

Householder Triangularization

Note Title

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Before discussing Householder triangularization, we need to interpret:

★ MGS as Triangular Orthogonalization

Recall the modified Gram-Schmidt (MGS) algorithm.

- Initial set up : $\psi_j^{(1)} = a_j \quad 1 \leq j \leq n$
- The first step in the outer for loop:

$$\underbrace{[\psi_1^{(1)} \psi_2^{(1)} \dots \psi_n^{(1)}]}_{=A} \underbrace{\begin{bmatrix} \frac{1}{r_{11}} & -\frac{r_{12}}{r_{11}} & \dots & -\frac{r_{1n}}{r_{11}} \\ 0 & & & \\ \vdots & & I_{n-1 \times n-1} & \\ 0 & & & \end{bmatrix}}_{\text{call this } R_1} = \underbrace{[\xi_1 \psi_2^{(2)} \dots \psi_n^{(2)}]}_{=AR_1}$$

- The second step:

$$\underbrace{[\xi_1 \psi_2^{(2)} \dots \psi_n^{(2)}]}_{=AR_1} \underbrace{\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{r_{22}} & -\frac{r_{23}}{r_{22}} & \dots & -\frac{r_{2n}}{r_{22}} \\ \vdots & & & & \\ 0 & & & I_{n-2 \times n-2} & \end{bmatrix}}_{\text{call this } R_2} = \underbrace{[\xi_1 \xi_2 \psi_3^{(3)} \dots \psi_n^{(3)}]}_{=AR_1 R_2}$$

⋮

In the end, we get

$$A \underbrace{R_1 R_2 \dots R_n}_{\text{call this } \hat{R}^{-1}} = \hat{Q} = [\xi_1 \dots \xi_n]$$

$$\text{Then } A = \hat{Q} \hat{R} !$$

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Hence, we can view

MGS = triangular orthogonalization

meaning: Applying triangular operations to reduce to orthonormal col' vectors.

Note: In practice, we do **not** form matrices R_i , $i=1, \dots, n$.

These are used to interpret the meaning of the MGS algorithm.

★ Householder Triangularization
= **orthogonal triangularization!**

Instead of triangular orthogonalization.

$$\text{MGS: } A \underbrace{R_1 R_2 \dots R_n}_{= \hat{R}^{-1}} = \underbrace{Q}_{\text{reduced QR}}$$

$$\text{Householder: } \underbrace{Q_n Q_{n-1} \dots Q_2 Q_1}_{= Q^T} A = R \quad \text{full QR}$$

In essence, it's a triangularization by introducing zeros (Householder, 1958)

$$\begin{array}{cccc}
 \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix} & \xrightarrow{Q_1} & \begin{bmatrix} \Delta & \Delta & \Delta \\ 0 & \Delta & \Delta \\ 0 & \Delta & \Delta \\ 0 & \Delta & \Delta \\ 0 & \Delta & \Delta \end{bmatrix} & \xrightarrow{Q_2} & \begin{bmatrix} \Delta & \Delta & \Delta \\ 0 & + & + \\ 0 & 0 & + \\ 0 & 0 & + \\ 0 & 0 & + \end{bmatrix} & \xrightarrow{Q_3} & \begin{bmatrix} \Delta & \Delta & \Delta \\ 0 & + & + \\ 0 & 0 & \nabla \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
 A & & Q_1 A & & Q_2 Q_1 A & & Q_3 Q_2 Q_1 A
 \end{array}$$

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How to construct Q_k ?

⇒ Householder Reflector

I_{k-1} is a short notation for $I_{k-1 \times k-1}$

$$Q_k = \begin{bmatrix} \underbrace{I_{k-1}}_{k-1} & \underbrace{0}_{m-(k-1)} \\ \underbrace{0}_{k-1} & \underbrace{F}_{m-(k-1)} \end{bmatrix} \begin{matrix} \}^{k-1} \\ \}^{m-(k-1)} \end{matrix}$$

$F \in \mathbb{R}^{(m-k+1) \times (m-k+1)}$, $F^T F = F F^T = I_{m-k+1}$
Householder Reflector, i.e., ortho. mat.

• What F does is the following:

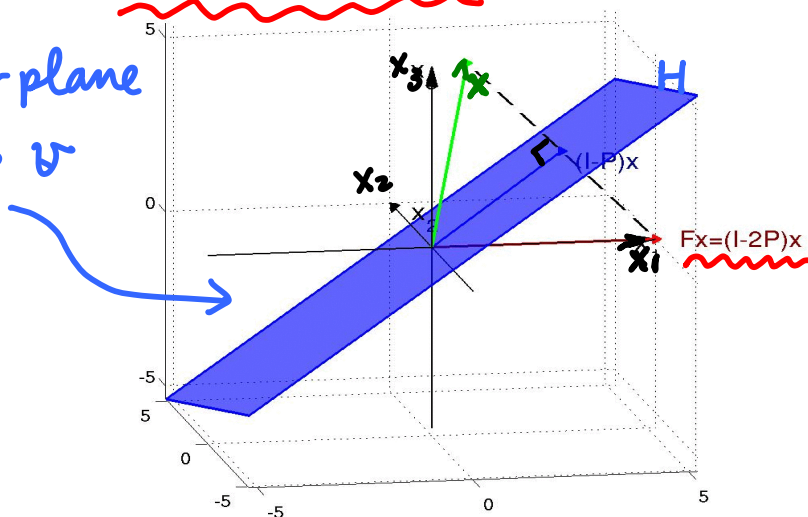
Suppose $x \in \mathbb{R}^{m-k+1}$, i.e.,

$$x = \begin{bmatrix} * \\ * \\ * \\ \vdots \\ * \end{bmatrix} \xrightarrow{F} Fx = \begin{bmatrix} \|x\| \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\| e_1$$

• Why F is called a reflector?

Define $v = \|x\| e_1 - x$

H : Hyperplane
normal to v



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$$P = P_v = \frac{vv^T}{v^T v} : \text{ortho. proj. onto } \langle v \rangle$$

But $v \perp H$.

Hence $I - P_v$: ortho. proj. onto H .

Now F can be written as

$$F = I - 2P_v = I - 2 \frac{vv^T}{v^T v}$$

Note F is not a projector.

but F is an orthogonal matrix.

why? $(I - 2P_v)^2 = (I - 2P_v)(I - 2P_v)$

$$= I - 2P_v - 2P_v + 4P_v^2$$

$$= I - 4P_v + 4P_v = I$$

$$\neq I - 2P_v \checkmark$$

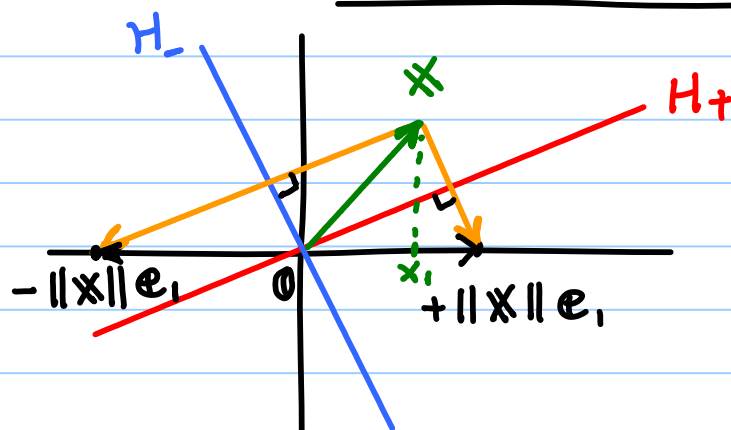
$$(I - 2P_v)^T (I - 2P_v) = (I^T - 2P_v^T)(I - 2P_v)$$

$$\text{red } P_v^T = P_v \rightarrow = (I - 2P_v)(I - 2P_v)$$

$$= I \checkmark$$

Similarly $(I - 2P_v)(I - 2P_v)^T = I. \checkmark$

★ Two possible reflectors :
which is better?



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Answer: In the above figure,

$-\|x\|e_1$ is a better choice.

Why? It's better numerically to move Fx as far from x as possible.

→ Why? Computing v involves

$v = \pm \|x\|e_1 - x$. If $\|x\|e_1 \approx x$ then $\|x\|e_1 - x$ loses numerical accuracy called **cancellation error**.

Hence in general, v should be chosen as

The first entry of $x = \begin{bmatrix} x_1 \\ \vdots \end{bmatrix}$

$$v = -\operatorname{sgn}(x_1) \|x\| e_1 - x$$

$$\text{where } \operatorname{sgn}(x_1) := \begin{cases} 1 & \text{if } x_1 \geq 0 \\ -1 & \text{if } x_1 < 0 \end{cases}$$

or equivalently,

$$v = \operatorname{sgn}(x_1) \|x\| e_1 + x.$$

★ Algorithm (Householder QR fact.)

for $k = 1:n$

$$\begin{cases} x = A[k:m, k] \\ v_k = \operatorname{sgn}(x_1) \|x\| e_1 + x \\ v_k = v_k / \|v_k\| \\ A[k:m, k:n] = A[k:m, k:n] \\ \quad - 2v_k (v_k^T A[k:m, k:n]) \\ \quad = F A[k:m, k:n] \end{cases}$$

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Note: In the end, A is replaced by the final R of $A = QR$.

Q has not constructed explicitly.

This is OK since QR fact. is usually used as an intermediate process for solving some other problem, e.g., $Ax = b$ or $\min. \|b - Ax\|^2$

As we showed before, this leads to $Rx = Q^T b$

Hence, as long as $Q^T b$ is computed we often do not need Q itself.

Algorithm (Implicit calculation of $Q^T b$)
for $k = 1:n$

$$b[k:m] = b[k:m] - 2\psi_k(\psi_k^T b[k:m])$$

↳ This should be included in the Householder QR fact. algorithm in the previous page.
Or, just store ψ_k , $k = 1:n$.

Do not store $Q_k = I - 2\psi_k\psi_k^T$

No need to store these.

ψ_k , $k = 1:n$ suffice.

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Example Let's consider the familiar example matrix.

$$A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix} \quad \begin{array}{l} \varepsilon : \text{small} \\ \text{s.t. } \varepsilon^2 \text{ can} \\ \text{be ignored.} \end{array}$$

I'm not going through the detailed computations by the Householder reflectors here (it would take several pages to do this by hand). But in the end, you get:

$$\begin{array}{c} Q_3 \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{3}} & \frac{\sqrt{2}}{\sqrt{3}} \\ 0 & 0 & \frac{\sqrt{2}}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix} \end{array} \begin{array}{c} Q_2 \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} Q_1 \\ \begin{bmatrix} -1 & -\varepsilon & 0 & 0 \\ -\varepsilon & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} A$$

$$= \begin{bmatrix} -1 & -1 & -1 \\ 0 & \sqrt{2}\varepsilon & \varepsilon/\sqrt{2} \\ 0 & 0 & (\frac{1}{\sqrt{3}} + \frac{\sqrt{2}}{\sqrt{3}})\varepsilon \\ 0 & 0 & 0 \end{bmatrix} R$$

If we want $A = QR$,
 then $\underbrace{Q_3 Q_2 Q_1}_{Q^T} A = R$ note each Q_i ortho mat.

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$$\begin{aligned}\text{So, } Q &= (Q_3 Q_2 Q_1)^T \\ &= Q_1^T Q_2^T Q_3^T \\ &= Q_1 Q_2 Q_3\end{aligned}$$

In this example, we have

$$Q = \begin{bmatrix} -1 & \varepsilon/\sqrt{2} & \varepsilon/\sqrt{6} & -\varepsilon/\sqrt{3} \\ -\varepsilon & -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 0 & \sqrt{2/3} & 1/\sqrt{3} \end{bmatrix}$$

Now let's check $Q^T Q$

$$Q^T Q = \begin{bmatrix} 1+\varepsilon^2 & 0 & 0 & 0 \\ 0 & 1+\varepsilon^2/2 & \varepsilon^2/2\sqrt{3} & -\varepsilon^2/\sqrt{6} \\ 0 & \varepsilon^2/2\sqrt{3} & 1+\varepsilon^2/6 & -\varepsilon^2/3\sqrt{2} \\ 0 & -\varepsilon^2/\sqrt{6} & -\varepsilon^2/3\sqrt{2} & 1+\varepsilon^2/3 \end{bmatrix}$$

$\approx I_{4 \times 4} !$

no loss of
orthogonality!

This is a big difference from
CGS and even MGS !

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★ Givens Rotations

Define

$$G(i, j, \theta) := i \begin{vmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{vmatrix}$$

⌈ all the other entries

We can choose θ s.t. $\theta \neq 0$.

$$G(i, j, \theta) \begin{bmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_j \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ \sqrt{x_i^2 + x_j^2} \\ \vdots \\ 0 \\ \vdots \\ x_m \end{bmatrix}$$

i.e., $\tan \theta = -x_j/x_i$

So, the Householder reflection can be written as successive applications of the Givens rotations:

$$Q_k = G(k, k+1, \theta_k) G(k+1, k+2, \theta_{k+1}) \dots G(m-1, m, \theta_{m-1})$$

= $m-k$ rotations!