Lecture 12: Householder QR factorizations

June 18, 2025

Outline

1. Householder Triangularization
2. Householder QR Factorization Algorithm
3. Example: Householder Reflector
4. Example: QR Factorization via Householder

Householder QR factorizations - Introduction

- Recall that in this course we consider three common algorithms for QR factorization:
  1. Gram-Schmidt orthogonalization,
  2. Householder reflections,
  3. Givens rotations.
- Gram-Schmidt orthogonalization was discussed in Lecture 11.
- This lecture will introduce the idea of Householder reflections for building the QR factorization.
- A final approach of Givens rotations will be presented in the next lecture.

Householder QR factorizations - Introduction

- Note that the QR factorization we produce here is similar, but not identical, to the one we produced last time:
  1. R is $m \times n$ and Q is square, instead of the other way around, and
  2. Negative entries can occur on R's "diagonal".

Householder Triangularization

- Note that Gram-Schmidt orthogonalization is a "triangular orthogonalization" process. In matrix form, Gram-Schmidt can be written as right-multiplication by triangular matrices that make the columns of A orthonormal (see end of Lecture 8 of Trefethen & Bau)

$$A \underbrace{R_1 R_2 \cdots R_n}_{\hat{R}^{-1}} = \hat{Q}.$$

- **Householder reflections** instead provide an "orthogonal triangularization" process. The matrix A is made to be triangular (R) by applying orthogonal matrices Q_j, i.e.,

$$\underbrace{Q_n \cdots Q_2 Q_1}_{Q^{-1}} A = R.$$

  Hence, the premise of Householder reflections (aka triangularization) is to find the orthogonal matrices $Q_j \in \mathbb{R}^{m\times m}$. This method is similar to LU-factorization, as each Q_j will zero the lower entries of column j.

Householder Triangularization

$$
\underset{A}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}} \xrightarrow{Q_1} \underset{Q_1 A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}} \xrightarrow{Q_2} \underset{Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{bmatrix}} \xrightarrow{Q_3} \underset{Q_3 Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix}}
$$

Householder Triangularization

We will build orthogonal matrices of the following form

$$Q_j = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix} \begin{matrix} \} \; j-1 \text{ rows, already done,} \\ \} \; m-(j-1) \text{ rows, still to be done.} \end{matrix}$$

where F is the **Householder reflector** matrix. F reflects a vector x across a (specific) hyperplane H to produce a vector **along the axis**.

Householder Triangularization

See Figure 1 for a visualization of applying the Householder reflector (note $e_1 = [1, 0, \ldots, 0]^T$).

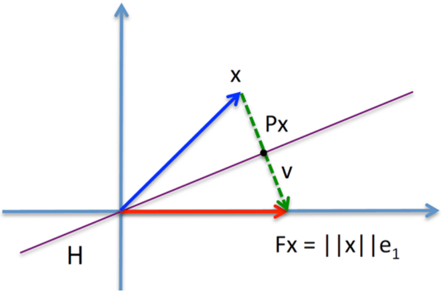

Figure: Applying the Householder reflector F to the vector x, which reflects x across the hyperplane H.

$$x + v^{-} = -\|x\|e_1 \Leftrightarrow v^{-} = -\|x\|e_1 - x.$$

Householder Triangularization

After reflection, the output vector has the same magnitude as x, and is parallel to e_1. It depends on both of x and e_1.
At step j, we start with x, and reflect onto the subspace spanned by $\{e_1, \ldots e_j\}$.
We find the Householder reflector matrix F, to perform the reflection, as follows.

Householder Triangularization

Suppose

$$x = \begin{bmatrix} \times \\ \times \\ \vdots \\ \times \end{bmatrix},$$

Find F such that

$$Fx = \begin{bmatrix} \|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\| e_1.$$

- The F reflects x across the hyperplane H **orthogonal to** $v = \|x\| e_1 - x$.
- That is because we want to produce a new vector of the same length as x, aligned with the axis e_1 (so all but the first entry are zeros).

Householder Triangularization

- The **orthogonal projection** P of x **onto** the hyperplane H (orthogonal to the vector v) is

$$Px = x - \left(\left(\frac{v}{\|v\|} \right)^T x \right) \frac{v}{\|v\|} = x - v \left(\frac{v^T x}{v^T v} \right).$$

- Note that this orthogonal projection P is similar to the steps in Gram-Schmidt orthogonalization.
- **Idea:** Subtract out the component of x **along** v.

Householder Triangularization

- To **reflect** x across H (instead of projecting onto H) we must go twice as far in the same direction (see Figure 1)

$$Fx = x - 2v\left(\frac{v^T x}{v^T v}\right).$$

- Therefore, the **Householder reflector** F is given by

$$F = I - 2\left(\frac{vv^T}{v^T v}\right)$$

where $v = \|x\|e_1 - x$.

Householder Triangularization

Remark that we could instead reflect to the point along the axis with a **negative** sign. That is, reflect to $-\|x\|e_1$ instead of $\|x\|e_1$, which gives

$$Fx = \begin{bmatrix} -\|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = -\|x\|e_1.$$

Either choice zeros out the desired entries of the active column. We just get a different v as shown in Figure 2.

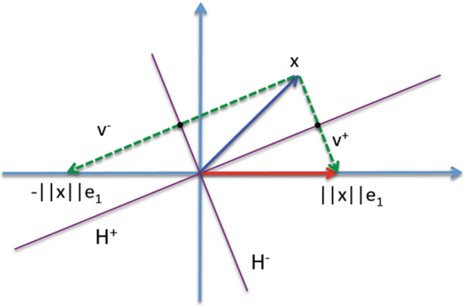

Figure: The two alternative Householder reflections.

Householder Triangularization

- Reflecting to either of $\|x\|e_i$ or $-\|x\|e_i$ will zero the remainder of the desired column.
- Which Householder reflector F should we choose?
- For numerical stability, we want the F that reflects x farther away from itself.
- Thus,
  - if $x_1 > 0$ we choose the negative one, $-\|x\|e_1$,
  - if $x_1 < 0$ we choose the positive one, $\|x\|e_1$.
- This gives $v = -\text{sign}(x_1)\|x\|e_1 - x$, or more simply (because only direction is important, and either choice gives the same F) $\text{sign}(x_1)\|x\|e_1 + x$.
- This choice of v avoids subtracting nearby quantities, which can introduce cancellation error.
- Therefore, choosing the F that reflects x farther away is more numerically stable.

Householder Triangularization

Alternative Derivation

- We will show an alternate derivation of Householder triangularization.
- Consider a reflection operator $F = I - 2\frac{vv^T}{v^T v}$ for an arbitrary vector v.
- We want to find v such that $Fx \in \text{span}\{e_1\}$ to zero the lower entries in column 1.
- Let $Fx \in \text{span}\{e_1\}$, in other words,

$$Fx = x - \frac{2vv^T x}{v^T v} = x - \left[\frac{2(v^T x)}{(v^T v)}\right] v \in \text{span}\{e_1\}.$$

Householder Triangularization

- Observe $v \in \text{span}\{e_1, x\}$ by construction, since $Fx \in \text{span}\{e_1\}$.
- Write $Fx = c_2 e_1$ for some scalar c_2.
- Hence,

$$\begin{aligned} c_2 e_1 &= x - c_1 v \\ \Rightarrow v &= \hat{c}_1 x + \hat{c}_2 e_1, \end{aligned}$$

(for scalars $\hat{c}_1$ and $\hat{c}_2$) which means $v \in \text{span}\{e_1, x\}$.

Householder Triangularization

- Now let $\hat{v} = x + \alpha e_1$ for some scalar α. (Note the length of v does not matter; only its direction matters.)
- We will write v for $\hat{v}$ from now on.
- Then,

$$\begin{aligned} v^T x &= (x + \alpha e_1)^T x \\ &= x^T x + \alpha e_1^T x \\ &= x^T x + \alpha \underbrace{x_{(1)}}_{\text{scalar}} \end{aligned}$$

and

$$\begin{aligned} v^T v &= (x + \alpha e_1)^T (x + \alpha e_1) \\ &= x^T x + 2\alpha x_{(1)} + \alpha^2. \end{aligned}$$

Householder Triangularization

Plugging into Fx to determine α, we have

$$
\begin{aligned}
Fx &= x - 2\left(\frac{v^T x}{v^T v}\right)(x + \alpha e_1), \\
&= \left(1 - \frac{2v^T x}{v^T v}\right) x - \left(2\alpha \frac{v^T x}{v^T v}\right) e_1, \\
&= \left(1 - \frac{2(x^T x + \alpha x_{(1)})}{x^T x + 2\alpha x_{(1)} + \alpha^2}\right) x - \left(2\alpha \frac{v^T x}{v^T v}\right) e_1, \\
&= \left(\frac{x^T x + \cancel{2\alpha x_{(1)}} + \alpha^2 - 2x^T x - \cancel{2\alpha x_{(1)}}}{x^T x + 2\alpha x_{(1)} + \alpha^2}\right) x - \left(2\alpha \frac{v^T x}{v^T v}\right) e_1, \\
&= \underbrace{\left(\frac{\alpha^2 - x^T x}{x^T x + 2\alpha x_{(1)} + \alpha^2}\right) x}_{\text{must be 0}} - \left(2\alpha \frac{v^T x}{v^T v}\right) e_1.
\end{aligned}
$$

Since $Fx \in \text{span}\{e_1\}$ the first term must be zero, so $\alpha^2 - x^T x = 0 \Rightarrow \alpha = \pm\|x\|$.

Householder Triangularization

Hence,

$$v = x \pm \|x\| e_1 \quad \text{and} \quad Fx = \mp \|x\| e_1,$$

as we saw last time.

Householder QR Factorization Algorithm

Algorithm 1 gives the QR factorization of A via Householder triangularization.

Algorithm 1 : Householder QR factorization algorithm

for $k = 1, 2, \ldots, n$
  $x = A(k:m, k)$ ▷ Get current column
  $v_k = \text{sign}(x_1)\|x\|e_1 + x$ ▷ Form the reflection vector
  $v_k = \frac{v_k}{\|v_k\|}$ ▷ Normalize
  for $j = k, k+1, \ldots, n$ ▷ Apply F to active lower-right block
    $A(k:m, j) = A(k:m, j) - 2v_k(v_k^T A(k:m, j))$
  end for
end for

Householder QR Factorization Algorithm

- The notation used follows Matlab, i.e., $A(k:m,j) = j^{\text{th}}$ column of A from row k to row m.
- The algorithm converts A into R (upper "triangular") using Householder reflections F.
- Note that one could **further** vectorize the inner loop (more efficient in Matlab) to the matrix operation

$$A(k:m,k:n) = A(k:m,k:n) - 2v_k(v_k^T A(k:m,k:n)).$$

Householder QR Factorization Algorithm

- Algorithm 1 does not construct Q, only the vectors v_k. Why is this not a problem in practice?
- We often do not need Q but just the products $Q^T b$ or Qx (e.g., for least squares we solve $Rx = Q^T b$). Since

$$
\begin{aligned}
Q^T &= Q_n Q_{n-1} \ldots Q_2 Q_1, \\
Q &= Q_1^T Q_2^T \ldots Q_{n-1}^T Q_n^T,
\end{aligned}
$$

we can efficiently (in $O(mn)$ flops) compute $Q^T b$ or Qx using just the v_k's to apply the appropriate reflections (see Algorithms 2 and 3). **Note the parentheses**, we compute $v(v^T b)$ rather than $(vv^T)b$ to avoid forming the matrix vv^T.

Algorithm 2 : Implicit $Q^T b$

for $k = 1, 2, \ldots, n$
$b(k : m) = b(k : m) - 2v_k \left(v_k^T b(k : m)\right)$
end for

Algorithm 3 : Implicit Qx

for $k = n, n-1, \ldots, 1$
$x(k : m) = x(k : m) - 2v_k \left(v_k^T x(k : m)\right)$
end for

Householder QR Factorization Algorithm

- Explicitly building the matrix Q may sometimes be necessary.
- So how **could** we use these implicit products to recover Q itself?
- We compute the product $QI = Q$ by applying Q to the columns of the identity matrix I $(e_1, e_2, \ldots)$, i.e., $q_1 = Qe_1, q_2 = Qe_2, \ldots$.
- For the reduced QR factorization

$$A = \hat{Q}\hat{R} = \begin{bmatrix} & \\ & \end{bmatrix}_{m \times n} \begin{bmatrix} & \end{bmatrix}_{n \times n}.$$

- So $\hat{Q}$ is given by just the first n columns of I

$$\hat{Q} = \begin{bmatrix} | & | & & | \\ Qe_1 & Qe_2 & \cdots & Qe_n \\ | & | & & | \end{bmatrix}.$$

Householder QR Factorization Algorithm

Complexity of Householder-Based QR Work is dominated by inner loop

$$A(k:m,j) = A(k:m,j) - 2v_k\left(v_k^T A(k:m,j)\right).$$

Tallying the cost gives:

- $v_k^T A(k:m,j) \approx 2(m-k+1)$ flops (dot product),
- $2v_k\left(v_k^T A(k:m,j)\right) \approx (m-k+1)$ flops (scalar multiply),
- $A(k:m,j) - 2v_k\left(v_k^T A(k:m,j)\right) \approx (m-k+1)$ flops (subtraction).

So it approximately costs $4(m-k+1)$ flops per inner step, which is done $(n-k+1)$ times (j-loop). This totals to $4(m-k+1)(n-k+1)$ flops per outer iteration. The outer k-loop runs from 1 to n, which means the total flops can be approximated by

$$\sum_{k=1}^{n} 4(m-k+1)(n-k+1) \approx 2mn^2 - \frac{2}{3}m^3.$$

Note that this does **not** include forming Q.

Householder QR Factorization Algorithm

- For $m = n$ (square),
  flops(Householder) $\approx \frac{4}{3}n^3 = 2 \times$ flops(LU).
- Recall from Lecture 11 that Gram-Schmidt orthogonalization cost $\approx 3 \times$ flops(LU).
- So Householder triangularization is faster than Gram-Schmidt orthogonalization.

Householder Reflector

- Given $x = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ find the Householder reflector F and the product Fx.
- **Answer:** We see that $\|x\| = \sqrt{1^2 + 2^2 + 2^2} = 3$. Therefore

$$v = \pm\|x\|e_1 + x = \pm 3 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix} \text{ or } \begin{bmatrix} -2 \\ 2 \\ 2 \end{bmatrix}.$$

- We choose $v = \text{sign}(x_1)\|x\|e_1 + x = 3 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix}$, for its numerical stability.

Householder Reflector

$$
\begin{aligned}
\frac{vv^T}{v^Tv} &= \left(\frac{1}{\begin{bmatrix} 4 & 2 & 2 \end{bmatrix} \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix}} \right) \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix} \begin{bmatrix} 4 & 2 & 2 \end{bmatrix} \\
&= \left(\frac{1}{24} \right) \begin{bmatrix} 16 & 8 & 8 \\ 8 & 4 & 4 \\ 8 & 4 & 4 \end{bmatrix} \\
&= \left(\frac{1}{6} \right) \begin{bmatrix} 4 & 2 & 2 \\ 2 & 1 & 1 \\ 2 & 1 & 1 \end{bmatrix}
\end{aligned}
$$

Householder Reflector

$$
\begin{aligned}
F &= I - 2\left(\frac{vv^T}{v^Tv}\right) \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{3}\begin{bmatrix} 4 & 2 & 2 \\ 2 & 1 & 1 \\ 2 & 1 & 1 \end{bmatrix} \\
&= \frac{1}{3}\begin{bmatrix} -1 & -2 & -2 \\ -2 & 2 & -1 \\ -2 & -1 & 2 \end{bmatrix}, \text{ so that} \\
Fx &= \frac{1}{3}\begin{bmatrix} -1 & -2 & -2 \\ -2 & 2 & -1 \\ -2 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \\
&= \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}.
\end{aligned}
$$

Householder Reflector

- Since we are computing exactly, we are not forced to consider numerical stability.
- We re-compute everything with the other possible choice, namely $v = \begin{bmatrix} -2 \\ 2 \\ 2 \end{bmatrix}$.

Householder Reflector

$$
\begin{aligned}
\frac{vv^T}{v^Tv} &= \left(\frac{1}{\begin{bmatrix} -2 & 2 & 2 \end{bmatrix} \begin{bmatrix} -2 \\ 2 \\ 2 \end{bmatrix}} \right) \begin{bmatrix} -2 \\ 2 \\ 2 \end{bmatrix} \begin{bmatrix} -2 & 2 & 2 \end{bmatrix} \\
&= \left(\frac{1}{12} \right) \begin{bmatrix} 4 & -4 & -4 \\ -4 & 4 & 4 \\ -4 & 4 & 4 \end{bmatrix} \\
&= \left(\frac{1}{3} \right) \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}
\end{aligned}
$$

Householder Reflector

$$\begin{aligned}
F &= I - 2\left(\frac{vv^T}{v^Tv}\right) \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{2}{3}\begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix} \\
&= \frac{1}{3}\begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & -2 \\ 2 & -2 & 1 \end{bmatrix}, \text{ so that} \\
Fx &= \frac{1}{3}\begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & -2 \\ 2 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \\
&= \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}.
\end{aligned}$$

Example: QR Factorization via Householder

Perform QR factorization using Householder reflections on the matrix

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$$

Example: QR Factorization via Householder

Step 1: $x = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}, v_- = \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix}, v_+ = \begin{bmatrix} 2 \\ -2 \\ -2 \end{bmatrix}$

(sign of v is irrelevant, since we only use vv^T and v^Tv.) Ordinarily we would use v_-, but let's use v_+ for variety.

Then $F_1 = \begin{bmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} & \frac{-2}{3} \\ \frac{2}{3} & \frac{-2}{3} & \frac{1}{3} \end{bmatrix} = Q_1$ and (by multiplying)

$Q_1 A = \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix}$

Example: QR Factorization via Householder

Step 2: $x = \begin{bmatrix} -3 \\ -4 \end{bmatrix}$ and so

$$\begin{aligned} v &= x + sign(x_1)\|x\|e_1 \\ &= \begin{bmatrix} -3 \\ -4 \end{bmatrix} + (-1) \cdot 5 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -8 \\ -4 \end{bmatrix} \end{aligned}$$

which lets us calculate

$$\begin{aligned} F_2 &= I - \frac{2vv^T}{v^Tv} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{2}{80} \begin{bmatrix} 64 & 32 \\ 32 & 16 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{5} \begin{bmatrix} 8 & 4 \\ 4 & 2 \end{bmatrix} \\ &= \begin{bmatrix} \frac{-3}{5} & \frac{-4}{5} \\ \frac{-4}{5} & \frac{3}{5} \end{bmatrix} \end{aligned}$$

Example: QR Factorization via Householder

Therefore $Q_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & & \\ 0 & \multicolumn{2}{c}{F_2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{-3}{5} & \frac{-4}{5} \\ 0 & \frac{-4}{5} & \frac{3}{5} \end{bmatrix}$

So $Q_2(Q_1 A) = R = \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix}$ (by multiplying)

Example: QR Factorization via Householder

Therefore

$$\begin{aligned} A &= Q_1^{-1} Q_2^{-1} R \\ &= Q_1^T Q_2^T R && \text{By orthogonality} \\ &= Q_1 Q_2 R && \text{by symmetry} \\ &= QR \end{aligned}$$

Example: QR Factorization via Householder

Orthogonality does not imply symmetry, but those Q's were constructed to be symmetric, $I - \frac{2vv^T}{v^Tv}$.

$$Q = Q_1 Q_2 = \begin{bmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} & \frac{-2}{3} \\ \frac{2}{3} & \frac{-2}{3} & \frac{1}{3} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{-3}{5} & \frac{-4}{5} \\ 0 & \frac{-4}{5} & \frac{3}{5} \end{bmatrix}$$

$$= \frac{1}{15} \begin{bmatrix} 5 & -14 & -2 \\ 10 & 5 & -10 \\ 10 & 2 & 11 \end{bmatrix}$$