properties of the Matrix transpose

$$(A^T)^T = A$$

$$(AB)^T = B^T A^T$$

$$(A^{-1})^T = (A^T)^{-1}$$

$$(A + B)^T = A^T + B^T$$

The first and the second property are similar to what holds for the matrix inverse A^{-1} .

Proof of the third property uses the second property:

$$(A^{-1}A)^T = A^T(A^{-1})^T$$

$$(A^{-1}A)^T = I^T = I \Rightarrow A^T(A^{-1})^T = I$$

Therefore $(A^{-1})^T$ must be the inverse of A^T , which is denoted as $(A^T)^{-1}$

When does the transpose occur ?

- Firstly, inside dot products:

If x and y are of shape $(d, 1)$ (columns), then

$$x \cdot y = x^{\top} y \text{ as matrix multiplication}$$

If x and y are of shape $(1, d)$, then

$$x \cdot y = xy^{\top} \text{ as matrix multiplication}$$

- secondly when matrices are used inside dot products:

$$\begin{aligned}(Ax) \cdot y &= (Ax)^{\top} y = x^{\top} A^{\top} y = x \cdot (A^{\top} y) = (A^{\top} y) \cdot x \\ x \cdot (Ay) &= x^{\top} Ay = (A^{\top} x)^{\top} y = (A^{\top} x)^{\top} y = (A^{\top} x) \cdot y = y \cdot (A^{\top} x)\end{aligned}$$

- it defines symmetric matrices which have special properties with respect to eigenvalues.

symmetric matrix

the matrix A is symmetric if:

$$A^{\top} = A$$

Note: any real number (or (1,1)-shaped matrix) is its own transpose, e.g. for shapes $(1, d), (d, e), (e, 1)$ we have:

$$w^{\top} A h = (w^{\top} A h)^{\top} = h^{\top} A^{\top} w$$

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- ◉ fourthly in combination with the inverse the matrix transpose defines orthogonal matrices

Definition: Orthogonal Matrices

Definition: A is an orthogonal matrix if $A^{-1} = A^T$

What for are they useful?

- if A is an orthogonal matrix, then it preserves the length of vectors when multiplied with them.
Proof:

$$\|Ax\|_2^2 = (Ax) \cdot (Ax) = (Ax)^\top Ax = x^\top \underbrace{A^\top A}_{=I} x = x^\top x = \|x\|_2^2$$

- Thus, if A is an orthogonal matrix, then Ax defines a rotation of vector x !

Orthogonal matrices define those linear operations on vectors which act as rotations.

What the float are they useful?

- A is an orthogonal matrix if and only if its columns define an orthonormal basis. Any orthonormal basis (orthogonal vectors with unit length) defines an orthogonal matrix. How to see this? Consider the equation:

$$A^T A = I$$

It translates to:

- the inner product of the i -th row of A^T and the i -th column of A is $= 1$:
 $(A^T)[i, :]A[:, i] = 1 = A[:, i] \cdot A[:, i]$
- the inner product of the i -th row of A^T and the k -th ($k \neq i$) column of A is $= 0$
 $(A^T)[i, :]A[:, k] = 0 = A[:, i] \cdot A[:, k]$

Note: the i -th row of A^T is equal to the i -th column of A .

Therefore: The inner product of two columns of A is zero, except we use the same column. This means: its columns form an orthonormal basis.

The other way round also holds:

- if $v^{\{0\}}, \dots, v^{\{d-1\}}$ are an orthonormal basis, then stacking them into a matrix results in an orthogonal matrix $A = (v^{\{0\}}, \dots, v^{\{d-1\}})$ with $A^\top A = I$.

The same can be proven for rows of A .

One uses $AA^\top = I$ and translates AA^\top to the inner product of the i -th row of A and the k -th column of A^\top , which is the k -th row of A .

$$A(a) = \begin{bmatrix} \cos a & \sin a \\ -\sin a & \cos a \end{bmatrix} \text{ and}$$
$$A(a) = \begin{bmatrix} \cos a & \sin a \\ \sin a & -\cos a \end{bmatrix}$$

are the orthogonal matrices of shape $(2, 2)$.

Proof: $(A^\top A)_{ii} = \cos^2 a + \sin^2 a = 1$ and $(A^\top A)_{01} = \cos a \sin a - \sin a \cos a = 0$

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Application of Householder matrices: obtaining upper triangular form of a matrix
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We have seen in lecture 2:

One important step to solve a linear equation system is to put it into a row echelon form (see section Main step 2). The row echelon form – is a special case of an upper triangular matrix.

Examples of upper triangular matrices are:

$$\begin{bmatrix} * & * \\ 0 & * \end{bmatrix}, \begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix}, \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix}$$

- We can use Householder rotations to obtain an upper triangular matrix without any swapping steps.

Goal of using Householder matrices:

- We want to rotate x onto a multiple of z where z is a unit vector $\|z\|_2 = 1$.
- note: A rotation does not change the vector norm, x has norm $\|x\|$, and $\|z\| = 1$.
Therefore x can be only rotated onto $\pm\|x\|z$.

Householder matrix

Given any vector x and any unit vector z , $\|z\| = 1$, define the Householder matrix H_u as:

$$u = x \pm \|x\|z \leftarrow \text{you can choose the sign}$$

$$H_u = I - \frac{2}{u \cdot u} uu^T$$

It has these three properties:

$$H_u x = \mp \|x\|z$$

rotates x to z

$$H_u^T H_u = I$$

orthogonal, it IS a rotation indeed

$$H_u = H_u^T$$

symmetric

$$\|z\| = 1$$

$$u = x \pm \|x\|z \leftarrow \text{you can choose the sign}$$

$$H_u = I - \underbrace{\frac{2}{u \cdot u}}_{\text{number}} \underbrace{uu^T}_{\text{matrix}}$$

What we want to achieve

Take any matrix A , and apply matrix multiplications (using Householder multiplications), such that it becomes an upper triangular matrix.

Learning goals

From the above section you need to remember how to define a Householder matrix, its three properties, the definition of an upper triangular matrix.

From this subsection you need also to remember that Householder matrices can be used to obtain an upper triangular matrix, and that you do this by rotating onto multiples of one-hot vectors $\|x\|e^{\{k\}}$

You can be expected to define a Householder matrix for a given vector x and a given unit vector $e^{\{k\}}$ and to multiply it to a target matrix or a submatrix of a given target matrix. – This requires you only to perform the three steps from the textbox above, and then to do a matrix multiplication

You do not need to remember how to prove that a Householder matrix transforms a vector into another. You do not need to remember how to prove that a Householder matrix is its own inverse.

We know that:

$$\text{If } z = e^{\{0\}} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \text{ then } H_u x = \mp \|x\| e^{\{0\}} = \begin{bmatrix} \mp \|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

We start with a matrix $A^{\{0\}} := A$ of shape (n, d)

$$A = \begin{bmatrix} A_{0,0} & A_{0,1} & A_{0,2} & \dots & A_{0,d-1} \\ A_{1,0} & A_{1,1} & A_{1,1} & \dots & A_{1,d-1} \\ A_{2,0} & A_{2,1} & A_{2,1} & \dots & A_{2,d-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{n-1,0} & A_{n-1,1} & A_{n-1,2} & \dots & A_{n-1,d-1} \end{bmatrix}$$

and choose $x = A[:, 0]$ – its zero-th column, $z = e^{\{0\}}$

Step 0: You can make the 0-th column $A_{:,0}$ of a matrix to be almost everywhere zero. You can achieve this by using:

$$x = A_{:,0}, z = e^{\{0\}} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Then, use

$$u = x \pm \|x\|z = A_{:,0} \pm \|A_{:,0}\|e^{\{0\}},$$

define $H_u^{\{0\}}$, multiply it to A and you obtain this:

$$A^{\{1\}} = H_u^{\{0\}} A = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \cdots & A_{0,d-1}^{\{1\}} \\ 0 & A_{1,1}^{\{1\}} & A_{1,1}^{\{1\}} & \cdots & A_{1,d-1}^{\{1\}} \\ 0 & A_{2,1}^{\{1\}} & A_{2,1}^{\{1\}} & \cdots & A_{2,d-1}^{\{1\}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & A_{n-1,1}^{\{1\}} & A_{n-1,2}^{\{1\}} & \cdots & A_{n-1,d-1}^{\{1\}} \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & \cdots & A_{0,d-1}^{\{1\}} \\ 0 & & & \\ \vdots & & [A_{1:end,1:end}^{\{1\}}] & \\ 0 & & & \end{bmatrix}$$

define $H_u^{\{0\}}$, multiply it to A and you obtain this:

$$A^{\{1\}} = H_v^{\{0\}} A = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \dots & A_{0,d-1}^{\{1\}} \\ 0 & A_{1,1}^{\{1\}} & A_{1,1}^{\{1\}} & \dots & A_{1,d-1}^{\{1\}} \\ 0 & A_{2,1}^{\{1\}} & A_{2,1}^{\{1\}} & \dots & A_{2,d-1}^{\{1\}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & A_{n-1,1}^{\{1\}} & A_{n-1,2}^{\{1\}} & \dots & A_{n-1,d-1}^{\{1\}} \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & \dots & A_{0,d-1}^{\{1\}} \\ 0 & & & \\ \vdots & & \begin{bmatrix} A_{1:end,1}^{\{1\}} \end{bmatrix} & \\ 0 & & & \end{bmatrix}$$

This is the start of creating an upper triangular matrix like

$$\begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix}$$

$$A^{\{1\}} = H_v^{\{0\}} A = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \cdots & A_{0,d-1}^{\{1\}} \\ 0 & A_{1,1}^{\{1\}} & A_{1,2}^{\{1\}} & \cdots & A_{1,d-1}^{\{1\}} \\ 0 & A_{2,1}^{\{1\}} & A_{2,2}^{\{1\}} & \cdots & A_{2,d-1}^{\{1\}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & A_{n-1,1}^{\{1\}} & A_{n-1,2}^{\{1\}} & \cdots & A_{n-1,d-1}^{\{1\}} \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & \cdots & A_{0,d-1}^{\{1\}} \\ 0 & & & \\ \vdots & & \begin{bmatrix} A_{1:end,1:end}^{\{1\}} \end{bmatrix} & \\ 0 & & & \end{bmatrix}$$

You will iterate this idea - on the next columns. In the next step you apply the same idea ... to the "lower-right" sub-matrix $\begin{bmatrix} A_{1:end,1:end}^{\{1\}} \end{bmatrix}$ of shape $(n-1, d-1)$, which is taken from the matrix $A^{\{1\}}$ ($A^{\{1\}}$ has shape (n, d)).

Step 1: In order to get the 1-st column into a good shape, do the following:

- we have this result from the previous step:

$$A^{\{1\}} = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \dots & A_{0,d-1}^{\{1\}} \\ 0 & & & & \\ \vdots & & [A_{1:end,1:end}^{\{1\}}] & & \\ 0 & & & & \end{bmatrix}$$

- take the vector of the 1-st column starting at the first row $A_{1:end,1}^{\{1\}}$. This has shape $(n-1, 1)$ and it is the zero-th column from $[A_{1:end,1:end}^{\{1\}}]$.

Note: you do **not take** anything from the zero-th row

$$\text{do not use: } A_{0,1:end}^{\{1\}} = \begin{bmatrix} \mp \|A_{:,0}\| & A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \dots & A_{0,d-1}^{\{1\}} \\ A_{0,1}^{\{1\}} & A_{0,2}^{\{1\}} & \dots & A_{0,d-1}^{\{1\}} \end{bmatrix}$$

- ⊙ make $u = A_{1:end,1}^{\{1\}} \pm \|A_{1:end,1}^{\{1\}}\| e^{\{0\}}$ into a Householder matrix $\widetilde{H}_v^{\{1\}}$ of shape $(n-1, n-1)$, which you will apply to $A^{\{1\}}$ only starting from the 1-st row and 1-st column $\left[A_{1:end,1:end}^{\{1\}} \right]$ - which has shape $(n-1, d-1)$.

$$A^{\{1\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & & & \\ \vdots & \left[A_{1:end,1:end}^{\{1\}} \right] & & \\ 0 & & & \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & \left[A_{1,1}^{\{1\}} & \dots & A_{1,d-1}^{\{1\}} \right] \\ \vdots & \left[A_{2,1}^{\{1\}} & \dots & A_{2,d-1}^{\{1\}} \right] \\ 0 & \left[A_{n-1,1}^{\{1\}} & \dots & A_{n-1,d-1}^{\{1\}} \right] \end{bmatrix}$$

$$A^{\{2\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & & & \\ \vdots & \widetilde{H}_v^{\{1\}} \left[A_{1:end,1:end}^{\{1\}} \right] & & \\ 0 & & & \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & \left[\mp \|A_{1:end,1}^{\{1\}}\| & A_{1,2}^{\{2\}} & \dots & A_{1,d-1}^{\{2\}} \right] \\ \vdots & \left[0 & & & \right] \\ 0 & \left[0 & & \left[A_{2:end,2:end}^{\{2\}} \right] \right] \end{bmatrix}$$

to achieve this, use $u = A_{1:end,1}^{\{1\}} \pm \|A_{1:end,1}^{\{1\}}\| e^{\{0\}}$, where e^0 is the zero-th one hot vector - now in $n - 1$ dimensions.

Note: $\widetilde{H}_v^{\{1\}}$ is a matrix of shape $(n - 1, n - 1)$.

$$A^{\{2\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & & & \\ \vdots & \widetilde{H}_v^{\{1\}} \begin{bmatrix} A_{1:end,1}^{\{1\}} \\ A_{1:end,2:end}^{\{1\}} \end{bmatrix} & & \\ 0 & & & \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & \begin{bmatrix} \mp \|A_{1:end,1}^{\{1\}}\| & A_{1,2}^{\{2\}} & \dots & A_{1,d-1}^{\{2\}} \\ 0 & & & \end{bmatrix} & & \\ \vdots & & \begin{bmatrix} A_{2:end,2:end}^{\{2\}} \end{bmatrix} & \\ 0 & & & \end{bmatrix}$$

We want to let $\widetilde{H}_v^{\{1\}}$ act only

- on rows $[1 : n - 1]$
- and columns $[1 : d - 1]$ of $A^{\{1\}}$ as shown above,
- not on the whole set of rows $[0 : n - 1]$ and columns $[0 : d - 1]$ of the matrix $A^{\{1\}}$

One thing is annoying here:

How to apply $\widetilde{H}_v^{\{1\}}$ only on a subset of rows and columns of $A^{\{1\}}$?

It is possible to embed $\widetilde{H}_v^{\{1\}}$ into an (n, n) -shaped matrix, such that the (n, n) -shaped matrix can be just multiplied with $A^{\{1\}}$:

We achieve this by defining:

$$H_v^{\{1\}} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & \begin{bmatrix} \widetilde{H}_v^{\{1\}} \end{bmatrix} \\ \vdots & \\ 0 & \end{bmatrix}$$

$$\text{then: } A^{\{2\}} = H_v^{\{1\}} A^{\{1\}}$$

Good news: This does not change anything in the zero-th column of $A^{\{1\}}$.

$$A^{\{2\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & \widetilde{H}_v^{\{1\}} & & \\ \vdots & \begin{bmatrix} A_{1:end,1:end}^{\{1\}} \end{bmatrix} & & \\ 0 & & & \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & * & \dots & * \\ 0 & \begin{bmatrix} \mp \|A_{1:end,1}^{\{1\}}\| & A_{1,2}^{\{2\}} & \dots & A_{1,d-1}^{\{2\}} \end{bmatrix} \\ \vdots & \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} & \begin{bmatrix} A_{2:end,2:end}^{\{2\}} \end{bmatrix} & \end{bmatrix}$$

You will iterate this idea - on the next columns, [again](#). In the next step you apply the same idea ... to the "lower-right" sub-matrix $\begin{bmatrix} A_{2:end,2:end}^{\{2\}} \end{bmatrix}$ of shape $(n-2, d-2)$, which is taken from the matrix $A^{\{2\}}$ ($A^{\{2\}}$ has shape (n, d)).

Step 2: In order to get the 2-nd column into a good shape, do the following:

- take the vector of the 2-nd column starting at the 2-nd row $A_{2:end,2}^{\{2\}}$. This has shape $(n-2, 1)$.
 $u = A_{2:end,2}^{\{2\}} \pm \|A_{2:end,2}^{\{2\}}\| e^{\{0\}}$. Note: $e^{\{0\}}$ is now a vector in $n-2$ dimensions
- make it into a Householder matrix $\widetilde{H}_v^{\{2\}}$, which you apply only from the 2-nd row and 2-nd column $\begin{bmatrix} A_{2:end,2}^{\{2\}} \end{bmatrix}$.

$$A^{\{2\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & * & \dots & * \\ 0 & \mp \|A_{1:end,1}^{\{1\}}\| & * & \dots & * \\ 0 & 0 & & & \\ \vdots & \vdots & & & \\ 0 & 0 & & & \begin{bmatrix} A_{2:end,2}^{\{2\}} \end{bmatrix} \end{bmatrix}$$

$$A^{\{3\}} = \begin{bmatrix} \mp \|A_{:,0}\| & * & * & \dots & * \\ 0 & \mp \|A_{1:end,1}^{\{1\}}\| & * & \dots & * \\ 0 & 0 & & & \\ \vdots & \vdots & & & \\ 0 & 0 & & & \begin{bmatrix} A_{2:end,2}^{\{2\}} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \mp \|A_{:,0}\| & * & * & * & \dots & * \\ 0 & \mp \|A_{1:end,1}^{\{1\}}\| & * & * & \dots & * \\ 0 & 0 & \mp \|A_{2:end,2}^{\{2\}}\| & A_{2,3}^{\{3\}} & \dots & A_{2,d-1}^{\{3\}} \\ 0 & 0 & 0 & & & \\ \vdots & \vdots & \vdots & & & \\ 0 & 0 & 0 & & & \begin{bmatrix} A_{3:end,3}^{\{3\}} \end{bmatrix} \end{bmatrix}$$

Note: $\widetilde{H}_v^{\{2\}}$ is a matrix of shape $(n-2, n-2)$.

It only acts on rows $[2 : n-1]$ and columns $[2 : d-1]$ as shown above.

It is possible to run $\widetilde{H}_v^{\{2\}}$ on the whole matrix of shape (n, d) by defining:

$$H_v^{\{2\}} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & \left[\begin{array}{c} \widetilde{H}_v^{\{2\}} \end{array} \right] \\ \vdots & \vdots & \\ 0 & 0 & \end{bmatrix}$$

$$\text{then: } A^{\{3\}} = H_v^{\{2\}} A^{\{2\}}$$

This does not change anything in the zero-th and 1-st column of $A^{\{2\}}$.

The general embedding of a matrix $\widetilde{H}_v^{\{k\}}$ at step k of shape (k, k) into shape (n, n) looks like:

$$\begin{bmatrix} [I_{n-k}] & [0_{n-k,k}] \\ [0_{k,n-k}] & [\widetilde{H}_v^{\{k\}}] \end{bmatrix}$$

Here I_{n-k} is the identity matrix for $n - k$ dimensions, $0_{n-k,k}$, $0_{k,n-k}$ are zero matrices of shapes $(n - k, k)$ and $(k, n - k)$.

When do you stop this algorithm? When either 2 rows or 2 columns are left, at the lower right end, then you apply it one last time.

- if the shape is (n, d) with $n = d$, then you apply it the last time on the bottom-right $(2, 2)$ -submatrix, \widetilde{H}_V of shape $(2, 2)$

$$\begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & * & * \end{bmatrix} \rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * \end{bmatrix}$$

- if the shape is (n, d) with $n < d$, then you apply it the last time on the bottom-right $(2, d - n + 2)$ submatrix, \widetilde{H}_V of shape $(2, 2)$
- if the shape is (n, d) with $n > d$, then you apply it the last time on the bottom-right $(n - d + 2, 2)$ submatrix, \widetilde{H}_V of shape $(n - d + 2, n - d + 2)$

$n < d$ case last time with result:

$$\begin{bmatrix} * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * \\ 0 & 0 & * & * & * & * & * \\ 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & * & * & * & * \end{bmatrix} \rightarrow \begin{bmatrix} * & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * \\ 0 & 0 & * & * & * & * & * \\ 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & * \end{bmatrix}$$

$n > d$ case last time with result:

$$\begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & * & * \end{bmatrix} \rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & * \end{bmatrix}$$

Householder rotations can be used

- for obtaining an upper triangular matrix used for solving affine equation systems and for computing the matrix inverse
- for computing QR matrix decompositions,
- to obtain a eigenvalue decomposition for a symmetric matrix ^a
- and for a singular value decomposition for any matrix ^b

^aout of exams: you transform it into a tridiagonal shape, you start in the first step one row down

^bout of exams: you transform it into a bi-diagonal shape

A QR-decomposition of a matrix A is about finding two matrices Q , R , such that

$$A = QR$$

and Q is an orthogonal matrix, and R is an upper triangular matrix

The above example to obtain a triangular matrix shows how to get a QR decomposition. R will be the resulting upper triangular matrix, you obtain Q as the product of the embedded Householder matrices $H_V^{\{i\}}$

$$\begin{aligned} A &= H_V^{\{0\}} (H_V^{\{0\}} A) = H_V^{\{0\}} H_V^{\{1\}} (H_V^{\{1\}} H_V^{\{0\}} A) \\ &= H_V^{\{0\}} H_V^{\{1\}} H_V^{\{2\}} (H_V^{\{2\}} H_V^{\{1\}} H_V^{\{0\}} A) \\ &= \underbrace{H_V^{\{0\}} H_V^{\{1\}} \dots H_V^{\{d-1\}}}_{=Q} \underbrace{H_V^{\{d-1\}} \dots H_V^{\{1\}} H_V^{\{0\}} A}_{=R} \end{aligned}$$

we used the property $HH = I$ of Householder matrices here.

Question:

- if we want to solve

$$Ax = b$$

and we apply a Householder transformation L

$$L Ax = L b$$

, why this does not change the space of solutions x ?

Reason: $L = H_v$ is invertible!

we show: $H_v H_v = I$

$$v = \frac{u}{\|u\|} \Rightarrow \|v\| = 1$$

$$\begin{aligned} (I - 2vv^T)(I - 2vv^T) &= I - 2Ivv^T - 2vv^T I + 4vv^T vv^T \\ &= I - 4vv^T + 4v \underbrace{v^T v}_{\substack{= \text{a number!} = \|v\|_2}} v^T \\ &= I - 4vv^T + 4 \underbrace{\|v\|_2^2}_{=1} vv^T = I - 4vv^T + 4vv^T = I \end{aligned}$$

means it is an invertible operation. That's why it does not change the solution.

$$\begin{aligned}
 H_v x &= x - 2vv^T x \\
 &= x - 2 \frac{u(u^T \cdot x)}{u \cdot u} \\
 &= x - 2 \frac{(x - \|x\|z)(x - \|x\|z) \cdot x}{(x - \|x\|z) \cdot (x - \|x\|z)} \\
 &= x - 2 \frac{(x - \|x\|z)(\|x\|^2 - \|x\|z \cdot x)}{(x - \|x\|z) \cdot (x - \|x\|z)} \\
 &= x - 2 \frac{\underbrace{(x - \|x\|z)}_{\text{vector}} \underbrace{(\|x\|^2 - \|x\|z \cdot x)}_{\text{number}}}{\|x\|^2 - 2\|x\|z \cdot x + \|x\|^2 \underbrace{\|z\|^2}_{=1}} \\
 &= x - (x - \|x\|z) 2 \frac{\|x\|^2 - \|x\|z \cdot x}{\|x\|^2 - 2\|x\|z \cdot x + \|x\|^2}
 \end{aligned}$$

$$\begin{aligned}
 &= x - (x - \|x\|z)2 \frac{\|x\|^2 - \|x\|z \cdot x}{2\|x\|^2 - 2\|x\|z \cdot x} \\
 &= x - (x - \|x\|z) = \|x\|z
 \end{aligned}$$

Same for

$$\begin{aligned}
 u &= x + \|x\|z \\
 v &= \frac{u}{\sqrt{u \cdot u}} \\
 H_v &= I - 2vv^\top \\
 H_v x &= x - 2vv^\top x \\
 &= x - 2 \frac{u(u^\top \cdot x)}{u \cdot u} \\
 &= x - 2 \frac{(x + \|x\|z)(x + \|x\|z) \cdot x}{(x + \|x\|z) \cdot (x + \|x\|z)}
 \end{aligned}$$

$$\begin{aligned}
 &= x - (x + \|x\|z)2 \frac{\|x\|^2 + \|x\|z \cdot x}{\|x\|^2 + 2\|x\|z \cdot x + \underbrace{\|x\|^2 \|z\|^2}_{=1}} \\
 &= x - (x + \|x\|z)2 \frac{\|x\|^2 + \|x\|z \cdot x}{2\|x\|^2 + 2\|x\|z \cdot x} \\
 &= -\|x\|z
 \end{aligned}$$

Result:

$$\begin{aligned}
 u &= x \pm \|x\|z \\
 v &= \frac{u}{\|u\|_2} \\
 H_v &= I - 2vv^\top \\
 H_v x &= \mp \|x\|z
 \end{aligned}$$

- ① Recap
- ② The Inverse and Determinant of a Matrix
- ③ Matrix transpose
- ④ Orthogonal matrices
- ⑤ Householder transformation
- ⑥ Bonus parts

See the pdf writeup.