STAT 309: MATHEMATICAL COMPUTATIONS I
FALL 2015
LECTURE 12

1. ORTHOGONALIZATION USING HOUSEHOLDER REFLECTIONS

- it is natural to ask whether we can introduce more zeros with each orthogonal rotation and to that end, we examine *Householder reflections*
- consider a matrix of the form $P = I - \tau \mathbf{u}\mathbf{u}^\mathsf{T}$, where $\mathbf{u} \neq \mathbf{0}$ and τ is a nonzero constant
- a P that has this form is called a *symmetric rank*-1 *change* of I
- can we choose τ so that P is also orthogonal?
- from the desired relation $P^\mathsf{T} P = I$ we obtain

$$\begin{aligned} P^\mathsf{T} P &= (I - \tau\mathbf{u}\mathbf{u}^\mathsf{T})^\mathsf{T}(I - \tau\mathbf{u}\mathbf{u}^\mathsf{T}) \\ &= I - 2\tau\mathbf{u}\mathbf{u}^\mathsf{T} + \tau^2\mathbf{u}\mathbf{u}^\mathsf{T}\mathbf{u}\mathbf{u}^\mathsf{T} \\ &= I - 2\tau\mathbf{u}\mathbf{u}^\mathsf{T} + \tau^2(\mathbf{u}^\mathsf{T}\mathbf{u})\mathbf{u}\mathbf{u}^\mathsf{T} \\ &= I - (\tau^2\mathbf{u}^\mathsf{T}\mathbf{u} - 2\tau)\mathbf{u}\mathbf{u}^\mathsf{T} \\ &= I + \tau(\tau\mathbf{u}^\mathsf{T}\mathbf{u} - 2)\mathbf{u}\mathbf{u}^\mathsf{T} \end{aligned}$$

- it follows that if $\tau = 2/\mathbf{u}^\mathsf{T}\mathbf{u}$, then $P^\mathsf{T} P = I$ for any nonzero $\mathbf{u}$
- without loss of generality, we can stipulate that $\mathbf{u}^\mathsf{T}\mathbf{u} = 1$, and therefore P takes the form $P = I - 2\mathbf{v}\mathbf{v}^\mathsf{T}$, where $\mathbf{v}^\mathsf{T}\mathbf{v} = 1$
- why is the matrix P called a reflection?
- this is because for any nonzero vector $\mathbf{x}$, $P\mathbf{x}$ is the reflection of $\mathbf{x}$ across the hyperplane that is normal to $\mathbf{v}$
- for example, consider the 2×2 case and set $\mathbf{v} = \begin{bmatrix} 1 & 0 \end{bmatrix}^\mathsf{T}$ and $\mathbf{x} = \begin{bmatrix} 1 & 2 \end{bmatrix}^\mathsf{T}$, then

$$P = I - 2\mathbf{v}\mathbf{v}^\mathsf{T} = I - 2\begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - 2\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

  and therefore

$$P\mathbf{x} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$$

- now, let $\mathbf{x}$ be any vector, we wish to construct P so that $P\mathbf{x} = \alpha\begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}^\mathsf{T} = \alpha\mathbf{e}_1$ for some α
- from the relations

$$\|P\mathbf{x}\|_2 = \|\mathbf{x}\|_2, \qquad \|\alpha\mathbf{e}_1\|_2 = |\alpha|\|\mathbf{e}_1\|_2 = |\alpha|$$

  we obtain $\alpha = \pm\|\mathbf{x}\|_2$
- to determine P, we observe that

$$\mathbf{x} = P^{-1}(\alpha\mathbf{e}_1) = \alpha P\mathbf{e}_1 = \alpha(I - 2\mathbf{v}\mathbf{v}^\mathsf{T})\mathbf{e}_1 = \alpha(\mathbf{e}_1 - 2\mathbf{v}\mathbf{v}^\mathsf{T}\mathbf{e}_1) = \alpha(\mathbf{e}_1 - 2\mathbf{v}v_1)$$

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which yields the system of equations

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \alpha \begin{bmatrix} 1 - 2v_1^2 \\ -2v_1v_2 \\ \vdots \\ -2v_1v_n \end{bmatrix}$$

- from the first equation $x_1 = \alpha(1 - 2v_1^2)$ we obtain

$$v_1 = \pm\sqrt{\frac{1}{2}\left(1 - \frac{x_1}{\alpha}\right)}$$

- for $i = 2, \ldots, n$, we have

$$v_i = -\frac{x_i}{2\alpha v_1}$$

- it is best to choose α to have the opposite sign of x_1 to avoid cancellation in v_1
- it is conventional to choose the $+$ sign for α if $x_1 = 0$
- note that the matrix P is never formed explicitly: for any vector $\mathbf{b}$, the product $P\mathbf{b}$ can be computed as follows

$$P\mathbf{b} = (I - 2\mathbf{v}\mathbf{v}^\top)\mathbf{b} = \mathbf{b} - 2(\mathbf{v}^\top\mathbf{b})\mathbf{v}$$

- this process requires only $O(2n)$ operations
- it is easy to see that we can represent P simply by storing only $\mathbf{v}$
- we showed how a Householder reflection of the form $P = I - 2\mathbf{u}\mathbf{u}^\top$ could be constructed so that given a vector $\mathbf{x}$, $P\mathbf{x} = \alpha\mathbf{e}_1$
- now, suppose that that $\mathbf{x} = \mathbf{a}_1$ is the first column of a matrix A, then we construct a Householder reflection $H_1 = I - 2\mathbf{u}_1\mathbf{u}_1^\top$ such that $H\mathbf{x} = \alpha\mathbf{e}_1$, and we have

$$A^{(2)} = H_1 A = \begin{bmatrix} r_{11} & & & \\ 0 & & & \\ \vdots & \mathbf{a}_2^{(2)} & \cdots & \mathbf{a}_n^{(2)} \\ 0 & & & \end{bmatrix}$$

where we denote the constant α by r_{11}, as it is the $(1,1)$ element of the updated matrix $A^{(2)}$
- now, we can construct H_2 such that

$$H_2\mathbf{a}^{(2)} = \begin{bmatrix} a_{12}^{(2)} \\ r_{22} \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad u_{12} = 0, \quad H_2 = \begin{bmatrix} 1 & 0 \\ 0 & \\ \vdots & h_{ij} \\ 0 & \end{bmatrix}$$

- note that the first column of $A^{(2)}$ is unchanged by H_2
- continuing this process, we obtain

$$H_{n-1} \cdots H_1 A = A^{(n)} = R$$

where R is an upper triangular matrix
- we have thus factored $A = QR$, where $Q = H_1 H_2 \cdots H_{n-1}$ is an orthogonal matrix
- note that

$$A^\top A = R^\top Q^\top Q R = R^\top R,$$

and thus R is the Cholesky factor of $A^\top A$ (we will discus Cholesky factorization next week)

2. GIVENS ROTATIONS VERSUS HOUSEHOLDER REFLECTIONS

- we showed how to construct Givens rotations in order to rotate two elements of a column vector so that one element would be zero, and that approximately $n^2/2$ such rotations could be used to transform A into an upper triangular matrix R
- because each rotation only modifies two rows of A, it is possible to interchange the order of rotations that affect different rows, and thus apply sets of rotations in parallel
- this is the main reason why Givens rotations can be preferable to Householder reflections
- other reasons are that they are easy to use when the QR factorization needs to be updated as a result of adding a row to A or deleting a column of A
- Givens rotations are also more efficient when A is sparse

3. COMPUTING THE COMPLETE ORTHOGONAL FACTORIZATION

- we first seek a decomposition of the form $A = QR\Pi$ where the permutation matrix Π is chosen so that the diagonal elements of R are maximized at each stage
- specifically, suppose

$$H_1 A = \begin{bmatrix} r_{11} & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ \vdots & \vdots & & \vdots \\ 0 & \times & \cdots & \times \end{bmatrix}, \quad r_{11} = \|\mathbf{a}_1\|_2$$

- so, we choose Π_1 so that $\|\mathbf{a}_1\|_2 \geq \|\mathbf{a}_j\|_2$ for $j \geq 2$
- for Π_2, look at the lengths of the columns of the submatrix; we don't need to recompute the lengths each time, because we can update by subtracting the square of the first component from the square of the total length
- eventually, we get

$$Q \begin{bmatrix} R & S \\ 0 & 0 \end{bmatrix} \Pi_1 \cdots \Pi_r = A$$

  where R is upper triangular
- suppose

$$A = Q \begin{bmatrix} R & S \\ 0 & 0 \end{bmatrix} \Pi$$

  where R is upper triangular, then

$$A^\mathsf{T} = \Pi^\mathsf{T} \begin{bmatrix} R^\mathsf{T} & 0 \\ S^\mathsf{T} & 0 \end{bmatrix} Q^\mathsf{T}$$

  where R^T is lower triangular
- we apply Householder reflections so that

$$H_i \cdots H_2 H_1 \begin{bmatrix} R^\mathsf{T} & 0 \\ S^\mathsf{T} & 0 \end{bmatrix} = \begin{bmatrix} U & 0 \\ 0 & 0 \end{bmatrix}$$

- then

$$A^\mathsf{T} = Z^\mathsf{T} \begin{bmatrix} U & 0 \\ 0 & 0 \end{bmatrix} Q^\mathsf{T}$$

  where $Z = H_i \cdots H_1 \Pi$
- we look at LU factorization and some of its variants: condensed LU, LDU, LDL^T, and Cholesky factorizations

4. Existence of LU factorization

- the solution method for a linear system $A\mathbf{x} = \mathbf{b}$ depends on the structure of A: A may be a sparse or dense matrix, or it may have one of many well-known structures, such as being a banded matrix, or a Hankel matrix
- for the general case of a dense, unstructured matrix A, the most common method is to obtain a decomposition $A = LU$, where L is lower triangular and U is upper triangular
- this decomposition is called the *LU factorization* or *LU decomposition*
- we deduce its existence via a constructive proof, namely, *Gaussian elimination*
- the motivation for this is something you learnt in middle school, i.e., solving $Ax = b$ by eliminating variables

$$\begin{array}{ccccccc}
a_{11}x_1 & + & \cdots & + & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & + & \cdots & + & a_{2n}x_n & = & b_2 \\
\vdots & & & & \vdots & & \vdots \\
a_{n1}x_1 & + & \cdots & + & a_{nn}x_n & = & b_n
\end{array}$$

- we proceed by multiplying the first equation by $-a_{21}/a_{11}$ and adding it to the second equation, and in general multiplying the first equation by $-a_{i1}/a_{11}$ and adding it to equation i and this leaves you with the equivalent system

$$\begin{array}{ccccccccc}
a_{11}x_1 & + & a_{12}x_2 & + & \cdots & + & a_{1n}x_n & = & b_1 \\
0x_1 & + & a'_{22}x_2 & + & \cdots & + & a'_{2n}x_n & = & b'_2 \\
\vdots & & & & & & \vdots & & \vdots \\
0x_1 & + & a'_{n2}x_2 & + & \cdots & + & a'_{nn}x_n & = & b'_n
\end{array}$$

- continuing in this fashion, adding multiples of the second equation to each subsequent equation to make all elements below the diagonal equal to zero, you obtain an upper triangular system and may then solve for all $x_n, x_{n-1}, \dots, x_1$ by back substitution
- getting the LU factorization $A = LU$ is very similar, the main difference is that you want not just the final upper triangular matrix (which is your U) but also to keep track of all the elimination steps (which is your L)

5. Gaussian elimination revisited

- we are going to look at Gaussian elimination in a slightly different light from what you learnt in your undergraduate linear algebra class
- we think of Gaussian elimination as the process of transforming A to an upper triangular matrix U is equivalent to multiplying A by a sequence of matrices to obtain U
- but instead of elementary matrices, we consider again a rank-1 change to I, i.e., a matrix of the form
$$I - \mathbf{u}\mathbf{v}^{\mathsf{T}}$$
where $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$
- in Householder QR, we used Householder reflection matrices of the form
$$H = I - 2\mathbf{u}\mathbf{u}^{\mathsf{T}}$$
- in Gaussian elimination, we use so-called *Gauss transformation* or *elimination matrices* of the form
$$M = I - \mathbf{m}\mathbf{e}_i^{\mathsf{T}}$$
where $\mathbf{e}_i = [0, \dots, 1, \dots 0]^{\mathsf{T}}$ is the ith standard basis vector

- the same trick that led us to the appropriate $\mathbf{u}$ in Householder matrix can be applied to find the appropriate $\mathbf{m}$ too: suppose we want $M_1 = I - \mathbf{m}_1\mathbf{e}_1^{\mathsf{T}}$ to 'zero out' all the entries beneath the first in a vector $\mathbf{a}$, i.e.,

$$M_1 \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \gamma \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

  i.e.,

$$\begin{aligned} (I - \mathbf{m}_1\mathbf{e}_1^{\mathsf{T}})\mathbf{a} &= \gamma\mathbf{e}_1 \\ \mathbf{a} - (\mathbf{e}_1^{\mathsf{T}}\mathbf{a}_1)\mathbf{m}_1 &= \gamma\mathbf{e}_1 \\ a_1\mathbf{m}_1 &= \mathbf{a} - \gamma\mathbf{e}_1 \end{aligned}$$

  and if $a_1 \neq 0$, then we may set

$$\gamma = a_1, \quad \mathbf{m}_1 = \begin{bmatrix} 0 \\ a_2/a_1 \\ \vdots \\ a_n/a_1 \end{bmatrix}$$

- so we get

$$M_1 = I - \mathbf{m}_1\mathbf{e}_1^{\mathsf{T}} = \begin{bmatrix} 1 & & & 0 \\ -a_2/a_1 & 1 & & \\ \vdots & 0 & \ddots & \\ -a_n/a_1 & & & 1 \end{bmatrix}$$

  and, as required,

$$M_1\mathbf{a} = \begin{bmatrix} 1 & & & 0 \\ -a_2/a_1 & 1 & & \\ \vdots & 0 & \ddots & \\ -a_n/a_1 & & & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = a_1\mathbf{e}_1$$

- applying this to zero out the entries beneath a_{11} in the first column of a matrix A, we get $M_1A = A_2$ where

$$A_2 = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} \end{bmatrix}$$

  where the superscript in parenthesis denote that the entries have changed
- we will write

$$M_1 = \begin{bmatrix} 1 & & & 0 \\ -\ell_{21} & 1 & & \\ \vdots & 0 & \ddots & \\ -\ell_{n1} & & & 1 \end{bmatrix}, \quad \ell_{i1} = \frac{a_{i1}}{a_{11}}$$

  for $i = 2, \dots, n$

- if we do this recursively, defining M_2 by

$$M_2 = \begin{bmatrix} 1 & & & & \\ 0 & 1 & & & \\ 0 & -\ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ 0 & -\ell_{n2} & & & 1 \end{bmatrix}, \quad \ell_{i2} = \frac{a_{i2}^{(2)}}{a_{22}^{(2)}}$$

for $i = 3, \ldots, n$, then

$$M_2 A_2 = A_3 = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & \cdots & a_{2n}^{(2)} \\ 0 & 0 & a_{33}^{(3)} & \cdots & a_{3n}^{(3)} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & a_{n3}^{(3)} & \cdots & a_{nn}^{(3)} \end{bmatrix}$$

- in general, we have

$$M_k = \begin{bmatrix} 1 & & & & & \\ 0 & \ddots & & & & \\ \vdots & \ddots & 1 & & & \\ \vdots & & -\ell_{k+1,k} & 1 & & \\ \vdots & & \vdots & & \ddots & \\ 0 & & -\ell_{nk} & & & 1 \end{bmatrix}, \quad \ell_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}$$

for $i = k+1, \ldots, n$, and

$$M_{n-1} M_{n-2} \cdots M_1 A = A_n \equiv \begin{bmatrix} u_{11} & \cdots & & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & u_{nn} \end{bmatrix}$$

or, equivalently,

$$A = M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1} U$$

- it turns out that M_j^{-1} is very easy to compute, we claim that

$$M_1^{-1} = \begin{bmatrix} 1 & & & 0 \\ \ell_{21} & 1 & & \\ \vdots & 0 & \ddots & \\ \ell_{n1} & & & 1 \end{bmatrix} \tag{5.1}$$

- to see this, consider the product

$$M_1 M_1^{-1} = \begin{bmatrix} 1 & & & 0 \\ -\ell_{21} & 1 & & \\ \vdots & 0 & \ddots & \\ -\ell_{n1} & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & 0 \\ \ell_{21} & 1 & & \\ \vdots & 0 & \ddots & \\ \ell_{n1} & & & 1 \end{bmatrix}$$

which can easily be verified to be equal to the identity matrix

- in general, we have

$$M_k^{-1} = \begin{bmatrix} 1 & & & & & \\ 0 & \ddots & & & & \\ \vdots & \ddots & 1 & & & \\ \vdots & & \ell_{k+1,k} & 1 & & \\ \vdots & & \vdots & & \ddots & \\ 0 & & \ell_{nk} & & & 1 \end{bmatrix} \tag{5.2}$$

- now, consider the product

$$\begin{aligned} M_1^{-1} M_2^{-1} &= \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & 0 & 1 & & \\ \vdots & \vdots & & \ddots & \\ \ell_{n1} & 0 & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & \\ 0 & 1 & & & \\ 0 & \ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ 0 & \ell_{n2} & & & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ \ell_{n1} & \ell_{n2} & & & 1 \end{bmatrix} \end{aligned}$$

- so inductively we get

$$M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & \ddots & & & \\ \vdots & \ell_{32} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{n1} & \ell_{n2} & \cdots & \ell_{n,n-1} & 1 \end{bmatrix}$$

- it follows that under proper circumstances, we can write $A = LU$ where

$$L = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \ell_{21} & 1 & 0 & \cdots & 0 \\ \ell_{31} & \ell_{32} & \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \ell_{n1} & \ell_{n2} & \cdots & \ell_{n,n-1} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} u_{11} & u_{12} & \cdots & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & \cdots & u_{2n} \\ 0 & 0 & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & u_{nn} \end{bmatrix}$$

- what exactly are proper circumstances?
- we will discuss them in the next lecture and also introduce *pivoting* to ensure that they are always satisfied